



# Full wwPDB NMR Structure Validation Report ⓘ

Mar 6, 2026 – 03:26 AM UTC

PDB ID : 5TGY / pdb\_00005tgy  
BMRB ID : 30186  
Title : NMR structure of holo-PS1  
Authors : Polizzi, N.F.; Wu, Y.  
Deposited on : 2016-09-28

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  
Mogul : 2022.3.0, CSD as543be (2022)  
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

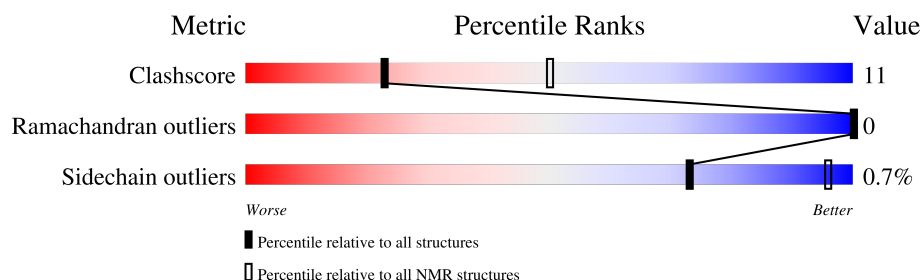
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 85%.

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     | 109    |                  |

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 15 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:5-A:51, A:60-A:105 (93) | 0.56              | 15           |

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

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

The models can be grouped into 3 clusters. No single-model clusters were found.

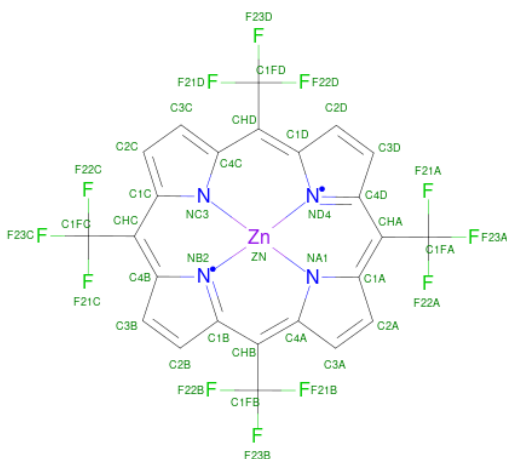
| Cluster number | Models                           |
|----------------|----------------------------------|
| 1              | 1, 3, 4, 6, 7, 8, 10, 14, 15, 17 |
| 2              | 5, 9, 11, 12, 18, 20             |
| 3              | 2, 13, 16, 19                    |

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- Molecule 1 is a protein called PS1.

| Total | C   | H   | N   | O   |
|-------|-----|-----|-----|-----|
| 1800  | 563 | 887 | 161 | 189 |

- Molecule 2 is [5,10,15,20-tetrakis(trifluoromethyl)porphyrinato(2-)-kappa 4 N 21 ,N 22 ,N 23 ,N 24 ]zinc (CCD ID: 7BU) (formula: C<sub>24</sub>H<sub>8</sub>F<sub>12</sub>N<sub>4</sub>Zn).



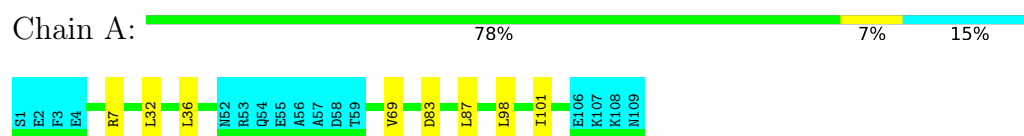
| Atoms |    |    |   |   |    |
|-------|----|----|---|---|----|
| Total | C  | F  | H | N | Zn |
| 49    | 24 | 12 | 8 | 4 | 1  |

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

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

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

- Molecule 1: PS1

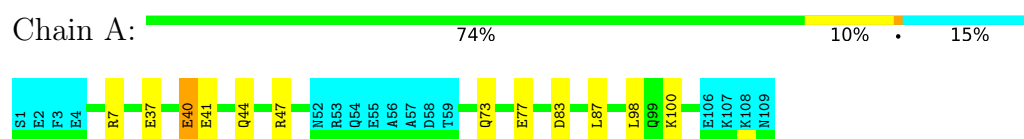


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

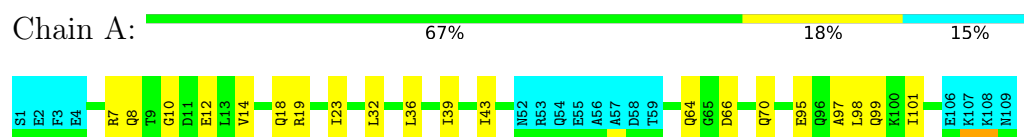
#### 4.2.1 Score per residue for model 1

- Molecule 1: PS1



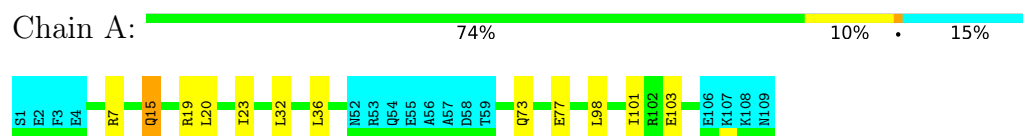
#### 4.2.2 Score per residue for model 2

- Molecule 1: PS1



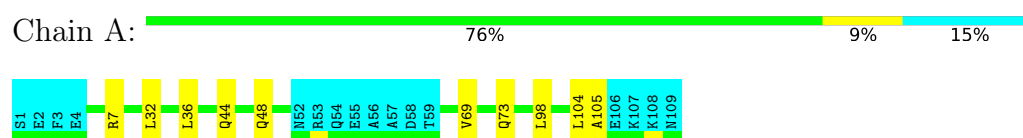
### 4.2.3 Score per residue for model 3

- Molecule 1: PS1



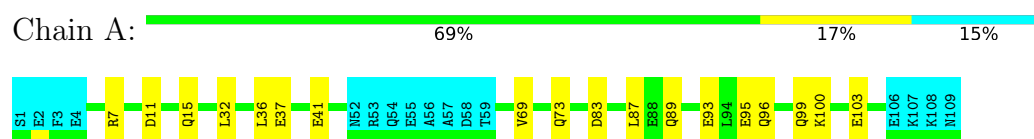
### 4.2.4 Score per residue for model 4

- Molecule 1: PS1



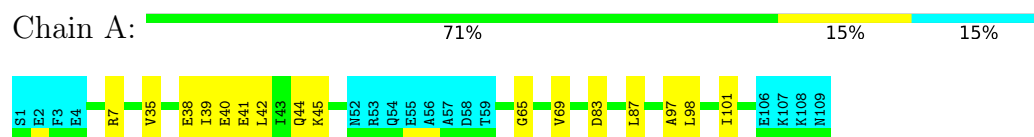
### 4.2.5 Score per residue for model 5

- Molecule 1: PS1



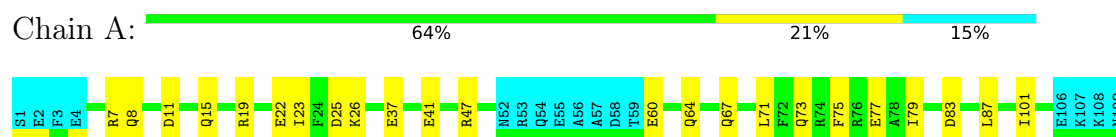
### 4.2.6 Score per residue for model 6

- Molecule 1: PS1



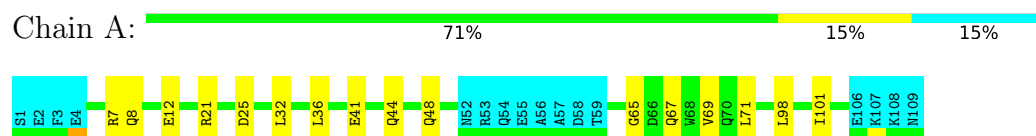
### 4.2.7 Score per residue for model 7

- Molecule 1: PS1



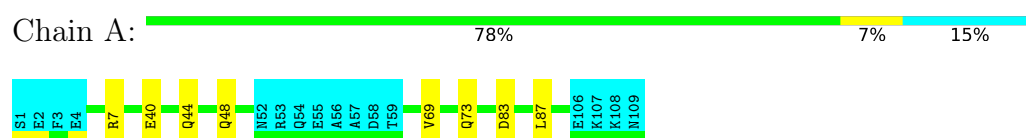
### 4.2.8 Score per residue for model 8

- Molecule 1: PS1



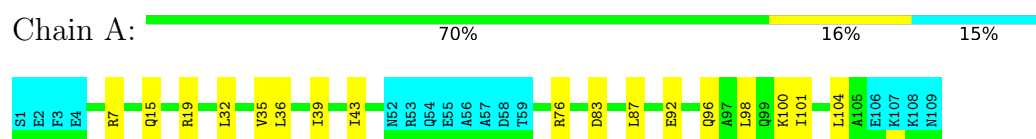
### 4.2.9 Score per residue for model 9

- Molecule 1: PS1



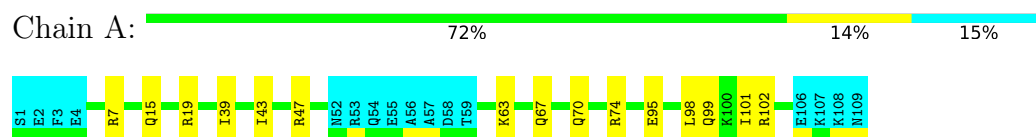
### 4.2.10 Score per residue for model 10

- Molecule 1: PS1



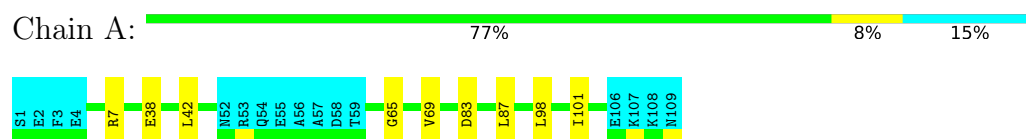
### 4.2.11 Score per residue for model 11

- Molecule 1: PS1



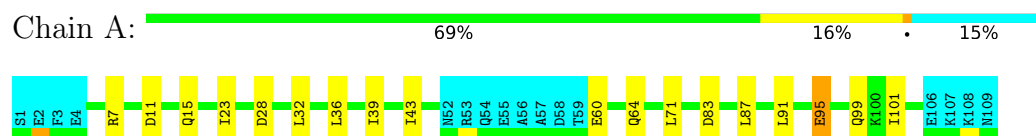
### 4.2.12 Score per residue for model 12

- Molecule 1: PS1



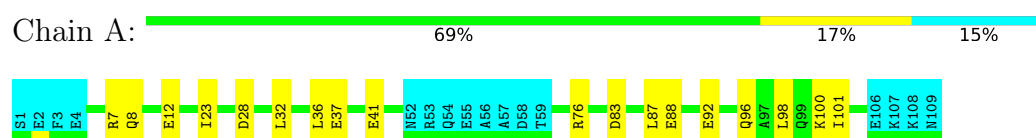
### 4.2.13 Score per residue for model 13

- Molecule 1: PS1



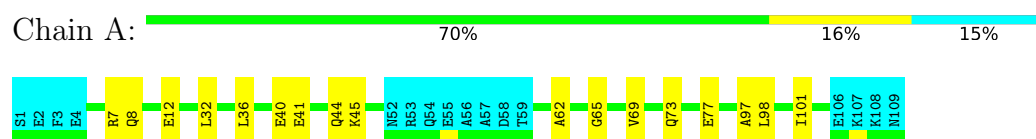
### 4.2.14 Score per residue for model 14

- Molecule 1: PS1



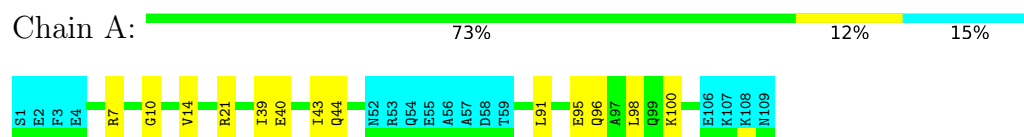
### 4.2.15 Score per residue for model 15 (medoid)

- Molecule 1: PS1



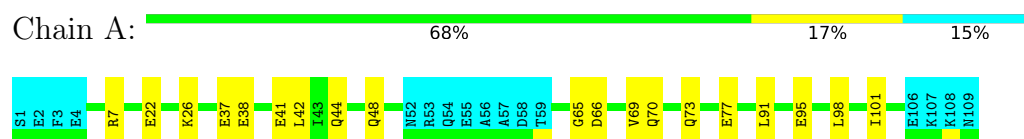
### 4.2.16 Score per residue for model 16

- Molecule 1: PS1



### 4.2.17 Score per residue for model 17

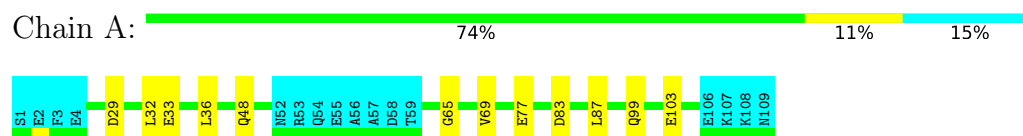
- Molecule 1: PS1





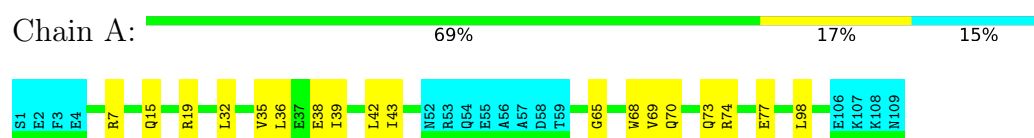
#### 4.2.18 Score per residue for model 18

- Molecule 1: PS1



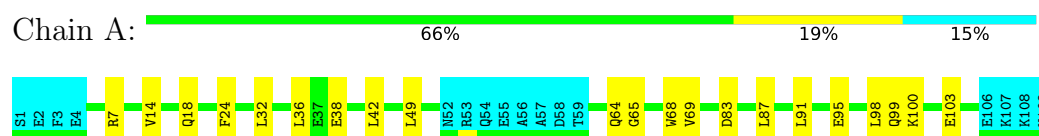
#### 4.2.19 Score per residue for model 19

- Molecule 1: PS1



#### 4.2.20 Score per residue for model 20

- Molecule 1: PS1



## 5 Refinement protocol and experimental data overview

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

Of the 20 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 |
|---------------|-----------------------|---------|
| CYANA         | 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                       | 1318           |
| Number of shifts mapped to atoms             | 1318           |
| Number of unparsed shifts                    | 0              |
| Number of shifts with mapping errors         | 0              |
| Number of shifts with mapping warnings       | 0              |
| Assignment completeness (well-defined parts) | 85%            |

## 6 Model quality

### 6.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 7BU

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 6.2 Too-close contacts

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     | 780   | 767      | 767      | 10±2    |
| 2   | A     | 41    | 8        | 0        | 11±1    |
| All | All   | 16420 | 15500    | 15340    | 356     |

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 11.

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

| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 2:A:201:7BU:F22A | 2:A:201:7BU:C2A  | 0.75     | 2.63        | 15     | 14    |
| 2:A:201:7BU:F22D | 2:A:201:7BU:C2D  | 0.75     | 2.65        | 14     | 14    |
| 2:A:201:7BU:C2D  | 2:A:201:7BU:F22D | 0.74     | 2.66        | 1      | 6     |
| 2:A:201:7BU:F21D | 2:A:201:7BU:C3C  | 0.72     | 2.65        | 19     | 20    |
| 2:A:201:7BU:C2A  | 2:A:201:7BU:F22A | 0.71     | 2.66        | 20     | 6     |
| 2:A:201:7BU:F23B | 2:A:201:7BU:C3A  | 0.70     | 2.68        | 7      | 20    |
| 2:A:201:7BU:C2C  | 2:A:201:7BU:F22C | 0.70     | 2.67        | 20     | 6     |
| 2:A:201:7BU:C3B  | 2:A:201:7BU:F21C | 0.67     | 2.73        | 11     | 14    |
| 2:A:201:7BU:F22C | 2:A:201:7BU:C2C  | 0.67     | 2.71        | 3      | 14    |
| 1:A:38:GLU:O     | 1:A:42:LEU:HG    | 0.66     | 1.91        | 17     | 5     |
| 2:A:201:7BU:F21B | 2:A:201:7BU:C2B  | 0.64     | 2.73        | 13     | 14    |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 2:A:201:7BU:F21C | 2:A:201:7BU:C3B  | 0.63     | 2.77        | 7      | 6     |
| 2:A:201:7BU:C3D  | 2:A:201:7BU:F23A | 0.63     | 2.76        | 10     | 14    |
| 2:A:201:7BU:F23A | 2:A:201:7BU:C3D  | 0.63     | 2.77        | 7      | 6     |
| 2:A:201:7BU:C2B  | 2:A:201:7BU:F21B | 0.63     | 2.76        | 17     | 6     |
| 1:A:95:GLU:O     | 1:A:99:GLN:HG2   | 0.61     | 1.95        | 5      | 5     |
| 1:A:47:ARG:HG3   | 2:A:201:7BU:F23B | 0.59     | 2.27        | 1      | 2     |
| 1:A:22:GLU:O     | 1:A:26:LYS:HD3   | 0.59     | 1.98        | 17     | 1     |
| 1:A:32:LEU:O     | 1:A:36:LEU:HG    | 0.58     | 1.98        | 5      | 12    |
| 1:A:44:GLN:O     | 1:A:48:GLN:HG3   | 0.57     | 2.00        | 17     | 3     |
| 1:A:83:ASP:O     | 1:A:87:LEU:HG    | 0.57     | 1.99        | 14     | 11    |
| 1:A:98:LEU:HG    | 2:A:201:7BU:F22C | 0.57     | 2.29        | 10     | 14    |
| 1:A:98:LEU:HA    | 2:A:201:7BU:F22C | 0.56     | 2.30        | 1      | 7     |
| 1:A:7:ARG:HA     | 2:A:201:7BU:F22D | 0.55     | 2.31        | 5      | 19    |
| 1:A:15:GLN:O     | 1:A:19:ARG:HG2   | 0.55     | 2.00        | 11     | 3     |
| 1:A:96:GLN:O     | 1:A:100:LYS:HG3  | 0.54     | 2.03        | 14     | 2     |
| 1:A:67:GLN:O     | 1:A:71:LEU:HG    | 0.53     | 2.03        | 8      | 1     |
| 1:A:37:GLU:O     | 1:A:41:GLU:HG2   | 0.52     | 2.05        | 17     | 3     |
| 1:A:40:GLU:O     | 1:A:44:GLN:HG2   | 0.51     | 2.05        | 9      | 4     |
| 1:A:47:ARG:HD2   | 2:A:201:7BU:F23B | 0.51     | 2.35        | 11     | 1     |
| 1:A:44:GLN:O     | 1:A:48:GLN:HG2   | 0.51     | 2.05        | 8      | 1     |
| 1:A:23:ILE:HG23  | 1:A:28:ASP:HB3   | 0.51     | 1.81        | 13     | 2     |
| 1:A:98:LEU:HD12  | 2:A:201:7BU:F23C | 0.51     | 2.36        | 3      | 1     |
| 1:A:7:ARG:HG3    | 2:A:201:7BU:F22D | 0.50     | 2.37        | 14     | 1     |
| 1:A:69:VAL:O     | 1:A:73:GLN:HG3   | 0.50     | 2.06        | 5      | 2     |
| 1:A:66:ASP:O     | 1:A:70:GLN:HG2   | 0.50     | 2.07        | 2      | 2     |
| 1:A:19:ARG:O     | 1:A:23:ILE:HG12  | 0.49     | 2.07        | 3      | 3     |
| 1:A:60:GLU:O     | 1:A:64:GLN:HG2   | 0.49     | 2.07        | 7      | 2     |
| 1:A:62:ALA:HB2   | 2:A:201:7BU:F22A | 0.48     | 2.38        | 15     | 1     |
| 1:A:96:GLN:O     | 1:A:100:LYS:HG2  | 0.48     | 2.07        | 5      | 1     |
| 1:A:99:GLN:O     | 1:A:103:GLU:HG2  | 0.48     | 2.08        | 5      | 1     |
| 1:A:8:GLN:O      | 1:A:12:GLU:HG2   | 0.48     | 2.09        | 14     | 3     |
| 1:A:7:ARG:HA     | 2:A:201:7BU:F21D | 0.47     | 2.39        | 4      | 4     |
| 1:A:101:ILE:HD12 | 2:A:201:7BU:F21C | 0.47     | 2.40        | 8      | 9     |
| 1:A:22:GLU:O     | 1:A:26:LYS:HG2   | 0.47     | 2.09        | 7      | 1     |
| 1:A:65:GLY:O     | 1:A:69:VAL:HG23  | 0.47     | 2.10        | 6      | 8     |
| 1:A:73:GLN:O     | 1:A:77:GLU:HG3   | 0.46     | 2.10        | 19     | 5     |
| 1:A:105:ALA:HB1  | 2:A:201:7BU:C2D  | 0.46     | 2.40        | 4      | 1     |
| 1:A:29:ASP:O     | 1:A:33:GLU:HG3   | 0.46     | 2.10        | 18     | 1     |
| 1:A:35:VAL:O     | 1:A:39:ILE:HG12  | 0.46     | 2.11        | 19     | 3     |
| 1:A:67:GLN:O     | 1:A:71:LEU:HD13  | 0.46     | 2.11        | 7      | 1     |
| 1:A:91:LEU:O     | 1:A:95:GLU:HG3   | 0.46     | 2.11        | 17     | 2     |

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| Atom-1          | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|-----------------|------------------|----------|-------------|--------|-------|
|                 |                  |          |             | Worst  | Total |
| 1:A:39:ILE:O    | 1:A:43:ILE:HG13  | 0.45     | 2.11        | 10     | 5     |
| 1:A:97:ALA:O    | 1:A:101:ILE:HG13 | 0.45     | 2.10        | 15     | 3     |
| 1:A:70:GLN:O    | 1:A:74:ARG:HG2   | 0.45     | 2.11        | 11     | 1     |
| 1:A:37:GLU:O    | 1:A:41:GLU:HG3   | 0.45     | 2.12        | 7      | 2     |
| 1:A:10:GLY:HA3  | 2:A:201:7BU:F21D | 0.45     | 2.42        | 2      | 1     |
| 1:A:88:GLU:O    | 1:A:92:GLU:HG2   | 0.45     | 2.12        | 14     | 1     |
| 1:A:7:ARG:HG2   | 2:A:201:7BU:F22D | 0.44     | 2.42        | 20     | 2     |
| 1:A:92:GLU:O    | 1:A:96:GLN:HG2   | 0.44     | 2.13        | 10     | 1     |
| 1:A:8:GLN:O     | 1:A:12:GLU:HG3   | 0.44     | 2.12        | 2      | 1     |
| 1:A:20:LEU:C    | 1:A:20:LEU:HD13  | 0.44     | 2.38        | 3      | 1     |
| 1:A:21:ARG:HG2  | 1:A:25:ASP:OD2   | 0.43     | 2.12        | 8      | 1     |
| 1:A:99:GLN:O    | 1:A:103:GLU:HG3  | 0.43     | 2.13        | 20     | 2     |
| 1:A:64:GLN:OE1  | 1:A:101:ILE:HA   | 0.43     | 2.13        | 2      | 1     |
| 1:A:11:ASP:O    | 1:A:15:GLN:HG3   | 0.43     | 2.13        | 5      | 3     |
| 1:A:75:PHE:CE2  | 1:A:79:ILE:HD11  | 0.43     | 2.48        | 7      | 1     |
| 1:A:64:GLN:OE1  | 1:A:100:LYS:HE3  | 0.42     | 2.14        | 20     | 1     |
| 1:A:14:VAL:O    | 1:A:18:GLN:HG3   | 0.42     | 2.14        | 20     | 2     |
| 1:A:15:GLN:HE21 | 1:A:15:GLN:HA    | 0.42     | 1.74        | 3      | 1     |
| 1:A:39:ILE:O    | 1:A:43:ILE:HG12  | 0.42     | 2.14        | 11     | 1     |
| 1:A:68:TRP:CG   | 2:A:201:7BU:F21C | 0.42     | 3.02        | 20     | 1     |
| 1:A:41:GLU:O    | 1:A:45:LYS:HG3   | 0.42     | 2.15        | 6      | 2     |
| 1:A:40:GLU:O    | 1:A:44:GLN:HG3   | 0.42     | 2.14        | 15     | 1     |
| 1:A:68:TRP:CD2  | 2:A:201:7BU:F21C | 0.42     | 3.03        | 20     | 2     |
| 1:A:100:LYS:HZ2 | 1:A:100:LYS:HB3  | 0.41     | 1.74        | 1      | 1     |
| 1:A:89:GLN:O    | 1:A:93:GLU:HG2   | 0.41     | 2.15        | 5      | 1     |
| 1:A:70:GLN:O    | 1:A:74:ARG:HG3   | 0.41     | 2.15        | 19     | 1     |
| 1:A:24:PHE:CD2  | 1:A:91:LEU:HD22  | 0.41     | 2.51        | 20     | 1     |
| 1:A:69:VAL:O    | 1:A:73:GLN:HG2   | 0.41     | 2.15        | 4      | 1     |
| 1:A:22:GLU:HA   | 1:A:25:ASP:OD2   | 0.41     | 2.16        | 7      | 1     |
| 1:A:100:LYS:O   | 1:A:104:LEU:HG   | 0.41     | 2.16        | 10     | 1     |
| 1:A:63:LYS:O    | 1:A:67:GLN:HG3   | 0.41     | 2.15        | 11     | 1     |
| 1:A:100:LYS:HB3 | 1:A:100:LYS:NZ   | 0.40     | 2.31        | 1      | 1     |
| 1:A:10:GLY:O    | 1:A:14:VAL:HG23  | 0.40     | 2.15        | 16     | 1     |
| 1:A:73:GLN:O    | 1:A:77:GLU:HG2   | 0.40     | 2.17        | 17     | 1     |

## 6.3 Torsion angles ⓘ

### 6.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR

entries. The Analysed column shows the number of residues for which the backbone conformation was analysed and the total number of residues.

| Mol | Chain | Analysed        | Favoured      | Allowed    | Outliers   | Percentiles |     |
|-----|-------|-----------------|---------------|------------|------------|-------------|-----|
| 1   | A     | 93/109 (85%)    | 93±0 (100±0%) | 0±0 (0±0%) | 0±0 (0±0%) | 100         | 100 |
| All | All   | 1860/2180 (85%) | 1860 (100%)   | 0 (0%)     | 0 (0%)     | 100         | 100 |

There are no Ramachandran outliers.

### 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     | 83/97 (86%)     | 82±1 (99±1%) | 1±1 (1±1%) | 73          | 96 |
| All | All   | 1660/1940 (86%) | 1649 (99%)   | 11 (1%)    | 73          | 96 |

All 10 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     | 76  | ARG  | 2              |
| 1   | A     | 40  | GLU  | 1              |
| 1   | A     | 15  | GLN  | 1              |
| 1   | A     | 41  | GLU  | 1              |
| 1   | A     | 71  | LEU  | 1              |
| 1   | A     | 91  | LEU  | 1              |
| 1   | A     | 95  | GLU  | 1              |
| 1   | A     | 21  | ARG  | 1              |
| 1   | A     | 48  | GLN  | 1              |
| 1   | A     | 77  | GLU  | 1              |

### 6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length is the number of standard deviations the observed value is removed from the expected value. A bond length with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

| Mol | Type | Chain | Res | Link | Bond lengths |           |            |
|-----|------|-------|-----|------|--------------|-----------|------------|
|     |      |       |     |      | Counts       | RMSZ      | #Z>2       |
| 2   | 7BU  | A     | 201 | 1    | 48,48,48     | 1.04±0.02 | 1±1 (2±1%) |

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

| Mol | Type | Chain | Res | Link | Bond angles |           |            |
|-----|------|-------|-----|------|-------------|-----------|------------|
|     |      |       |     |      | Counts      | RMSZ      | #Z>2       |
| 2   | 7BU  | A     | 201 | 1    | 64,86,86    | 0.52±0.01 | 0±0 (0±0%) |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res | Link | Chirals | Torsions     | Rings |
|-----|------|-------|-----|------|---------|--------------|-------|
| 2   | 7BU  | A     | 201 | 1    | -       | 0±0,24,80,80 | -     |

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

| Mol | Chain | Res | Type | Atoms    | Z    | Observed(Å) | Ideal(Å) | Models |       |
|-----|-------|-----|------|----------|------|-------------|----------|--------|-------|
|     |       |     |      |          |      |             |          | Worst  | Total |
| 2   | A     | 201 | 7BU  | ZN-ND4   | 2.24 | 2.10        | 2.03     | 14     | 18    |
| 2   | A     | 201 | 7BU  | C1FA-CHA | 2.12 | 1.55        | 1.50     | 3      | 9     |

There are no bond-angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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 85% for the well-defined parts and 84% for the entire structure.

### 7.1 Chemical shift list 1

File name: working\_cs.cif

Chemical shift list name: *hologood.bmr*

#### 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                  | 1318 |
| Number of shifts mapped to atoms        | 1318 |
| Number of unparsed shifts               | 0    |
| Number of shifts with mapping errors    | 0    |
| Number of shifts with mapping warnings  | 0    |
| Number of shift outliers (ShiftChecker) | 17   |

#### 7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

| Nucleus                | # values | Correction $\pm$ precision, ppm | Suggested action           |
|------------------------|----------|---------------------------------|----------------------------|
| $^{13}\text{C}_\alpha$ | 108      | $-0.58 \pm 0.16$                | Should be checked          |
| $^{13}\text{C}_\beta$  | 104      | $0.29 \pm 0.08$                 | None needed ( $< 0.5$ ppm) |
| $^{13}\text{C}'$       | 0        | —                               | None (insufficient data)   |
| $^{15}\text{N}$        | 108      | $-0.12 \pm 0.11$                | 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 85%, i.e. 1152 atoms were assigned a chemical shift out of a possible 1357. 0 out of 17 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total         | $^1\text{H}$   | $^{13}\text{C}$ | $^{15}\text{N}$ |
|-----------|---------------|----------------|-----------------|-----------------|
| Backbone  | 376/469 (80%) | 190/190 (100%) | 93/186 (50%)    | 93/93 (100%)    |
| Sidechain | 718/819 (88%) | 487/519 (94%)  | 215/259 (83%)   | 16/41 (39%)     |

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|          | <b>Total</b>    | <b><sup>1</sup>H</b> | <b><sup>13</sup>C</b> | <b><sup>15</sup>N</b> |
|----------|-----------------|----------------------|-----------------------|-----------------------|
| Aromatic | 58/69 (84%)     | 34/35 (97%)          | 22/32 (69%)           | 2/2 (100%)            |
| Overall  | 1152/1357 (85%) | 711/744 (96%)        | 330/477 (69%)         | 111/136 (82%)         |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 84%, i.e. 1318 atoms were assigned a chemical shift out of a possible 1567. 0 out of 17 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | <b>Total</b>    | <b><sup>1</sup>H</b> | <b><sup>13</sup>C</b> | <b><sup>15</sup>N</b> |
|-----------|-----------------|----------------------|-----------------------|-----------------------|
| Backbone  | 436/549 (79%)   | 220/222 (99%)        | 108/218 (50%)         | 108/109 (99%)         |
| Sidechain | 816/939 (87%)   | 553/592 (93%)        | 244/298 (82%)         | 19/49 (39%)           |
| Aromatic  | 66/79 (84%)     | 39/40 (98%)          | 25/37 (68%)           | 2/2 (100%)            |
| Overall   | 1318/1567 (84%) | 812/854 (95%)        | 377/553 (68%)         | 129/160 (81%)         |

#### 7.1.4 Statistically unusual chemical shifts ⓘ

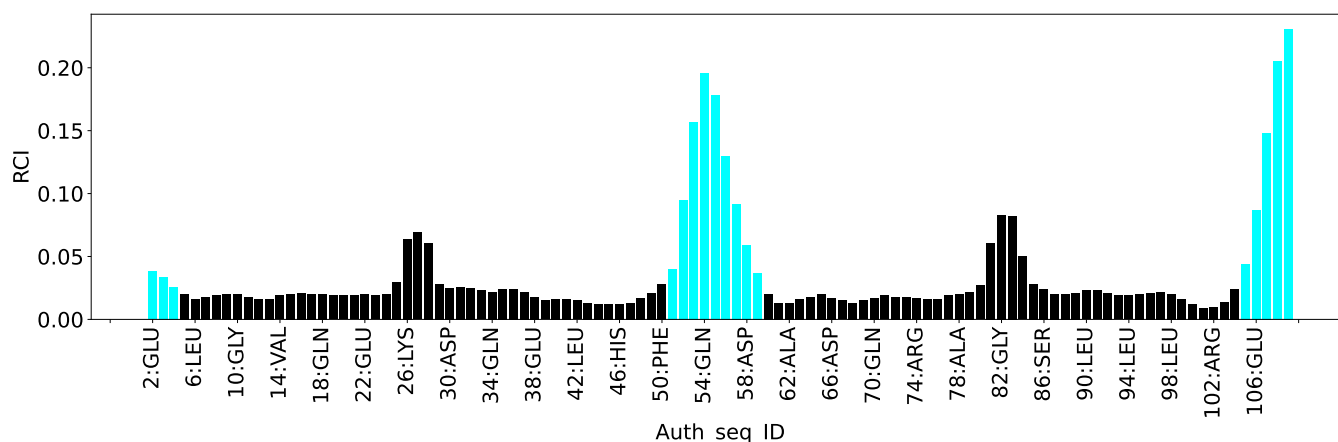
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

| List Id | Chain | Res | Type | Atom | Shift, ppm | Expected range, ppm | Z-score |
|---------|-------|-----|------|------|------------|---------------------|---------|
| 1       | A     | 101 | ILE  | HG21 | -3.92      | -0.56 – 2.11        | -17.6   |
| 1       | A     | 101 | ILE  | HG22 | -3.92      | -0.56 – 2.11        | -17.6   |
| 1       | A     | 101 | ILE  | HG23 | -3.92      | -0.56 – 2.11        | -17.6   |
| 1       | A     | 46  | HIS  | HD2  | 1.10       | 4.65 – 9.35         | -12.6   |
| 1       | A     | 46  | HIS  | HE1  | 2.64       | 5.13 – 10.76        | -9.4    |
| 1       | A     | 46  | HIS  | ND1  | 31.03      | 97.69 – 289.13      | -8.5    |
| 1       | A     | 10  | GLY  | HA2  | 1.01       | 2.15 – 5.77         | -8.2    |
| 1       | A     | 101 | ILE  | HD11 | -1.57      | -0.72 – 2.09        | -8.0    |
| 1       | A     | 101 | ILE  | HD12 | -1.57      | -0.72 – 2.09        | -8.0    |
| 1       | A     | 101 | ILE  | HD13 | -1.57      | -0.72 – 2.09        | -8.0    |
| 1       | A     | 101 | ILE  | HG12 | -1.58      | -0.69 – 3.24        | -7.2    |
| 1       | A     | 65  | GLY  | HA2  | 1.62       | 2.15 – 5.77         | -6.5    |
| 1       | A     | 101 | ILE  | HB   | 0.01       | 0.35 – 3.22         | -6.2    |
| 1       | A     | 61  | ALA  | HB1  | -0.08      | 0.14 – 2.58         | -5.9    |
| 1       | A     | 61  | ALA  | HB2  | -0.08      | 0.14 – 2.58         | -5.9    |
| 1       | A     | 61  | ALA  | HB3  | -0.08      | 0.14 – 2.58         | -5.9    |
| 1       | A     | 10  | GLY  | HA3  | 2.05       | 2.08 – 5.71         | -5.1    |

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

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

Random coil index (RCI) for chain A:



## 8 NMR restraints analysis

### 8.1 Conformationally restricting restraints

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

| Description                                              | Value |
|----------------------------------------------------------|-------|
| Total distance restraints                                | 2143  |
| Intra-residue ( $ i-j =0$ )                              | 467   |
| Sequential ( $ i-j =1$ )                                 | 498   |
| Medium range ( $ i-j >1$ and $ i-j <5$ )                 | 616   |
| Long range ( $ i-j \geq 5$ )                             | 526   |
| Inter-chain                                              | 26    |
| Hydrogen bond restraints                                 | 10    |
| Disulfide bond restraints                                | 0     |
| Total dihedral-angle restraints                          | 228   |
| Number of unmapped restraints                            | 0     |
| Number of restraints per residue                         | 21.6  |
| Number of long range restraints per residue <sup>1</sup> | 4.8   |

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

### 8.2 Residual restraint violations

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

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

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

| Bins (Å)         | Average number of violations per model | Max (Å) |
|------------------|----------------------------------------|---------|
| 0.1-0.2 (Small)  | 8.2                                    | 0.2     |
| 0.2-0.5 (Medium) | 1.6                                    | 0.4     |
| >0.5 (Large)     | None                                   | None    |

### 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)   | 45.0                                   | 7.27    |
| 10.0-20.0 (Medium) | None                                   | None    |
| >20.0 (Large)      | None                                   | None    |

## 9 Distance violation analysis ⓘ

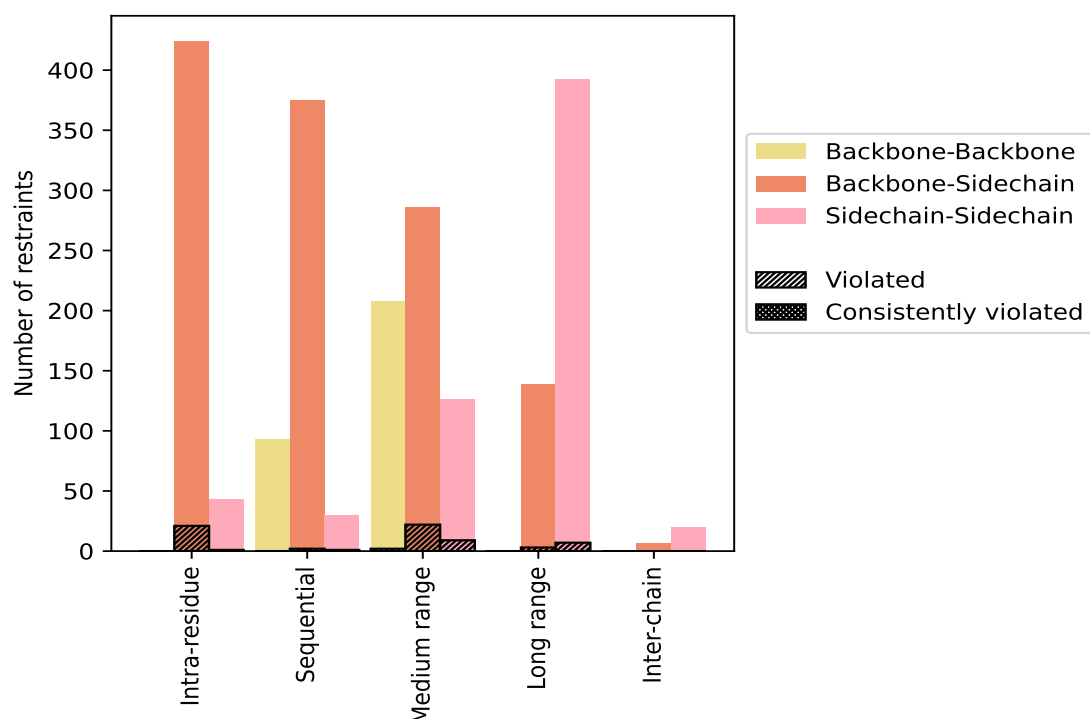
### 9.1 Summary of distance violations ⓘ

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

| Restrains type                                             | Count                | % <sup>1</sup>        | Violated <sup>3</sup> |                      |                     | Consistently Violated <sup>4</sup> |                     |                     |
|------------------------------------------------------------|----------------------|-----------------------|-----------------------|----------------------|---------------------|------------------------------------|---------------------|---------------------|
|                                                            |                      |                       | Count                 | % <sup>2</sup>       | % <sup>1</sup>      | Count                              | % <sup>2</sup>      | % <sup>1</sup>      |
| <a href="#">Intra-residue ( i-j =0)</a>                    | <a href="#">467</a>  | <a href="#">21.8</a>  | <a href="#">22</a>    | <a href="#">4.7</a>  | <a href="#">1.0</a> | <a href="#">0</a>                  | <a href="#">0.0</a> | <a href="#">0.0</a> |
| Backbone-Backbone                                          | 0                    | 0.0                   | 0                     | 0.0                  | 0.0                 | 0                                  | 0.0                 | 0.0                 |
| Backbone-Sidechain                                         | 424                  | 19.8                  | 21                    | 5.0                  | 1.0                 | 0                                  | 0.0                 | 0.0                 |
| Sidechain-Sidechain                                        | 43                   | 2.0                   | 1                     | 2.3                  | 0.0                 | 0                                  | 0.0                 | 0.0                 |
| <a href="#">Sequential ( i-j =1)</a>                       | <a href="#">498</a>  | <a href="#">23.2</a>  | <a href="#">3</a>     | <a href="#">0.6</a>  | <a href="#">0.1</a> | <a href="#">0</a>                  | <a href="#">0.0</a> | <a href="#">0.0</a> |
| Backbone-Backbone                                          | 93                   | 4.3                   | 0                     | 0.0                  | 0.0                 | 0                                  | 0.0                 | 0.0                 |
| Backbone-Sidechain                                         | 375                  | 17.5                  | 2                     | 0.5                  | 0.1                 | 0                                  | 0.0                 | 0.0                 |
| Sidechain-Sidechain                                        | 30                   | 1.4                   | 1                     | 3.3                  | 0.0                 | 0                                  | 0.0                 | 0.0                 |
| <a href="#">Medium range ( i-j &gt;1 &amp;  i-j &lt;5)</a> | <a href="#">616</a>  | <a href="#">28.7</a>  | <a href="#">29</a>    | <a href="#">4.7</a>  | <a href="#">1.4</a> | <a href="#">0</a>                  | <a href="#">0.0</a> | <a href="#">0.0</a> |
| Backbone-Backbone                                          | 208                  | 9.7                   | 2                     | 1.0                  | 0.1                 | 0                                  | 0.0                 | 0.0                 |
| Backbone-Sidechain                                         | 286                  | 13.3                  | 22                    | 7.7                  | 1.0                 | 0                                  | 0.0                 | 0.0                 |
| Sidechain-Sidechain                                        | 122                  | 5.7                   | 5                     | 4.1                  | 0.2                 | 0                                  | 0.0                 | 0.0                 |
| <a href="#">Long range ( i-j ≥5)</a>                       | <a href="#">526</a>  | <a href="#">24.5</a>  | <a href="#">9</a>     | <a href="#">1.7</a>  | <a href="#">0.4</a> | <a href="#">0</a>                  | <a href="#">0.0</a> | <a href="#">0.0</a> |
| Backbone-Backbone                                          | 1                    | 0.0                   | 0                     | 0.0                  | 0.0                 | 0                                  | 0.0                 | 0.0                 |
| Backbone-Sidechain                                         | 139                  | 6.5                   | 3                     | 2.2                  | 0.1                 | 0                                  | 0.0                 | 0.0                 |
| Sidechain-Sidechain                                        | 386                  | 18.0                  | 6                     | 1.6                  | 0.3                 | 0                                  | 0.0                 | 0.0                 |
| <a href="#">Inter-chain</a>                                | <a href="#">26</a>   | <a href="#">1.2</a>   | <a href="#">0</a>     | <a href="#">0.0</a>  | <a href="#">0.0</a> | <a href="#">0</a>                  | <a href="#">0.0</a> | <a href="#">0.0</a> |
| Backbone-Backbone                                          | 0                    | 0.0                   | 0                     | 0.0                  | 0.0                 | 0                                  | 0.0                 | 0.0                 |
| Backbone-Sidechain                                         | 6                    | 0.3                   | 0                     | 0.0                  | 0.0                 | 0                                  | 0.0                 | 0.0                 |
| Sidechain-Sidechain                                        | 20                   | 0.9                   | 0                     | 0.0                  | 0.0                 | 0                                  | 0.0                 | 0.0                 |
| <a href="#">Hydrogen bond</a>                              | <a href="#">10</a>   | <a href="#">0.5</a>   | <a href="#">5</a>     | <a href="#">50.0</a> | <a href="#">0.2</a> | <a href="#">0</a>                  | <a href="#">0.0</a> | <a href="#">0.0</a> |
| <a href="#">Disulfide bond</a>                             | <a href="#">0</a>    | <a href="#">0.0</a>   | <a href="#">0</a>     | <a href="#">0.0</a>  | <a href="#">0.0</a> | <a href="#">0</a>                  | <a href="#">0.0</a> | <a href="#">0.0</a> |
| <a href="#">Total</a>                                      | <a href="#">2143</a> | <a href="#">100.0</a> | <a href="#">68</a>    | <a href="#">3.2</a>  | <a href="#">3.2</a> | <a href="#">0</a>                  | <a href="#">0.0</a> | <a href="#">0.0</a> |
| Backbone-Backbone                                          | 302                  | 14.1                  | 2                     | 0.7                  | 0.1                 | 0                                  | 0.0                 | 0.0                 |
| Backbone-Sidechain                                         | 1230                 | 57.4                  | 48                    | 3.9                  | 2.2                 | 0                                  | 0.0                 | 0.0                 |
| Sidechain-Sidechain                                        | 611                  | 28.5                  | 18                    | 2.9                  | 0.8                 | 0                                  | 0.0                 | 0.0                 |

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

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



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

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

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

| Model ID | Number of violations |                 |                 |                 |                 |       | Mean (Å) | Max (Å) | SD <sup>6</sup> (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
|          | IR <sup>1</sup>      | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total |          |         |                     |            |
| 1        | 1                    | 0               | 5               | 2               | 0               | 8     | 0.16     | 0.25    | 0.04                | 0.15       |
| 2        | 3                    | 0               | 4               | 1               | 0               | 8     | 0.15     | 0.25    | 0.05                | 0.12       |
| 3        | 4                    | 1               | 5               | 1               | 0               | 11    | 0.17     | 0.28    | 0.05                | 0.17       |
| 4        | 5                    | 0               | 3               | 2               | 0               | 10    | 0.15     | 0.23    | 0.05                | 0.12       |
| 5        | 6                    | 0               | 4               | 0               | 0               | 10    | 0.14     | 0.19    | 0.03                | 0.14       |
| 6        | 5                    | 1               | 3               | 4               | 0               | 13    | 0.14     | 0.23    | 0.04                | 0.13       |
| 7        | 4                    | 0               | 8               | 1               | 0               | 13    | 0.18     | 0.29    | 0.06                | 0.18       |
| 8        | 4                    | 0               | 5               | 1               | 0               | 10    | 0.14     | 0.22    | 0.03                | 0.14       |
| 9        | 5                    | 0               | 3               | 1               | 0               | 9     | 0.15     | 0.23    | 0.04                | 0.15       |
| 10       | 9                    | 0               | 4               | 3               | 0               | 16    | 0.17     | 0.4     | 0.07                | 0.15       |

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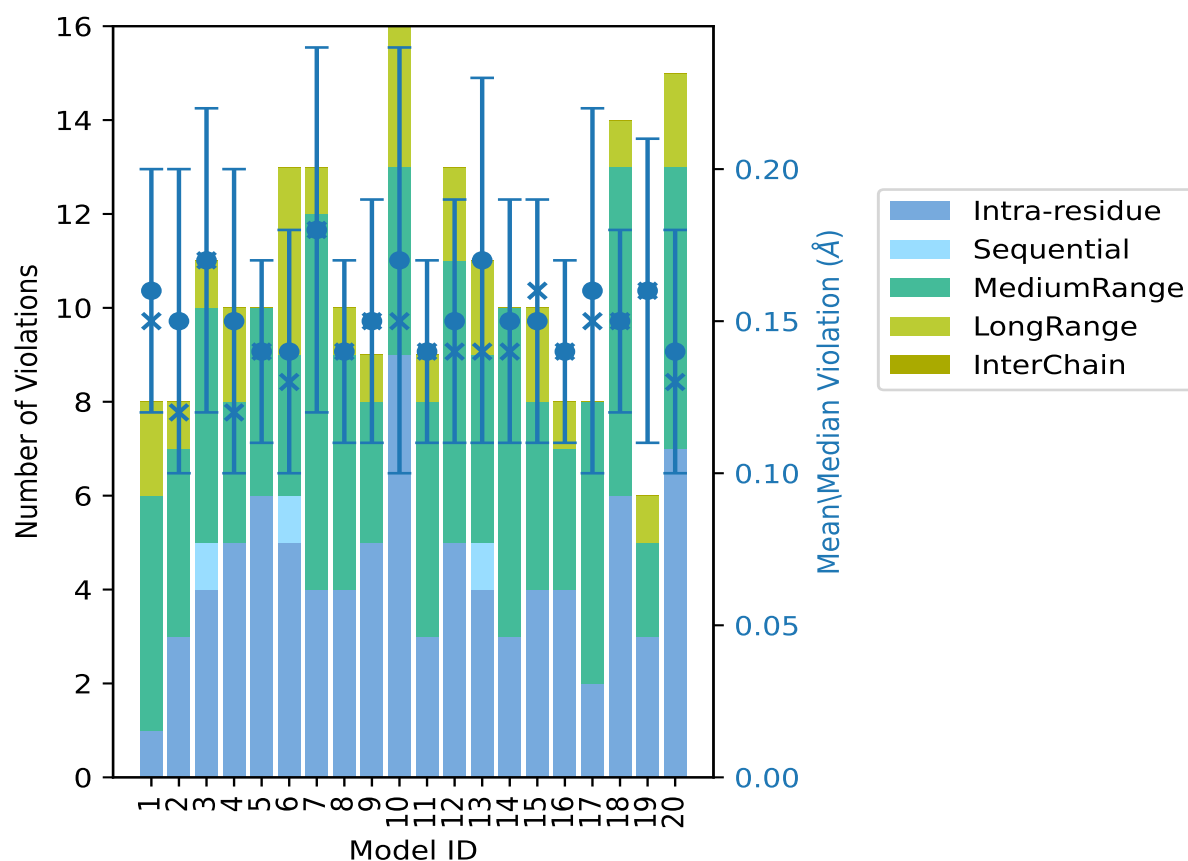
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| Model ID | Number of violations |                 |                 |                 |                 |       | Mean (Å) | Max (Å) | SD <sup>6</sup> (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
|          | IR <sup>1</sup>      | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total |          |         |                     |            |
| 11       | 3                    | 0               | 5               | 1               | 0               | 9     | 0.14     | 0.2     | 0.03                | 0.14       |
| 12       | 5                    | 0               | 6               | 2               | 0               | 13    | 0.15     | 0.25    | 0.04                | 0.14       |
| 13       | 4                    | 1               | 4               | 2               | 0               | 11    | 0.17     | 0.32    | 0.06                | 0.14       |
| 14       | 3                    | 0               | 7               | 0               | 0               | 10    | 0.15     | 0.21    | 0.04                | 0.14       |
| 15       | 4                    | 0               | 4               | 2               | 0               | 10    | 0.15     | 0.23    | 0.04                | 0.16       |
| 16       | 4                    | 0               | 3               | 1               | 0               | 8     | 0.14     | 0.21    | 0.03                | 0.14       |
| 17       | 2                    | 0               | 6               | 0               | 0               | 8     | 0.16     | 0.27    | 0.06                | 0.15       |
| 18       | 6                    | 0               | 7               | 1               | 0               | 14    | 0.15     | 0.21    | 0.03                | 0.15       |
| 19       | 3                    | 0               | 2               | 1               | 0               | 6     | 0.16     | 0.24    | 0.05                | 0.16       |
| 20       | 7                    | 0               | 6               | 2               | 0               | 15    | 0.14     | 0.26    | 0.04                | 0.13       |

<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

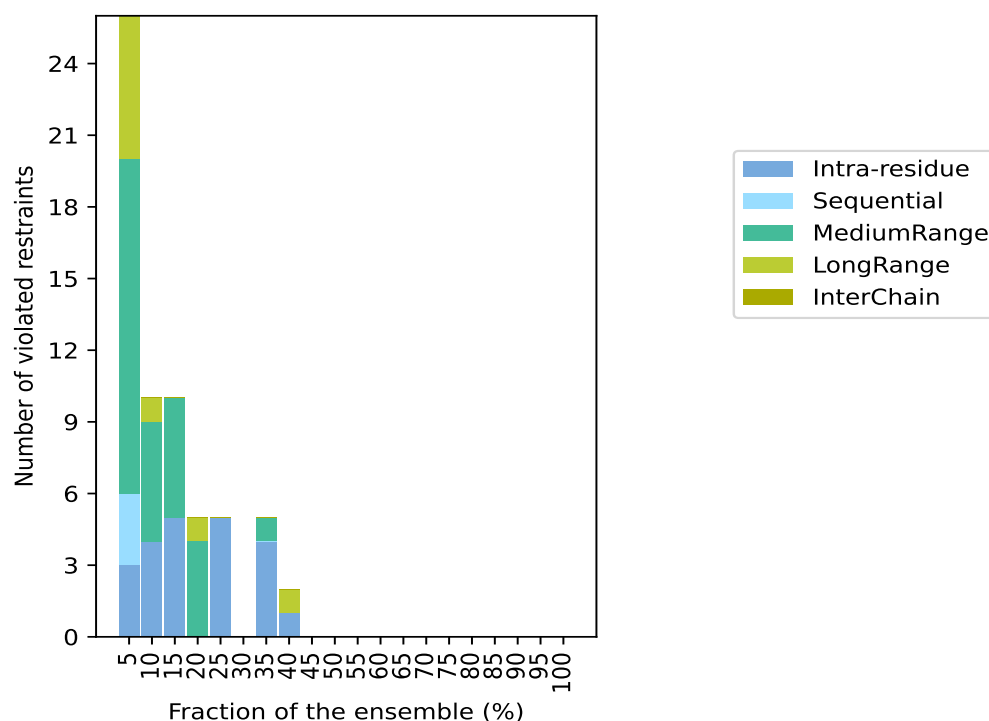
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 2070(IR:445, SQ:495, MR:587, LR:517, IC:26) restraints are 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>       | %     |
| 3                             | 3               | 14              | 6               | 0               | 26    | 1                        | 5.0   |
| 4                             | 0               | 5               | 1               | 0               | 10    | 2                        | 10.0  |
| 5                             | 0               | 5               | 0               | 0               | 10    | 3                        | 15.0  |
| 0                             | 0               | 4               | 1               | 0               | 5     | 4                        | 20.0  |
| 5                             | 0               | 0               | 0               | 0               | 5     | 5                        | 25.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 6                        | 30.0  |
| 4                             | 0               | 1               | 0               | 0               | 5     | 7                        | 35.0  |
| 1                             | 0               | 0               | 1               | 0               | 2     | 8                        | 40.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 9                        | 45.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 10                       | 50.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 11                       | 55.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 12                       | 60.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 13                       | 65.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 14                       | 70.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 15                       | 75.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 16                       | 80.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 17                       | 85.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 18                       | 90.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 19                       | 95.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 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

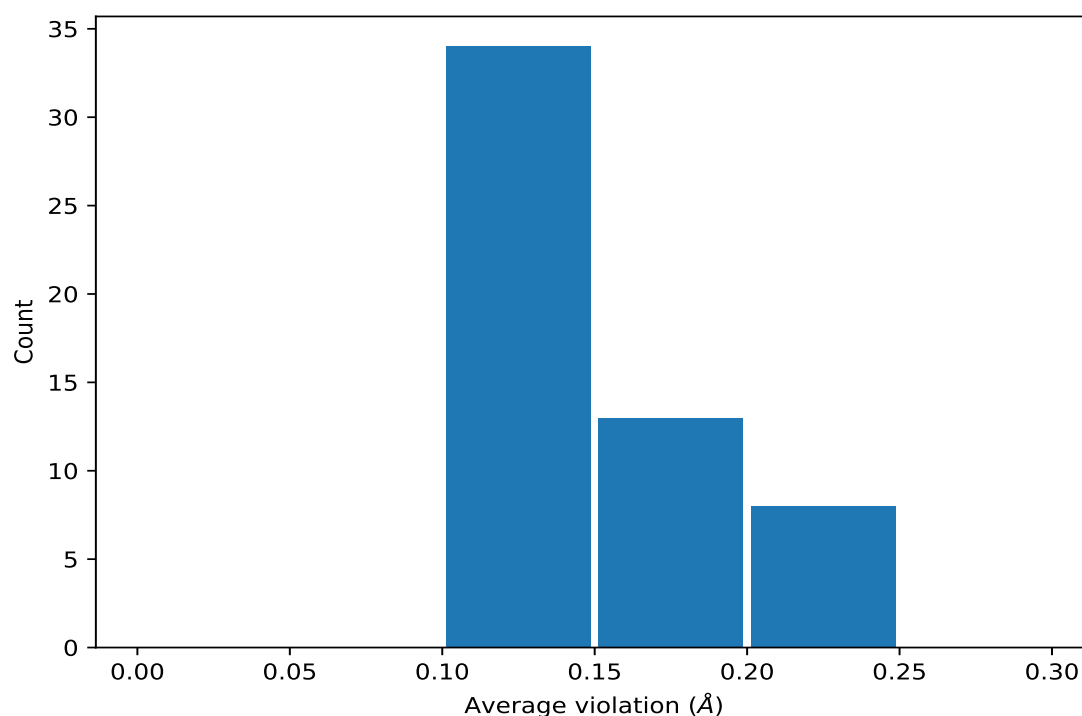
### 9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



## 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) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (2,7)    | 1:25:A:ASP:OD1   | 1:21:A:ARG:HE    | 15                  | 0.18     | 0.09                | 0.15       |
| (2,9)    | 1:80:A:ASP:OD1   | 1:76:A:ARG:HE    | 15                  | 0.17     | 0.04                | 0.17       |
| (2,1)    | 1:6:A:LEU:O      | 1:46:A:HIS:HD1   | 8                   | 0.18     | 0.04                | 0.17       |
| (1,375)  | 1:70:A:GLN:H     | 1:70:A:GLN:HG2   | 8                   | 0.16     | 0.04                | 0.13       |
| (1,1674) | 1:71:A:LEU:HD21  | 1:94:A:LEU:HA    | 8                   | 0.11     | 0.01                | 0.11       |
| (1,1674) | 1:71:A:LEU:HD22  | 1:94:A:LEU:HA    | 8                   | 0.11     | 0.01                | 0.11       |
| (1,1674) | 1:71:A:LEU:HD23  | 1:94:A:LEU:HA    | 8                   | 0.11     | 0.01                | 0.11       |
| (1,893)  | 1:41:A:GLU:H     | 1:41:A:GLU:HG2   | 7                   | 0.18     | 0.04                | 0.17       |
| (1,1031) | 1:8:A:GLN:HA     | 1:11:A:ASP:HB3   | 7                   | 0.15     | 0.03                | 0.15       |
| (1,328)  | 1:41:A:GLU:H     | 1:41:A:GLU:HG3   | 7                   | 0.14     | 0.02                | 0.14       |
| (1,376)  | 1:70:A:GLN:H     | 1:70:A:GLN:HG3   | 7                   | 0.13     | 0.02                | 0.13       |
| (1,2097) | 2:201:A:7BU:H3B1 | 2:201:A:7BU:F23C | 7                   | 0.11     | 0.01                | 0.11       |
| (1,319)  | 1:37:A:GLU:H     | 1:37:A:GLU:HG3   | 5                   | 0.2      | 0.03                | 0.23       |
| (1,290)  | 1:22:A:GLU:H     | 1:22:A:GLU:HG2   | 5                   | 0.18     | 0.01                | 0.19       |
| (1,437)  | 1:99:A:GLN:H     | 1:99:A:GLN:HG2   | 5                   | 0.18     | 0.01                | 0.17       |
| (1,437)  | 1:99:A:GLN:H     | 1:99:A:GLN:HG3   | 5                   | 0.18     | 0.01                | 0.17       |

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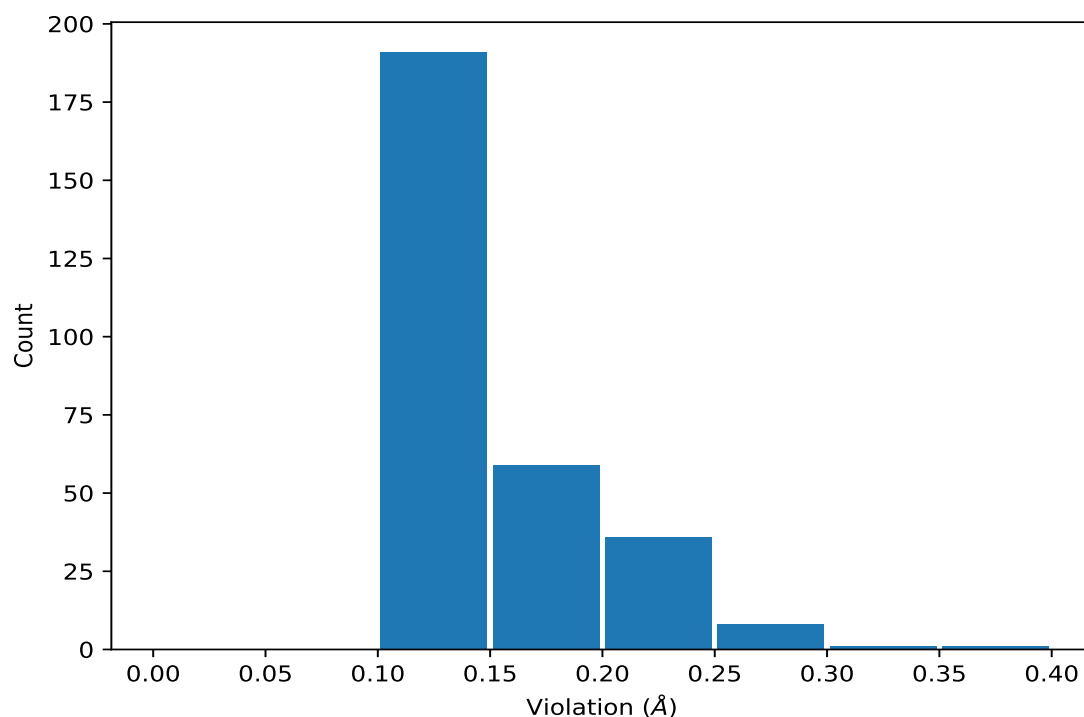
| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,268)  | 1:15:A:GLN:H    | 1:15:A:GLN:HG2  | 5                   | 0.16     | 0.03                | 0.16       |
| (1,318)  | 1:37:A:GLU:H    | 1:37:A:GLU:HG2  | 5                   | 0.16     | 0.03                | 0.15       |
| (1,1059) | 1:28:A:ASP:HA   | 1:31:A:SER:HB2  | 4                   | 0.24     | 0.03                | 0.25       |
| (1,1525) | 1:97:A:ALA:HA   | 1:100:A:LYS:HD2 | 4                   | 0.2      | 0.04                | 0.21       |
| (1,1525) | 1:97:A:ALA:HA   | 1:100:A:LYS:HD3 | 4                   | 0.2      | 0.04                | 0.21       |
| (1,1438) | 1:69:A:VAL:HG11 | 1:73:A:GLN:HG3  | 4                   | 0.14     | 0.04                | 0.13       |
| (1,1438) | 1:69:A:VAL:HG12 | 1:73:A:GLN:HG3  | 4                   | 0.14     | 0.04                | 0.13       |
| (1,1438) | 1:69:A:VAL:HG13 | 1:73:A:GLN:HG3  | 4                   | 0.14     | 0.04                | 0.13       |
| (1,1295) | 1:16:A:ALA:HA   | 1:35:A:VAL:HG21 | 4                   | 0.14     | 0.02                | 0.14       |
| (1,1295) | 1:16:A:ALA:HA   | 1:35:A:VAL:HG22 | 4                   | 0.14     | 0.02                | 0.14       |
| (1,1295) | 1:16:A:ALA:HA   | 1:35:A:VAL:HG23 | 4                   | 0.14     | 0.02                | 0.14       |
| (1,1070) | 1:35:A:VAL:HA   | 1:38:A:GLU:HB3  | 4                   | 0.12     | 0.01                | 0.12       |
| (1,1426) | 1:71:A:LEU:HA   | 1:74:A:ARG:HD2  | 3                   | 0.21     | 0.07                | 0.23       |
| (1,851)  | 1:12:A:GLU:H    | 1:12:A:GLU:HG2  | 3                   | 0.16     | 0.02                | 0.17       |
| (1,269)  | 1:15:A:GLN:H    | 1:15:A:GLN:HG3  | 3                   | 0.15     | 0.03                | 0.16       |
| (1,450)  | 1:106:A:GLU:H   | 1:106:A:GLU:HG2 | 3                   | 0.14     | 0.04                | 0.11       |
| (1,871)  | 1:22:A:GLU:H    | 1:22:A:GLU:HG3  | 3                   | 0.13     | 0.03                | 0.11       |
| (1,1127) | 1:77:A:GLU:HA   | 1:80:A:ASP:HB3  | 3                   | 0.13     | 0.0                 | 0.13       |
| (1,386)  | 1:73:A:GLN:H    | 1:73:A:GLN:HG2  | 3                   | 0.12     | 0.01                | 0.12       |
| (1,1150) | 1:97:A:ALA:HA   | 1:100:A:LYS:HB3 | 3                   | 0.12     | 0.02                | 0.11       |
| (1,1060) | 1:28:A:ASP:HA   | 1:31:A:SER:HB3  | 3                   | 0.12     | 0.01                | 0.11       |
| (1,1864) | 1:28:A:ASP:HA   | 1:31:A:SER:HB2  | 3                   | 0.1      | 0.0                 | 0.1        |
| (1,1864) | 1:28:A:ASP:HA   | 1:31:A:SER:HB3  | 3                   | 0.1      | 0.0                 | 0.1        |
| (1,379)  | 1:71:A:LEU:H    | 1:71:A:LEU:HG   | 2                   | 0.2      | 0.03                | 0.2        |
| (1,722)  | 1:53:A:ARG:HB2  | 1:55:A:GLU:H    | 2                   | 0.2      | 0.02                | 0.2        |
| (1,722)  | 1:53:A:ARG:HB3  | 1:55:A:GLU:H    | 2                   | 0.2      | 0.02                | 0.2        |
| (1,1299) | 1:32:A:LEU:HG   | 1:36:A:LEU:HD11 | 2                   | 0.14     | 0.03                | 0.14       |
| (1,1299) | 1:32:A:LEU:HG   | 1:36:A:LEU:HD12 | 2                   | 0.14     | 0.03                | 0.14       |
| (1,1299) | 1:32:A:LEU:HG   | 1:36:A:LEU:HD13 | 2                   | 0.14     | 0.03                | 0.14       |
| (1,400)  | 1:77:A:GLU:H    | 1:77:A:GLU:HG2  | 2                   | 0.14     | 0.04                | 0.14       |
| (1,1636) | 1:78:A:ALA:HA   | 1:81:A:LYS:HD2  | 2                   | 0.14     | 0.01                | 0.14       |
| (1,1636) | 1:78:A:ALA:HA   | 1:81:A:LYS:HD3  | 2                   | 0.14     | 0.01                | 0.14       |
| (1,259)  | 1:12:A:GLU:H    | 1:12:A:GLU:HG3  | 2                   | 0.13     | 0.01                | 0.13       |
| (1,533)  | 1:28:A:ASP:HA   | 1:30:A:ASP:H    | 2                   | 0.12     | 0.01                | 0.12       |
| (1,844)  | 1:7:A:ARG:HA    | 1:7:A:ARG:HD3   | 2                   | 0.12     | 0.02                | 0.12       |
| (1,735)  | 1:64:A:GLN:HE21 | 1:100:A:LYS:HB2 | 2                   | 0.12     | 0.02                | 0.12       |
| (1,1282) | 1:32:A:LEU:HA   | 1:35:A:VAL:HG11 | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1282) | 1:32:A:LEU:HA   | 1:35:A:VAL:HG12 | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1282) | 1:32:A:LEU:HA   | 1:35:A:VAL:HG13 | 2                   | 0.11     | 0.0                 | 0.11       |

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

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

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

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



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

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

| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (2,7)    | 1:25:A:ASP:OD1 | 1:21:A:ARG:HE  | 10       | 0.4           |
| (2,7)    | 1:25:A:ASP:OD1 | 1:21:A:ARG:HE  | 13       | 0.32          |
| (1,1426) | 1:71:A:LEU:HA  | 1:74:A:ARG:HD2 | 7        | 0.29          |
| (2,7)    | 1:25:A:ASP:OD1 | 1:21:A:ARG:HE  | 3        | 0.28          |
| (1,1059) | 1:28:A:ASP:HA  | 1:31:A:SER:HB2 | 17       | 0.27          |
| (2,7)    | 1:25:A:ASP:OD1 | 1:21:A:ARG:HE  | 7        | 0.26          |
| (1,893)  | 1:41:A:GLU:H   | 1:41:A:GLU:HG2 | 20       | 0.26          |
| (2,1)    | 1:6:A:LEU:O    | 1:46:A:HIS:HD1 | 1        | 0.25          |
| (1,1059) | 1:28:A:ASP:HA  | 1:31:A:SER:HB2 | 2        | 0.25          |
| (1,1059) | 1:28:A:ASP:HA  | 1:31:A:SER:HB2 | 12       | 0.25          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (2,9)    | 1:80:A:ASP:OD1  | 1:76:A:ARG:HE    | 7        | 0.24          |
| (2,9)    | 1:80:A:ASP:OD1  | 1:76:A:ARG:HE    | 10       | 0.24          |
| (1,1525) | 1:97:A:ALA:HA   | 1:100:A:LYS:HD2  | 19       | 0.24          |
| (1,1525) | 1:97:A:ALA:HA   | 1:100:A:LYS:HD3  | 19       | 0.24          |
| (2,9)    | 1:80:A:ASP:OD1  | 1:76:A:ARG:HE    | 15       | 0.23          |
| (2,1)    | 1:6:A:LEU:O     | 1:46:A:HIS:HD1   | 7        | 0.23          |
| (1,1426) | 1:71:A:LEU:HA   | 1:74:A:ARG:HD2   | 6        | 0.23          |
| (1,379)  | 1:71:A:LEU:H    | 1:71:A:LEU:HG    | 13       | 0.23          |
| (1,319)  | 1:37:A:GLU:H    | 1:37:A:GLU:HG3   | 4        | 0.23          |
| (1,319)  | 1:37:A:GLU:H    | 1:37:A:GLU:HG3   | 9        | 0.23          |
| (1,319)  | 1:37:A:GLU:H    | 1:37:A:GLU:HG3   | 10       | 0.23          |
| (1,893)  | 1:41:A:GLU:H    | 1:41:A:GLU:HG2   | 4        | 0.22          |
| (1,375)  | 1:70:A:GLN:H    | 1:70:A:GLN:HG2   | 8        | 0.22          |
| (1,268)  | 1:15:A:GLN:H    | 1:15:A:GLN:HG2   | 3        | 0.22          |
| (2,9)    | 1:80:A:ASP:OD1  | 1:76:A:ARG:HE    | 14       | 0.21          |
| (1,1525) | 1:97:A:ALA:HA   | 1:100:A:LYS:HD2  | 10       | 0.21          |
| (1,1525) | 1:97:A:ALA:HA   | 1:100:A:LYS:HD3  | 10       | 0.21          |
| (1,1525) | 1:97:A:ALA:HA   | 1:100:A:LYS:HD2  | 18       | 0.21          |
| (1,1525) | 1:97:A:ALA:HA   | 1:100:A:LYS:HD3  | 18       | 0.21          |
| (1,1390) | 1:60:A:GLU:HB3  | 1:104:A:LEU:HD21 | 4        | 0.21          |
| (1,1390) | 1:60:A:GLU:HB3  | 1:104:A:LEU:HD22 | 4        | 0.21          |
| (1,1390) | 1:60:A:GLU:HB3  | 1:104:A:LEU:HD23 | 4        | 0.21          |
| (1,1271) | 1:20:A:LEU:HG   | 1:24:A:PHE:HB3   | 3        | 0.21          |
| (1,722)  | 1:53:A:ARG:HB2  | 1:55:A:GLU:H     | 13       | 0.21          |
| (1,722)  | 1:53:A:ARG:HB3  | 1:55:A:GLU:H     | 13       | 0.21          |
| (1,375)  | 1:70:A:GLN:H    | 1:70:A:GLN:HG2   | 6        | 0.21          |
| (1,375)  | 1:70:A:GLN:H    | 1:70:A:GLN:HG2   | 16       | 0.21          |
| (1,1438) | 1:69:A:VAL:HG11 | 1:73:A:GLN:HG3   | 11       | 0.2           |
| (1,1438) | 1:69:A:VAL:HG12 | 1:73:A:GLN:HG3   | 11       | 0.2           |
| (1,1438) | 1:69:A:VAL:HG13 | 1:73:A:GLN:HG3   | 11       | 0.2           |
| (1,1059) | 1:28:A:ASP:HA   | 1:31:A:SER:HB2   | 7        | 0.2           |
| (1,721)  | 1:50:A:PHE:HA   | 1:53:A:ARG:H     | 14       | 0.2           |
| (1,450)  | 1:106:A:GLU:H   | 1:106:A:GLU:HG2  | 19       | 0.2           |
| (1,318)  | 1:37:A:GLU:H    | 1:37:A:GLU:HG2   | 7        | 0.2           |
| (1,290)  | 1:22:A:GLU:H    | 1:22:A:GLU:HG2   | 17       | 0.2           |
| (1,43)   | 1:20:A:LEU:HG   | 1:21:A:ARG:H     | 3        | 0.2           |
| (2,1)    | 1:6:A:LEU:O     | 1:46:A:HIS:HD1   | 18       | 0.19          |
| (1,893)  | 1:41:A:GLU:H    | 1:41:A:GLU:HG2   | 19       | 0.19          |
| (1,437)  | 1:99:A:GLN:H    | 1:99:A:GLN:HG2   | 14       | 0.19          |
| (1,437)  | 1:99:A:GLN:H    | 1:99:A:GLN:HG3   | 14       | 0.19          |
| (1,318)  | 1:37:A:GLU:H    | 1:37:A:GLU:HG2   | 5        | 0.19          |
| (1,290)  | 1:22:A:GLU:H    | 1:22:A:GLU:HG2   | 2        | 0.19          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,290)  | 1:22:A:GLU:H   | 1:22:A:GLU:HG2  | 3        | 0.19          |
| (2,9)    | 1:80:A:ASP:OD1 | 1:76:A:ARG:HE   | 1        | 0.18          |
| (2,9)    | 1:80:A:ASP:OD1 | 1:76:A:ARG:HE   | 17       | 0.18          |
| (1,1031) | 1:8:A:GLN:HA   | 1:11:A:ASP:HB3  | 15       | 0.18          |
| (1,851)  | 1:12:A:GLU:H   | 1:12:A:GLU:HG2  | 12       | 0.18          |
| (1,722)  | 1:53:A:ARG:HB2 | 1:55:A:GLU:H    | 17       | 0.18          |
| (1,722)  | 1:53:A:ARG:HB3 | 1:55:A:GLU:H    | 17       | 0.18          |
| (1,437)  | 1:99:A:GLN:H   | 1:99:A:GLN:HG2  | 7        | 0.18          |
| (1,437)  | 1:99:A:GLN:H   | 1:99:A:GLN:HG3  | 7        | 0.18          |
| (1,379)  | 1:71:A:LEU:H   | 1:71:A:LEU:HG   | 20       | 0.18          |
| (1,319)  | 1:37:A:GLU:H   | 1:37:A:GLU:HG3  | 5        | 0.18          |
| (1,269)  | 1:15:A:GLN:H   | 1:15:A:GLN:HG3  | 10       | 0.18          |
| (2,9)    | 1:80:A:ASP:OD1 | 1:76:A:ARG:HE   | 3        | 0.17          |
| (2,9)    | 1:80:A:ASP:OD1 | 1:76:A:ARG:HE   | 20       | 0.17          |
| (2,1)    | 1:6:A:LEU:O    | 1:46:A:HIS:HD1  | 6        | 0.17          |
| (2,1)    | 1:6:A:LEU:O    | 1:46:A:HIS:HD1  | 9        | 0.17          |
| (2,1)    | 1:6:A:LEU:O    | 1:46:A:HIS:HD1  | 13       | 0.17          |
| (1,1299) | 1:32:A:LEU:HG  | 1:36:A:LEU:HD11 | 12       | 0.17          |
| (1,1299) | 1:32:A:LEU:HG  | 1:36:A:LEU:HD12 | 12       | 0.17          |
| (1,1299) | 1:32:A:LEU:HG  | 1:36:A:LEU:HD13 | 12       | 0.17          |
| (1,1291) | 1:33:A:GLU:HA  | 1:36:A:LEU:HD11 | 11       | 0.17          |
| (1,1291) | 1:33:A:GLU:HA  | 1:36:A:LEU:HD12 | 11       | 0.17          |
| (1,1291) | 1:33:A:GLU:HA  | 1:36:A:LEU:HD13 | 11       | 0.17          |
| (1,1031) | 1:8:A:GLN:HA   | 1:11:A:ASP:HB3  | 1        | 0.17          |
| (1,893)  | 1:41:A:GLU:H   | 1:41:A:GLU:HG2  | 10       | 0.17          |
| (1,893)  | 1:41:A:GLU:H   | 1:41:A:GLU:HG2  | 15       | 0.17          |
| (1,871)  | 1:22:A:GLU:H   | 1:22:A:GLU:HG3  | 15       | 0.17          |
| (1,851)  | 1:12:A:GLU:H   | 1:12:A:GLU:HG2  | 18       | 0.17          |
| (1,437)  | 1:99:A:GLN:H   | 1:99:A:GLN:HG2  | 10       | 0.17          |
| (1,437)  | 1:99:A:GLN:H   | 1:99:A:GLN:HG3  | 10       | 0.17          |
| (1,437)  | 1:99:A:GLN:H   | 1:99:A:GLN:HG2  | 15       | 0.17          |
| (1,437)  | 1:99:A:GLN:H   | 1:99:A:GLN:HG3  | 15       | 0.17          |
| (1,437)  | 1:99:A:GLN:H   | 1:99:A:GLN:HG2  | 16       | 0.17          |
| (1,437)  | 1:99:A:GLN:H   | 1:99:A:GLN:HG3  | 16       | 0.17          |
| (1,400)  | 1:77:A:GLU:H   | 1:77:A:GLU:HG2  | 6        | 0.17          |
| (1,376)  | 1:70:A:GLN:H   | 1:70:A:GLN:HG3  | 18       | 0.17          |
| (1,328)  | 1:41:A:GLU:H   | 1:41:A:GLU:HG3  | 2        | 0.17          |
| (1,328)  | 1:41:A:GLU:H   | 1:41:A:GLU:HG3  | 9        | 0.17          |
| (1,290)  | 1:22:A:GLU:H   | 1:22:A:GLU:HG2  | 5        | 0.17          |
| (1,290)  | 1:22:A:GLU:H   | 1:22:A:GLU:HG2  | 8        | 0.17          |
| (1,268)  | 1:15:A:GLN:H   | 1:15:A:GLN:HG2  | 12       | 0.17          |
| (2,7)    | 1:25:A:ASP:OD1 | 1:21:A:ARG:HE   | 8        | 0.16          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,7)    | 1:25:A:ASP:OD1  | 1:21:A:ARG:HE   | 9        | 0.16          |
| (2,7)    | 1:25:A:ASP:OD1  | 1:21:A:ARG:HE   | 14       | 0.16          |
| (2,1)    | 1:6:A:LEU:O     | 1:46:A:HIS:HD1  | 10       | 0.16          |
| (1,1336) | 1:42:A:LEU:HA   | 1:45:A:LYS:HD2  | 18       | 0.16          |
| (1,1336) | 1:42:A:LEU:HA   | 1:45:A:LYS:HD3  | 18       | 0.16          |
| (1,1031) | 1:8:A:GLN:HA    | 1:11:A:ASP:HB3  | 3        | 0.16          |
| (1,827)  | 1:64:A:GLN:HG2  | 1:101:A:ILE:H   | 1        | 0.16          |
| (1,827)  | 1:64:A:GLN:HG3  | 1:101:A:ILE:H   | 1        | 0.16          |
| (1,328)  | 1:41:A:GLU:H    | 1:41:A:GLU:HG3  | 18       | 0.16          |
| (1,269)  | 1:15:A:GLN:H    | 1:15:A:GLN:HG3  | 12       | 0.16          |
| (1,268)  | 1:15:A:GLN:H    | 1:15:A:GLN:HG2  | 20       | 0.16          |
| (2,9)    | 1:80:A:ASP:OD1  | 1:76:A:ARG:HE   | 9        | 0.15          |
| (2,9)    | 1:80:A:ASP:OD1  | 1:76:A:ARG:HE   | 12       | 0.15          |
| (2,9)    | 1:80:A:ASP:OD1  | 1:76:A:ARG:HE   | 18       | 0.15          |
| (2,7)    | 1:25:A:ASP:OD1  | 1:21:A:ARG:HE   | 5        | 0.15          |
| (1,1295) | 1:16:A:ALA:HA   | 1:35:A:VAL:HG21 | 20       | 0.15          |
| (1,1295) | 1:16:A:ALA:HA   | 1:35:A:VAL:HG22 | 20       | 0.15          |
| (1,1295) | 1:16:A:ALA:HA   | 1:35:A:VAL:HG23 | 20       | 0.15          |
| (1,1150) | 1:97:A:ALA:HA   | 1:100:A:LYS:HB3 | 13       | 0.15          |
| (1,1031) | 1:8:A:GLN:HA    | 1:11:A:ASP:HB3  | 11       | 0.15          |
| (1,893)  | 1:41:A:GLU:H    | 1:41:A:GLU:HG2  | 18       | 0.15          |
| (1,667)  | 1:60:A:GLU:HG2  | 1:64:A:GLN:H    | 16       | 0.15          |
| (1,667)  | 1:60:A:GLU:HG3  | 1:64:A:GLN:H    | 16       | 0.15          |
| (1,376)  | 1:70:A:GLN:H    | 1:70:A:GLN:HG3  | 11       | 0.15          |
| (1,325)  | 1:40:A:GLU:H    | 1:40:A:GLU:HG2  | 16       | 0.15          |
| (1,325)  | 1:40:A:GLU:H    | 1:40:A:GLU:HG3  | 16       | 0.15          |
| (1,319)  | 1:37:A:GLU:H    | 1:37:A:GLU:HG3  | 7        | 0.15          |
| (1,318)  | 1:37:A:GLU:H    | 1:37:A:GLU:HG2  | 4        | 0.15          |
| (2,8)    | 1:25:A:ASP:OD1  | 1:21:A:ARG:NE   | 8        | 0.14          |
| (2,7)    | 1:25:A:ASP:OD1  | 1:21:A:ARG:HE   | 11       | 0.14          |
| (2,7)    | 1:25:A:ASP:OD1  | 1:21:A:ARG:HE   | 15       | 0.14          |
| (1,1706) | 1:9:A:THR:HG21  | 1:45:A:LYS:HE2  | 3        | 0.14          |
| (1,1706) | 1:9:A:THR:HG21  | 1:45:A:LYS:HE3  | 3        | 0.14          |
| (1,1706) | 1:9:A:THR:HG22  | 1:45:A:LYS:HE2  | 3        | 0.14          |
| (1,1706) | 1:9:A:THR:HG22  | 1:45:A:LYS:HE3  | 3        | 0.14          |
| (1,1706) | 1:9:A:THR:HG23  | 1:45:A:LYS:HE2  | 3        | 0.14          |
| (1,1706) | 1:9:A:THR:HG23  | 1:45:A:LYS:HE3  | 3        | 0.14          |
| (1,1636) | 1:78:A:ALA:HA   | 1:81:A:LYS:HD2  | 1        | 0.14          |
| (1,1636) | 1:78:A:ALA:HA   | 1:81:A:LYS:HD3  | 1        | 0.14          |
| (1,1525) | 1:97:A:ALA:HA   | 1:100:A:LYS:HD2 | 8        | 0.14          |
| (1,1525) | 1:97:A:ALA:HA   | 1:100:A:LYS:HD3 | 8        | 0.14          |
| (1,1438) | 1:69:A:VAL:HG11 | 1:73:A:GLN:HG3  | 14       | 0.14          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1438) | 1:69:A:VAL:HG12  | 1:73:A:GLN:HG3   | 14       | 0.14          |
| (1,1438) | 1:69:A:VAL:HG13  | 1:73:A:GLN:HG3   | 14       | 0.14          |
| (1,1425) | 1:71:A:LEU:HD11  | 1:93:A:GLU:HB2   | 10       | 0.14          |
| (1,1425) | 1:71:A:LEU:HD12  | 1:93:A:GLU:HB2   | 10       | 0.14          |
| (1,1425) | 1:71:A:LEU:HD13  | 1:93:A:GLU:HB2   | 10       | 0.14          |
| (1,1295) | 1:16:A:ALA:HA    | 1:35:A:VAL:HG21  | 6        | 0.14          |
| (1,1295) | 1:16:A:ALA:HA    | 1:35:A:VAL:HG22  | 6        | 0.14          |
| (1,1295) | 1:16:A:ALA:HA    | 1:35:A:VAL:HG23  | 6        | 0.14          |
| (1,1295) | 1:16:A:ALA:HA    | 1:35:A:VAL:HG21  | 12       | 0.14          |
| (1,1295) | 1:16:A:ALA:HA    | 1:35:A:VAL:HG22  | 12       | 0.14          |
| (1,1295) | 1:16:A:ALA:HA    | 1:35:A:VAL:HG23  | 12       | 0.14          |
| (1,1051) | 1:18:A:GLN:HA    | 1:21:A:ARG:HB3   | 13       | 0.14          |
| (1,1033) | 1:9:A:THR:HA     | 1:12:A:GLU:HB2   | 1        | 0.14          |
| (1,1033) | 1:9:A:THR:HA     | 1:12:A:GLU:HB3   | 1        | 0.14          |
| (1,1031) | 1:8:A:GLN:HA     | 1:11:A:ASP:HB3   | 20       | 0.14          |
| (1,851)  | 1:12:A:GLU:H     | 1:12:A:GLU:HG2   | 19       | 0.14          |
| (1,844)  | 1:7:A:ARG:HA     | 1:7:A:ARG:HD3    | 12       | 0.14          |
| (1,386)  | 1:73:A:GLN:H     | 1:73:A:GLN:HG2   | 7        | 0.14          |
| (1,376)  | 1:70:A:GLN:H     | 1:70:A:GLN:HG3   | 5        | 0.14          |
| (1,328)  | 1:41:A:GLU:H     | 1:41:A:GLU:HG3   | 13       | 0.14          |
| (1,268)  | 1:15:A:GLN:H     | 1:15:A:GLN:HG2   | 6        | 0.14          |
| (1,259)  | 1:12:A:GLU:H     | 1:12:A:GLU:HG3   | 18       | 0.14          |
| (1,211)  | 1:91:A:LEU:HG    | 1:92:A:GLU:H     | 13       | 0.14          |
| (2,9)    | 1:80:A:ASP:OD1   | 1:76:A:ARG:HE    | 5        | 0.13          |
| (2,7)    | 1:25:A:ASP:OD1   | 1:21:A:ARG:HE    | 2        | 0.13          |
| (2,7)    | 1:25:A:ASP:OD1   | 1:21:A:ARG:HE    | 6        | 0.13          |
| (1,2097) | 2:201:A:7BU:H3B1 | 2:201:A:7BU:F23C | 12       | 0.13          |
| (1,1684) | 1:98:A:LEU:HD21  | 1:102:A:ARG:H    | 18       | 0.13          |
| (1,1684) | 1:98:A:LEU:HD22  | 1:102:A:ARG:H    | 18       | 0.13          |
| (1,1684) | 1:98:A:LEU:HD23  | 1:102:A:ARG:H    | 18       | 0.13          |
| (1,1636) | 1:78:A:ALA:HA    | 1:81:A:LYS:HD2   | 18       | 0.13          |
| (1,1636) | 1:78:A:ALA:HA    | 1:81:A:LYS:HD3   | 18       | 0.13          |
| (1,1251) | 1:19:A:ARG:HD2   | 1:35:A:VAL:HG21  | 8        | 0.13          |
| (1,1251) | 1:19:A:ARG:HD2   | 1:35:A:VAL:HG22  | 8        | 0.13          |
| (1,1251) | 1:19:A:ARG:HD2   | 1:35:A:VAL:HG23  | 8        | 0.13          |
| (1,1251) | 1:19:A:ARG:HD3   | 1:35:A:VAL:HG21  | 8        | 0.13          |
| (1,1251) | 1:19:A:ARG:HD3   | 1:35:A:VAL:HG22  | 8        | 0.13          |
| (1,1251) | 1:19:A:ARG:HD3   | 1:35:A:VAL:HG23  | 8        | 0.13          |
| (1,1127) | 1:77:A:GLU:HA    | 1:80:A:ASP:HB3   | 7        | 0.13          |
| (1,1127) | 1:77:A:GLU:HA    | 1:80:A:ASP:HB3   | 16       | 0.13          |
| (1,1070) | 1:35:A:VAL:HA    | 1:38:A:GLU:HB3   | 5        | 0.13          |
| (1,1060) | 1:28:A:ASP:HA    | 1:31:A:SER:HB3   | 8        | 0.13          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,735)  | 1:64:A:GLN:HE21  | 1:100:A:LYS:HB2  | 20       | 0.13          |
| (1,533)  | 1:28:A:ASP:HA    | 1:30:A:ASP:H     | 14       | 0.13          |
| (1,452)  | 1:107:A:LYS:H    | 1:107:A:LYS:HG2  | 13       | 0.13          |
| (1,376)  | 1:70:A:GLN:H     | 1:70:A:GLN:HG3   | 20       | 0.13          |
| (1,375)  | 1:70:A:GLN:H     | 1:70:A:GLN:HG2   | 3        | 0.13          |
| (1,375)  | 1:70:A:GLN:H     | 1:70:A:GLN:HG2   | 10       | 0.13          |
| (1,375)  | 1:70:A:GLN:H     | 1:70:A:GLN:HG2   | 20       | 0.13          |
| (1,328)  | 1:41:A:GLU:H     | 1:41:A:GLU:HG3   | 20       | 0.13          |
| (1,318)  | 1:37:A:GLU:H     | 1:37:A:GLU:HG2   | 9        | 0.13          |
| (1,268)  | 1:15:A:GLN:H     | 1:15:A:GLN:HG2   | 4        | 0.13          |
| (2,10)   | 1:80:A:ASP:OD1   | 1:76:A:ARG:NE    | 18       | 0.12          |
| (2,9)    | 1:80:A:ASP:OD1   | 1:76:A:ARG:HE    | 8        | 0.12          |
| (1,2097) | 2:201:A:7BU:H3B1 | 2:201:A:7BU:F23C | 11       | 0.12          |
| (1,1674) | 1:71:A:LEU:HD21  | 1:94:A:LEU:HA    | 11       | 0.12          |
| (1,1674) | 1:71:A:LEU:HD22  | 1:94:A:LEU:HA    | 11       | 0.12          |
| (1,1674) | 1:71:A:LEU:HD23  | 1:94:A:LEU:HA    | 11       | 0.12          |
| (1,1674) | 1:71:A:LEU:HD21  | 1:94:A:LEU:HA    | 15       | 0.12          |
| (1,1674) | 1:71:A:LEU:HD22  | 1:94:A:LEU:HA    | 15       | 0.12          |
| (1,1674) | 1:71:A:LEU:HD23  | 1:94:A:LEU:HA    | 15       | 0.12          |
| (1,1674) | 1:71:A:LEU:HD21  | 1:94:A:LEU:HA    | 19       | 0.12          |
| (1,1674) | 1:71:A:LEU:HD22  | 1:94:A:LEU:HA    | 19       | 0.12          |
| (1,1674) | 1:71:A:LEU:HD23  | 1:94:A:LEU:HA    | 19       | 0.12          |
| (1,1500) | 1:24:A:PHE:HZ    | 1:88:A:GLU:HG3   | 10       | 0.12          |
| (1,1438) | 1:69:A:VAL:HG11  | 1:73:A:GLN:HG3   | 7        | 0.12          |
| (1,1438) | 1:69:A:VAL:HG12  | 1:73:A:GLN:HG3   | 7        | 0.12          |
| (1,1438) | 1:69:A:VAL:HG13  | 1:73:A:GLN:HG3   | 7        | 0.12          |
| (1,1426) | 1:71:A:LEU:HA    | 1:74:A:ARG:HD2   | 11       | 0.12          |
| (1,1372) | 1:43:A:ILE:HG21  | 1:47:A:ARG:HD3   | 9        | 0.12          |
| (1,1372) | 1:43:A:ILE:HG22  | 1:47:A:ARG:HD3   | 9        | 0.12          |
| (1,1372) | 1:43:A:ILE:HG23  | 1:47:A:ARG:HD3   | 9        | 0.12          |
| (1,1127) | 1:77:A:GLU:HA    | 1:80:A:ASP:HB3   | 20       | 0.12          |
| (1,1073) | 1:37:A:GLU:HA    | 1:40:A:GLU:HB3   | 18       | 0.12          |
| (1,1070) | 1:35:A:VAL:HA    | 1:38:A:GLU:HB3   | 2        | 0.12          |
| (1,1058) | 1:22:A:GLU:HA    | 1:25:A:ASP:HB3   | 16       | 0.12          |
| (1,893)  | 1:41:A:GLU:H     | 1:41:A:GLU:HG2   | 9        | 0.12          |
| (1,675)  | 1:14:A:VAL:HG11  | 1:15:A:GLN:HE22  | 6        | 0.12          |
| (1,675)  | 1:14:A:VAL:HG12  | 1:15:A:GLN:HE22  | 6        | 0.12          |
| (1,675)  | 1:14:A:VAL:HG13  | 1:15:A:GLN:HE22  | 6        | 0.12          |
| (1,533)  | 1:28:A:ASP:HA    | 1:30:A:ASP:H     | 7        | 0.12          |
| (1,386)  | 1:73:A:GLN:H     | 1:73:A:GLN:HG2   | 20       | 0.12          |
| (1,328)  | 1:41:A:GLU:H     | 1:41:A:GLU:HG3   | 15       | 0.12          |
| (1,318)  | 1:37:A:GLU:H     | 1:37:A:GLU:HG2   | 10       | 0.12          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,259)  | 1:12:A:GLU:H     | 1:12:A:GLU:HG3   | 17       | 0.12          |
| (2,7)    | 1:25:A:ASP:OD1   | 1:21:A:ARG:HE    | 17       | 0.11          |
| (2,1)    | 1:6:A:LEU:O      | 1:46:A:HIS:HD1   | 2        | 0.11          |
| (1,2097) | 2:201:A:7BU:H3B1 | 2:201:A:7BU:F23C | 6        | 0.11          |
| (1,2097) | 2:201:A:7BU:H3B1 | 2:201:A:7BU:F23C | 10       | 0.11          |
| (1,2097) | 2:201:A:7BU:H3B1 | 2:201:A:7BU:F23C | 13       | 0.11          |
| (1,2097) | 2:201:A:7BU:H3B1 | 2:201:A:7BU:F23C | 14       | 0.11          |
| (1,1864) | 1:28:A:ASP:HA    | 1:31:A:SER:HB2   | 12       | 0.11          |
| (1,1864) | 1:28:A:ASP:HA    | 1:31:A:SER:HB3   | 12       | 0.11          |
| (1,1674) | 1:71:A:LEU:HD21  | 1:94:A:LEU:HA    | 4        | 0.11          |
| (1,1674) | 1:71:A:LEU:HD22  | 1:94:A:LEU:HA    | 4        | 0.11          |
| (1,1674) | 1:71:A:LEU:HD23  | 1:94:A:LEU:HA    | 4        | 0.11          |
| (1,1674) | 1:71:A:LEU:HD21  | 1:94:A:LEU:HA    | 6        | 0.11          |
| (1,1674) | 1:71:A:LEU:HD22  | 1:94:A:LEU:HA    | 6        | 0.11          |
| (1,1674) | 1:71:A:LEU:HD23  | 1:94:A:LEU:HA    | 6        | 0.11          |
| (1,1674) | 1:71:A:LEU:HD21  | 1:94:A:LEU:HA    | 16       | 0.11          |
| (1,1674) | 1:71:A:LEU:HD22  | 1:94:A:LEU:HA    | 16       | 0.11          |
| (1,1674) | 1:71:A:LEU:HD23  | 1:94:A:LEU:HA    | 16       | 0.11          |
| (1,1299) | 1:32:A:LEU:HG    | 1:36:A:LEU:HD11  | 7        | 0.11          |
| (1,1299) | 1:32:A:LEU:HG    | 1:36:A:LEU:HD12  | 7        | 0.11          |
| (1,1299) | 1:32:A:LEU:HG    | 1:36:A:LEU:HD13  | 7        | 0.11          |
| (1,1295) | 1:16:A:ALA:HA    | 1:35:A:VAL:HG21  | 15       | 0.11          |
| (1,1295) | 1:16:A:ALA:HA    | 1:35:A:VAL:HG22  | 15       | 0.11          |
| (1,1295) | 1:16:A:ALA:HA    | 1:35:A:VAL:HG23  | 15       | 0.11          |
| (1,1282) | 1:32:A:LEU:HA    | 1:35:A:VAL:HG11  | 10       | 0.11          |
| (1,1282) | 1:32:A:LEU:HA    | 1:35:A:VAL:HG12  | 10       | 0.11          |
| (1,1282) | 1:32:A:LEU:HA    | 1:35:A:VAL:HG13  | 10       | 0.11          |
| (1,1150) | 1:97:A:ALA:HA    | 1:100:A:LYS:HB3  | 4        | 0.11          |
| (1,1150) | 1:97:A:ALA:HA    | 1:100:A:LYS:HB3  | 5        | 0.11          |
| (1,1070) | 1:35:A:VAL:HA    | 1:38:A:GLU:HB3   | 3        | 0.11          |
| (1,1070) | 1:35:A:VAL:HA    | 1:38:A:GLU:HB3   | 15       | 0.11          |
| (1,1060) | 1:28:A:ASP:HA    | 1:31:A:SER:HB3   | 12       | 0.11          |
| (1,1060) | 1:28:A:ASP:HA    | 1:31:A:SER:HB3   | 20       | 0.11          |
| (1,1031) | 1:8:A:GLN:HA     | 1:11:A:ASP:HB3   | 12       | 0.11          |
| (1,1031) | 1:8:A:GLN:HA     | 1:11:A:ASP:HB3   | 17       | 0.11          |
| (1,871)  | 1:22:A:GLU:H     | 1:22:A:GLU:HG3   | 5        | 0.11          |
| (1,871)  | 1:22:A:GLU:H     | 1:22:A:GLU:HG3   | 8        | 0.11          |
| (1,844)  | 1:7:A:ARG:HA     | 1:7:A:ARG:HD3    | 6        | 0.11          |
| (1,450)  | 1:106:A:GLU:H    | 1:106:A:GLU:HG2  | 2        | 0.11          |
| (1,450)  | 1:106:A:GLU:H    | 1:106:A:GLU:HG2  | 18       | 0.11          |
| (1,401)  | 1:77:A:GLU:H     | 1:77:A:GLU:HG3   | 4        | 0.11          |
| (1,386)  | 1:73:A:GLN:H     | 1:73:A:GLN:HG2   | 14       | 0.11          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,376)  | 1:70:A:GLN:H     | 1:70:A:GLN:HG3   | 3        | 0.11          |
| (1,376)  | 1:70:A:GLN:H     | 1:70:A:GLN:HG3   | 10       | 0.11          |
| (1,376)  | 1:70:A:GLN:H     | 1:70:A:GLN:HG3   | 16       | 0.11          |
| (1,375)  | 1:70:A:GLN:H     | 1:70:A:GLN:HG2   | 5        | 0.11          |
| (1,375)  | 1:70:A:GLN:H     | 1:70:A:GLN:HG2   | 11       | 0.11          |
| (1,269)  | 1:15:A:GLN:H     | 1:15:A:GLN:HG3   | 1        | 0.11          |
| (2,9)    | 1:80:A:ASP:OD1   | 1:76:A:ARG:HE    | 4        | 0.1           |
| (2,9)    | 1:80:A:ASP:OD1   | 1:76:A:ARG:HE    | 6        | 0.1           |
| (2,7)    | 1:25:A:ASP:OD1   | 1:21:A:ARG:HE    | 4        | 0.1           |
| (2,7)    | 1:25:A:ASP:OD1   | 1:21:A:ARG:HE    | 20       | 0.1           |
| (1,2097) | 2:201:A:7BU:H3B1 | 2:201:A:7BU:F23C | 9        | 0.1           |
| (1,1864) | 1:28:A:ASP:HA    | 1:31:A:SER:HB2   | 2        | 0.1           |
| (1,1864) | 1:28:A:ASP:HA    | 1:31:A:SER:HB3   | 2        | 0.1           |
| (1,1864) | 1:28:A:ASP:HA    | 1:31:A:SER:HB2   | 17       | 0.1           |
| (1,1864) | 1:28:A:ASP:HA    | 1:31:A:SER:HB3   | 17       | 0.1           |
| (1,1674) | 1:71:A:LEU:HD21  | 1:94:A:LEU:HA    | 12       | 0.1           |
| (1,1674) | 1:71:A:LEU:HD22  | 1:94:A:LEU:HA    | 12       | 0.1           |
| (1,1674) | 1:71:A:LEU:HD23  | 1:94:A:LEU:HA    | 12       | 0.1           |
| (1,1674) | 1:71:A:LEU:HD21  | 1:94:A:LEU:HA    | 13       | 0.1           |
| (1,1674) | 1:71:A:LEU:HD22  | 1:94:A:LEU:HA    | 13       | 0.1           |
| (1,1674) | 1:71:A:LEU:HD23  | 1:94:A:LEU:HA    | 13       | 0.1           |
| (1,1447) | 1:72:A:PHE:HE1   | 1:76:A:ARG:HD3   | 14       | 0.1           |
| (1,1447) | 1:72:A:PHE:HE2   | 1:76:A:ARG:HD3   | 14       | 0.1           |
| (1,1438) | 1:69:A:VAL:HG11  | 1:73:A:GLN:HG3   | 20       | 0.1           |
| (1,1438) | 1:69:A:VAL:HG12  | 1:73:A:GLN:HG3   | 20       | 0.1           |
| (1,1438) | 1:69:A:VAL:HG13  | 1:73:A:GLN:HG3   | 20       | 0.1           |
| (1,1427) | 1:71:A:LEU:HA    | 1:74:A:ARG:HD3   | 14       | 0.1           |
| (1,1282) | 1:32:A:LEU:HA    | 1:35:A:VAL:HG11  | 1        | 0.1           |
| (1,1282) | 1:32:A:LEU:HA    | 1:35:A:VAL:HG12  | 1        | 0.1           |
| (1,1282) | 1:32:A:LEU:HA    | 1:35:A:VAL:HG13  | 1        | 0.1           |
| (1,1045) | 1:16:A:ALA:HA    | 1:19:A:ARG:HB3   | 19       | 0.1           |
| (1,735)  | 1:64:A:GLN:HE21  | 1:100:A:LYS:HB2  | 6        | 0.1           |
| (1,400)  | 1:77:A:GLU:H     | 1:77:A:GLU:HG2   | 8        | 0.1           |
| (1,328)  | 1:41:A:GLU:H     | 1:41:A:GLU:HG3   | 10       | 0.1           |

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

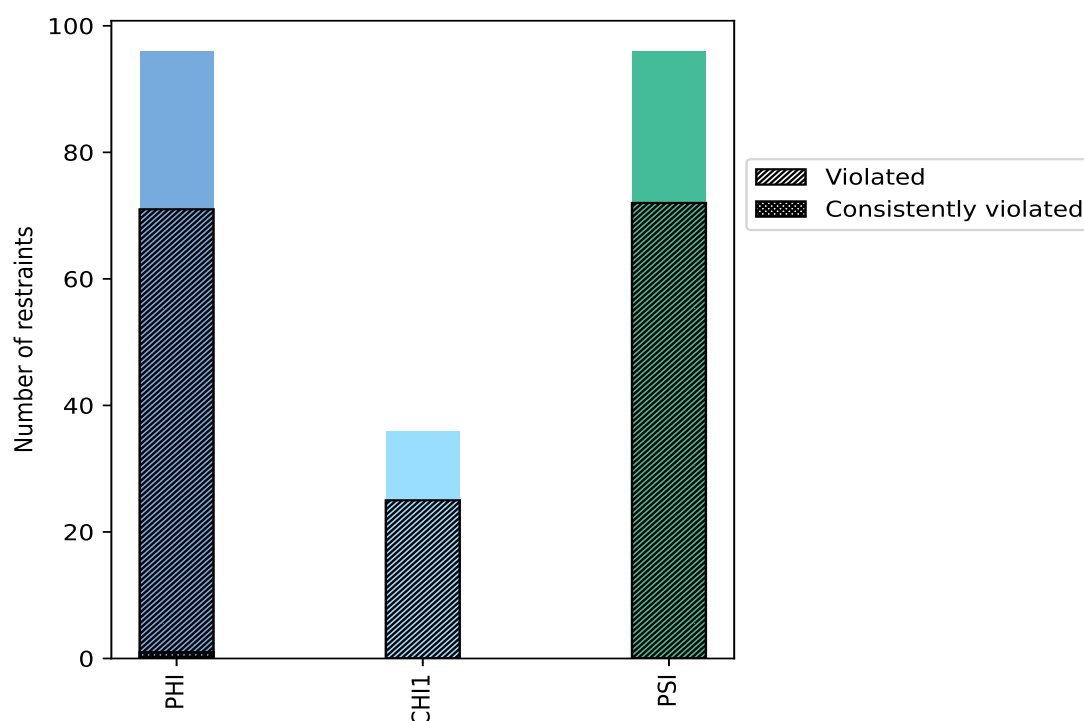
### 10.1 Summary of dihedral-angle violations [i](#)

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> |
| PHI        | 96    | 42.1           | 71                    | 74.0           | 31.1           | 1                                  | 1.0            | 0.4            |
| CHI1       | 36    | 15.8           | 25                    | 69.4           | 11.0           | 0                                  | 0.0            | 0.0            |
| PSI        | 96    | 42.1           | 72                    | 75.0           | 31.6           | 0                                  | 0.0            | 0.0            |
| Total      | 228   | 100.0          | 168                   | 73.7           | 73.7           | 1                                  | 0.4            | 0.4            |

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

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



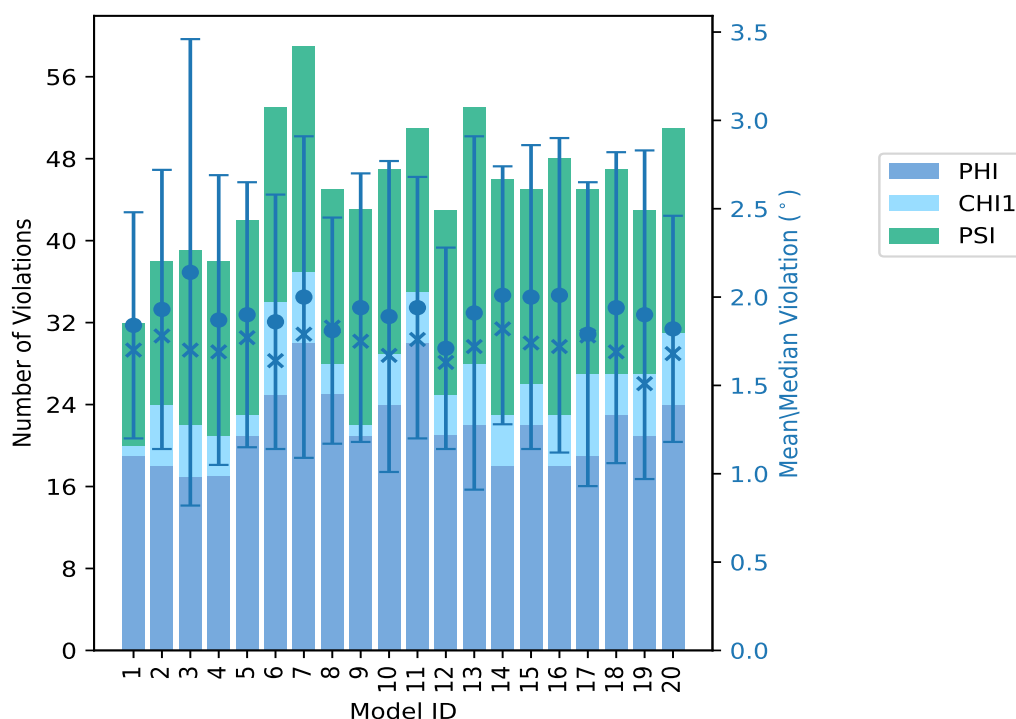
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

## 10.2 Dihedral-angle violation statistics for each model

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

| Model ID | Number of violations |      |     |       | Mean (°) | Max (°) | SD (°) | Median (°) |
|----------|----------------------|------|-----|-------|----------|---------|--------|------------|
|          | PHI                  | CHI1 | PSI | Total |          |         |        |            |
| 1        | 19                   | 1    | 12  | 32    | 1.84     | 3.2     | 0.64   | 1.7        |
| 2        | 18                   | 6    | 14  | 38    | 1.93     | 4.11    | 0.79   | 1.78       |
| 3        | 17                   | 5    | 17  | 39    | 2.14     | 6.39    | 1.32   | 1.7        |
| 4        | 17                   | 4    | 17  | 38    | 1.87     | 4.36    | 0.82   | 1.69       |
| 5        | 21                   | 2    | 19  | 42    | 1.9      | 5.04    | 0.75   | 1.77       |
| 6        | 25                   | 9    | 19  | 53    | 1.86     | 3.88    | 0.72   | 1.64       |
| 7        | 30                   | 7    | 22  | 59    | 2.0      | 5.16    | 0.91   | 1.79       |
| 8        | 25                   | 3    | 17  | 45    | 1.81     | 3.17    | 0.64   | 1.83       |
| 9        | 21                   | 1    | 21  | 43    | 1.94     | 4.39    | 0.76   | 1.75       |
| 10       | 24                   | 5    | 18  | 47    | 1.89     | 5.0     | 0.88   | 1.67       |
| 11       | 30                   | 5    | 16  | 51    | 1.94     | 4.08    | 0.74   | 1.76       |
| 12       | 21                   | 4    | 18  | 43    | 1.71     | 3.32    | 0.57   | 1.63       |
| 13       | 22                   | 6    | 25  | 53    | 1.91     | 7.27    | 1.0    | 1.72       |
| 14       | 18                   | 5    | 23  | 46    | 2.01     | 4.5     | 0.73   | 1.82       |
| 15       | 22                   | 4    | 19  | 45    | 2.0      | 4.82    | 0.86   | 1.74       |
| 16       | 18                   | 5    | 25  | 48    | 2.01     | 4.21    | 0.89   | 1.72       |
| 17       | 19                   | 8    | 18  | 45    | 1.79     | 6.23    | 0.86   | 1.78       |
| 18       | 23                   | 4    | 20  | 47    | 1.94     | 5.06    | 0.88   | 1.69       |
| 19       | 21                   | 6    | 16  | 43    | 1.9      | 4.67    | 0.93   | 1.51       |
| 20       | 24                   | 7    | 20  | 51    | 1.82     | 3.42    | 0.64   | 1.68       |

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



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

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

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

| Number of violated restraints |      |     |       | Fraction of the ensemble |      |
|-------------------------------|------|-----|-------|--------------------------|------|
| PHI                           | CHI1 | PSI | Total | Count <sup>1</sup>       | %    |
| 19                            | 7    | 14  | 40    | 1                        | 5.0  |
| 6                             | 4    | 12  | 22    | 2                        | 10.0 |
| 7                             | 3    | 8   | 18    | 3                        | 15.0 |
| 4                             | 3    | 5   | 12    | 4                        | 20.0 |
| 4                             | 3    | 8   | 15    | 5                        | 25.0 |
| 5                             | 1    | 3   | 9     | 6                        | 30.0 |
| 1                             | 1    | 3   | 5     | 7                        | 35.0 |
| 3                             | 1    | 3   | 7     | 8                        | 40.0 |
| 1                             | 0    | 4   | 5     | 9                        | 45.0 |
| 4                             | 0    | 4   | 8     | 10                       | 50.0 |
| 4                             | 0    | 1   | 5     | 11                       | 55.0 |

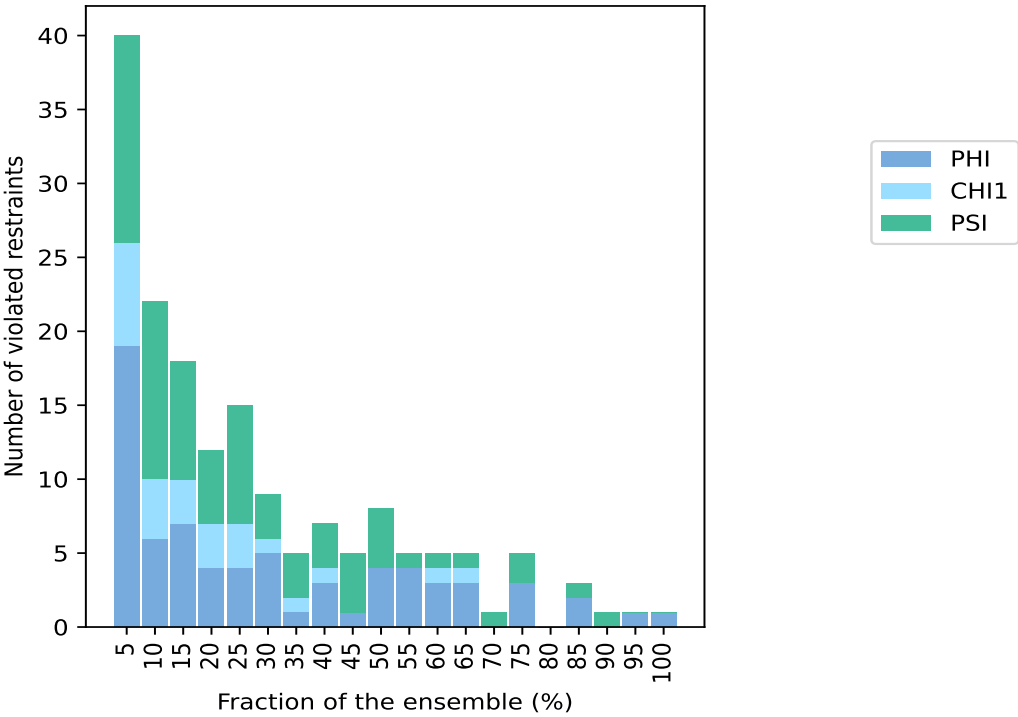
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| Number of violated restraints |      |     |       | Fraction of the ensemble |       |
|-------------------------------|------|-----|-------|--------------------------|-------|
| PHI                           | CHI1 | PSI | Total | Count <sup>1</sup>       | %     |
| 3                             | 1    | 1   | 5     | 12                       | 60.0  |
| 3                             | 1    | 1   | 5     | 13                       | 65.0  |
| 0                             | 0    | 1   | 1     | 14                       | 70.0  |
| 3                             | 0    | 2   | 5     | 15                       | 75.0  |
| 0                             | 0    | 0   | 0     | 16                       | 80.0  |
| 2                             | 0    | 1   | 3     | 17                       | 85.0  |
| 0                             | 0    | 1   | 1     | 18                       | 90.0  |
| 1                             | 0    | 0   | 1     | 19                       | 95.0  |
| 1                             | 0    | 0   | 1     | 20                       | 100.0 |

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

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



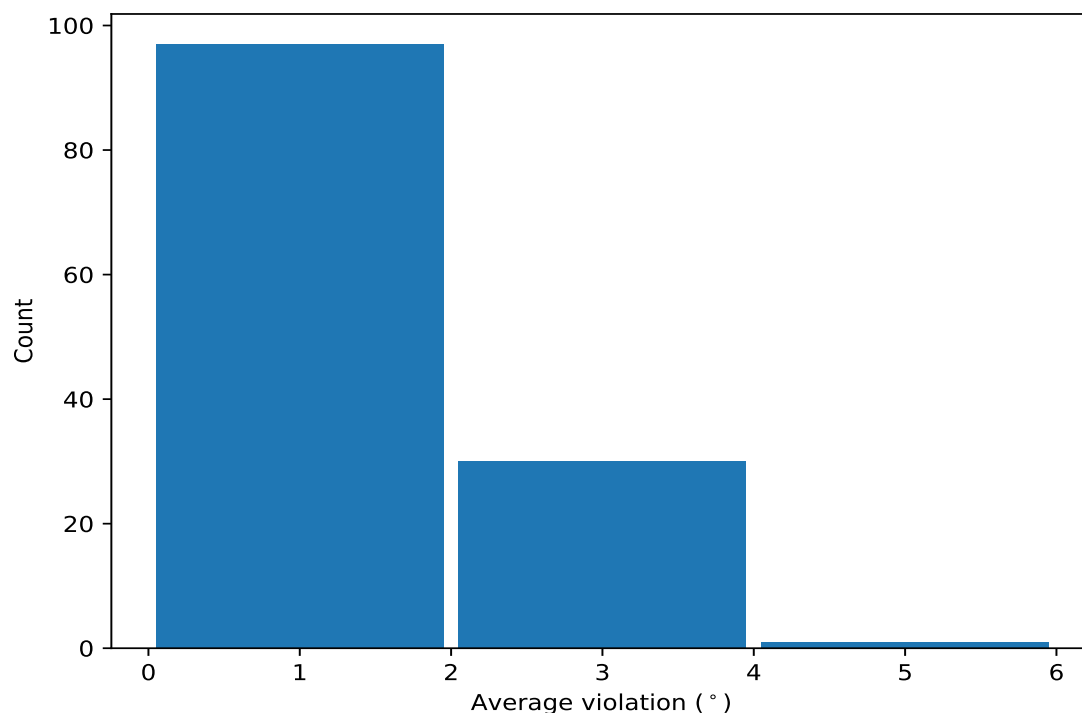
10.4 Most violated dihedral-angle restraints in the ensemble ⓘ

10.4.1 Histogram : Distribution of mean dihedral-angle violations ⓘ

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



in the ensemble



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

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

| Key     | Atom-1       | Atom-2        | Atom-3        | Atom-4        | Models <sup>1</sup> | Mean | SD <sup>2</sup> | Median |
|---------|--------------|---------------|---------------|---------------|---------------------|------|-----------------|--------|
| (1,57)  | 1:31:A:SER:C | 1:32:A:LEU:N  | 1:32:A:LEU:CA | 1:32:A:LEU:C  | 20                  | 2.99 | 0.91            | 3.08   |
| (1,19)  | 1:12:A:GLU:C | 1:13:A:LEU:N  | 1:13:A:LEU:CA | 1:13:A:LEU:C  | 19                  | 2.03 | 0.43            | 1.97   |
| (1,152) | 1:86:A:SER:N | 1:86:A:SER:CA | 1:86:A:SER:C  | 1:87:A:LEU:N  | 18                  | 2.08 | 0.65            | 1.98   |
| (1,38)  | 1:22:A:GLU:N | 1:22:A:GLU:CA | 1:22:A:GLU:C  | 1:23:A:ILE:N  | 17                  | 2.61 | 0.83            | 2.73   |
| (1,65)  | 1:35:A:VAL:C | 1:36:A:LEU:N  | 1:36:A:LEU:CA | 1:36:A:LEU:C  | 17                  | 2.15 | 0.64            | 2.17   |
| (1,153) | 1:86:A:SER:C | 1:87:A:LEU:N  | 1:87:A:LEU:CA | 1:87:A:LEU:C  | 17                  | 2.09 | 0.63            | 1.92   |
| (1,147) | 1:83:A:ASP:C | 1:84:A:LYS:N  | 1:84:A:LYS:CA | 1:84:A:LYS:C  | 15                  | 3.12 | 1.46            | 3.05   |
| (1,40)  | 1:23:A:ILE:N | 1:23:A:ILE:CA | 1:23:A:ILE:C  | 1:24:A:PHE:N  | 15                  | 2.59 | 0.94            | 2.32   |
| (1,116) | 1:68:A:TRP:N | 1:68:A:TRP:CA | 1:68:A:TRP:C  | 1:69:A:VAL:N  | 15                  | 2.03 | 0.53            | 2.38   |
| (1,89)  | 1:47:A:ARG:C | 1:48:A:GLN:N  | 1:48:A:GLN:CA | 1:48:A:GLN:C  | 15                  | 1.95 | 0.6             | 1.82   |
| (1,51)  | 1:28:A:ASP:C | 1:29:A:ASP:N  | 1:29:A:ASP:CA | 1:29:A:ASP:C  | 15                  | 1.89 | 0.8             | 1.75   |
| (1,12)  | 1:8:A:GLN:N  | 1:8:A:GLN:CA  | 1:8:A:GLN:C   | 1:9:A:THR:N   | 14                  | 2.72 | 1.0             | 2.74   |
| (1,137) | 1:78:A:ALA:C | 1:79:A:ILE:N  | 1:79:A:ILE:CA | 1:79:A:ILE:C  | 13                  | 2.31 | 0.94            | 2.1    |
| (1,11)  | 1:7:A:ARG:C  | 1:8:A:GLN:N   | 1:8:A:GLN:CA  | 1:8:A:GLN:C   | 13                  | 2.29 | 0.6             | 2.1    |
| (1,216) | 1:68:A:TRP:N | 1:68:A:TRP:CA | 1:68:A:TRP:CB | 1:68:A:TRP:CG | 13                  | 1.86 | 0.62            | 1.6    |
| (1,72)  | 1:39:A:ILE:N | 1:39:A:ILE:CA | 1:39:A:ILE:C  | 1:40:A:GLU:N  | 13                  | 1.74 | 0.46            | 1.69   |
| (1,23)  | 1:14:A:VAL:C | 1:15:A:GLN:N  | 1:15:A:GLN:CA | 1:15:A:GLN:C  | 13                  | 1.54 | 0.42            | 1.56   |
| (1,7)   | 1:5:A:LYS:C  | 1:6:A:LEU:N   | 1:6:A:LEU:CA  | 1:6:A:LEU:C   | 12                  | 3.1  | 0.95            | 3.04   |
| (1,41)  | 1:23:A:ILE:C | 1:24:A:PHE:N  | 1:24:A:PHE:CA | 1:24:A:PHE:C  | 12                  | 2.77 | 1.27            | 2.41   |
| (1,202) | 1:28:A:ASP:N | 1:28:A:ASP:CA | 1:28:A:ASP:CB | 1:28:A:ASP:CG | 12                  | 1.96 | 0.9             | 1.78   |

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| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4          | Models <sup>1</sup> | Mean | SD <sup>2</sup> | Median |
|---------|---------------|----------------|----------------|-----------------|---------------------|------|-----------------|--------|
| (1,73)  | 1:39:A:ILE:C  | 1:40:A:GLU:N   | 1:40:A:GLU:CA  | 1:40:A:GLU:C    | 12                  | 1.7  | 0.38            | 1.81   |
| (1,78)  | 1:42:A:LEU:N  | 1:42:A:LEU:CA  | 1:42:A:LEU:C   | 1:43:A:ILE:N    | 12                  | 1.64 | 0.57            | 1.5    |
| (1,39)  | 1:22:A:GLU:C  | 1:23:A:ILE:N   | 1:23:A:ILE:CA  | 1:23:A:ILE:C    | 11                  | 3.24 | 1.94            | 2.67   |
| (1,43)  | 1:24:A:PHE:C  | 1:25:A:ASP:N   | 1:25:A:ASP:CA  | 1:25:A:ASP:C    | 11                  | 2.11 | 0.76            | 1.84   |
| (1,143) | 1:81:A:LYS:C  | 1:82:A:GLY:N   | 1:82:A:GLY:CA  | 1:82:A:GLY:C    | 11                  | 2.09 | 0.71            | 2.05   |
| (1,64)  | 1:35:A:VAL:N  | 1:35:A:VAL:CA  | 1:35:A:VAL:C   | 1:36:A:LEU:N    | 11                  | 1.9  | 0.61            | 1.93   |
| (1,85)  | 1:45:A:LYS:C  | 1:46:A:HIS:N   | 1:46:A:HIS:CA  | 1:46:A:HIS:C    | 11                  | 1.5  | 0.6             | 1.21   |
| (1,109) | 1:64:A:GLN:C  | 1:65:A:GLY:N   | 1:65:A:GLY:CA  | 1:65:A:GLY:C    | 10                  | 2.75 | 0.59            | 2.85   |
| (1,82)  | 1:44:A:GLN:N  | 1:44:A:GLN:CA  | 1:44:A:GLN:C   | 1:45:A:LYS:N    | 10                  | 2.1  | 0.79            | 1.71   |
| (1,54)  | 1:30:A:ASP:N  | 1:30:A:ASP:CA  | 1:30:A:ASP:C   | 1:31:A:SER:N    | 10                  | 2.0  | 0.44            | 1.94   |
| (1,37)  | 1:21:A:ARG:C  | 1:22:A:GLU:N   | 1:22:A:GLU:CA  | 1:22:A:GLU:C    | 10                  | 1.89 | 0.33            | 1.81   |
| (1,179) | 1:99:A:GLN:C  | 1:100:A:LYS:N  | 1:100:A:LYS:CA | 1:100:A:LYS:C   | 10                  | 1.89 | 0.64            | 1.73   |
| (1,154) | 1:87:A:LEU:N  | 1:87:A:LEU:CA  | 1:87:A:LEU:C   | 1:88:A:GLU:N    | 10                  | 1.86 | 0.59            | 1.82   |
| (1,177) | 1:98:A:LEU:C  | 1:99:A:GLN:N   | 1:99:A:GLN:CA  | 1:99:A:GLN:C    | 10                  | 1.7  | 0.61            | 1.52   |
| (1,158) | 1:89:A:GLN:N  | 1:89:A:GLN:CA  | 1:89:A:GLN:C   | 1:90:A:LEU:N    | 10                  | 1.55 | 0.5             | 1.4    |
| (1,146) | 1:83:A:ASP:N  | 1:83:A:ASP:CA  | 1:83:A:ASP:C   | 1:84:A:LYS:N    | 9                   | 2.83 | 1.52            | 2.6    |
| (1,55)  | 1:30:A:ASP:C  | 1:31:A:SER:N   | 1:31:A:SER:CA  | 1:31:A:SER:C    | 9                   | 1.79 | 0.53            | 1.81   |
| (1,28)  | 1:17:A:PHE:N  | 1:17:A:PHE:CA  | 1:17:A:PHE:C   | 1:18:A:GLN:N    | 9                   | 1.59 | 0.33            | 1.62   |
| (1,32)  | 1:19:A:ARG:N  | 1:19:A:ARG:CA  | 1:19:A:ARG:C   | 1:20:A:LEU:N    | 9                   | 1.58 | 0.39            | 1.56   |
| (1,48)  | 1:27:A:GLY:N  | 1:27:A:GLY:CA  | 1:27:A:GLY:C   | 1:28:A:ASP:N    | 9                   | 1.52 | 0.34            | 1.57   |
| (1,56)  | 1:31:A:SER:N  | 1:31:A:SER:CA  | 1:31:A:SER:C   | 1:32:A:LEU:N    | 8                   | 1.89 | 0.56            | 1.86   |
| (1,84)  | 1:45:A:LYS:N  | 1:45:A:LYS:CA  | 1:45:A:LYS:C   | 1:46:A:HIS:N    | 8                   | 1.76 | 0.32            | 1.68   |
| (1,183) | 1:101:A:ILE:C | 1:102:A:ARG:N  | 1:102:A:ARG:CA | 1:102:A:ARG:C   | 8                   | 1.71 | 0.55            | 1.81   |
| (1,105) | 1:62:A:ALA:C  | 1:63:A:LYS:N   | 1:63:A:LYS:CA  | 1:63:A:LYS:C    | 8                   | 1.69 | 0.49            | 1.63   |
| (1,186) | 1:103:A:GLU:N | 1:103:A:GLU:CA | 1:103:A:GLU:C  | 1:104:A:LEU:N   | 8                   | 1.61 | 0.4             | 1.58   |
| (1,47)  | 1:26:A:LYS:C  | 1:27:A:GLY:N   | 1:27:A:GLY:CA  | 1:27:A:GLY:C    | 8                   | 1.53 | 0.35            | 1.63   |
| (1,220) | 1:79:A:ILE:N  | 1:79:A:ILE:CA  | 1:79:A:ILE:CB  | 1:79:A:ILE:CG1  | 8                   | 1.22 | 0.12            | 1.2    |
| (1,136) | 1:78:A:ALA:N  | 1:78:A:ALA:CA  | 1:78:A:ALA:C   | 1:79:A:ILE:N    | 7                   | 2.16 | 0.5             | 2.17   |
| (1,210) | 1:49:A:LEU:N  | 1:49:A:LEU:CA  | 1:49:A:LEU:CB  | 1:49:A:LEU:CG   | 7                   | 1.67 | 0.34            | 1.66   |
| (1,110) | 1:65:A:GLY:N  | 1:65:A:GLY:CA  | 1:65:A:GLY:C   | 1:66:A:ASP:N    | 7                   | 1.62 | 0.36            | 1.52   |
| (1,170) | 1:95:A:GLU:N  | 1:95:A:GLU:CA  | 1:95:A:GLU:C   | 1:96:A:GLN:N    | 7                   | 1.6  | 0.3             | 1.6    |
| (1,175) | 1:97:A:ALA:C  | 1:98:A:LEU:N   | 1:98:A:LEU:CA  | 1:98:A:LEU:C    | 7                   | 1.35 | 0.17            | 1.32   |
| (1,6)   | 1:5:A:LYS:N   | 1:5:A:LYS:CA   | 1:5:A:LYS:C    | 1:6:A:LEU:N     | 6                   | 2.56 | 0.66            | 2.52   |
| (1,35)  | 1:20:A:LEU:C  | 1:21:A:ARG:N   | 1:21:A:ARG:CA  | 1:21:A:ARG:C    | 6                   | 1.66 | 0.49            | 1.59   |
| (1,157) | 1:88:A:GLU:C  | 1:89:A:GLN:N   | 1:89:A:GLN:CA  | 1:89:A:GLN:C    | 6                   | 1.65 | 0.26            | 1.74   |
| (1,108) | 1:64:A:GLN:N  | 1:64:A:GLN:CA  | 1:64:A:GLN:C   | 1:65:A:GLY:N    | 6                   | 1.54 | 0.39            | 1.52   |
| (1,101) | 1:60:A:GLU:C  | 1:61:A:ALA:N   | 1:61:A:ALA:CA  | 1:61:A:ALA:C    | 6                   | 1.52 | 0.53            | 1.3    |
| (1,155) | 1:87:A:LEU:C  | 1:88:A:GLU:N   | 1:88:A:GLU:CA  | 1:88:A:GLU:C    | 6                   | 1.47 | 0.23            | 1.35   |
| (1,33)  | 1:19:A:ARG:C  | 1:20:A:LEU:N   | 1:20:A:LEU:CA  | 1:20:A:LEU:C    | 6                   | 1.42 | 0.33            | 1.25   |
| (1,26)  | 1:16:A:ALA:N  | 1:16:A:ALA:CA  | 1:16:A:ALA:C   | 1:17:A:PHE:N    | 6                   | 1.28 | 0.25            | 1.27   |
| (1,227) | 1:101:A:ILE:N | 1:101:A:ILE:CA | 1:101:A:ILE:CB | 1:101:A:ILE:CG1 | 6                   | 1.19 | 0.11            | 1.17   |
| (1,36)  | 1:21:A:ARG:N  | 1:21:A:ARG:CA  | 1:21:A:ARG:C   | 1:22:A:GLU:N    | 5                   | 2.07 | 0.63            | 1.79   |
| (1,156) | 1:88:A:GLU:N  | 1:88:A:GLU:CA  | 1:88:A:GLU:C   | 1:89:A:GLN:N    | 5                   | 2.0  | 0.89            | 1.74   |
| (1,224) | 1:85:A:ASP:N  | 1:85:A:ASP:CA  | 1:85:A:ASP:CB  | 1:85:A:ASP:CG   | 5                   | 1.93 | 0.39            | 2.05   |
| (1,135) | 1:77:A:GLU:C  | 1:78:A:ALA:N   | 1:78:A:ALA:CA  | 1:78:A:ALA:C    | 5                   | 1.65 | 0.48            | 1.7    |
| (1,42)  | 1:24:A:PHE:N  | 1:24:A:PHE:CA  | 1:24:A:PHE:C   | 1:25:A:ASP:N    | 5                   | 1.62 | 0.33            | 1.67   |
| (1,150) | 1:85:A:ASP:N  | 1:85:A:ASP:CA  | 1:85:A:ASP:C   | 1:86:A:SER:N    | 5                   | 1.61 | 0.43            | 1.57   |
| (1,58)  | 1:32:A:LEU:N  | 1:32:A:LEU:CA  | 1:32:A:LEU:C   | 1:33:A:GLU:N    | 5                   | 1.46 | 0.22            | 1.59   |
| (1,171) | 1:95:A:GLU:C  | 1:96:A:GLN:N   | 1:96:A:GLN:CA  | 1:96:A:GLN:C    | 5                   | 1.46 | 0.35            | 1.29   |
| (1,100) | 1:60:A:GLU:N  | 1:60:A:GLU:CA  | 1:60:A:GLU:C   | 1:61:A:ALA:N    | 5                   | 1.44 | 0.23            | 1.45   |
| (1,17)  | 1:11:A:ASP:C  | 1:12:A:GLU:N   | 1:12:A:GLU:CA  | 1:12:A:GLU:C    | 5                   | 1.42 | 0.26            | 1.37   |

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| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4         | Models <sup>1</sup> | Mean | SD <sup>2</sup> | Median |
|---------|---------------|----------------|----------------|----------------|---------------------|------|-----------------|--------|
| (1,79)  | 1:42:A:LEU:C  | 1:43:A:ILE:N   | 1:43:A:ILE:CA  | 1:43:A:ILE:C   | 5                   | 1.4  | 0.34            | 1.3    |
| (1,76)  | 1:41:A:GLU:N  | 1:41:A:GLU:CA  | 1:41:A:GLU:C   | 1:42:A:LEU:N   | 5                   | 1.39 | 0.27            | 1.26   |
| (1,223) | 1:83:A:ASP:N  | 1:83:A:ASP:CA  | 1:83:A:ASP:CB  | 1:83:A:ASP:CG  | 5                   | 1.36 | 0.35            | 1.24   |
| (1,228) | 1:104:A:LEU:N | 1:104:A:LEU:CA | 1:104:A:LEU:CB | 1:104:A:LEU:CG | 5                   | 1.36 | 0.38            | 1.33   |
| (1,106) | 1:63:A:LYS:N  | 1:63:A:LYS:CA  | 1:63:A:LYS:C   | 1:64:A:GLN:N   | 5                   | 1.35 | 0.2             | 1.28   |
| (1,50)  | 1:28:A:ASP:N  | 1:28:A:ASP:CA  | 1:28:A:ASP:C   | 1:29:A:ASP:N   | 4                   | 4.14 | 0.41            | 4.12   |
| (1,94)  | 1:50:A:PHE:N  | 1:50:A:PHE:CA  | 1:50:A:PHE:C   | 1:51:A:ASP:N   | 4                   | 2.51 | 1.09            | 2.54   |
| (1,139) | 1:79:A:ILE:C  | 1:80:A:ASP:N   | 1:80:A:ASP:CA  | 1:80:A:ASP:C   | 4                   | 1.92 | 0.82            | 1.64   |
| (1,80)  | 1:43:A:ILE:N  | 1:43:A:ILE:CA  | 1:43:A:ILE:C   | 1:44:A:GLN:N   | 4                   | 1.64 | 0.32            | 1.73   |
| (1,200) | 1:25:A:ASP:N  | 1:25:A:ASP:CA  | 1:25:A:ASP:CB  | 1:25:A:ASP:CG  | 4                   | 1.59 | 0.37            | 1.6    |
| (1,187) | 1:103:A:GLU:C | 1:104:A:LEU:N  | 1:104:A:LEU:CA | 1:104:A:LEU:C  | 4                   | 1.38 | 0.27            | 1.36   |
| (1,91)  | 1:48:A:GLN:C  | 1:49:A:LEU:N   | 1:49:A:LEU:CA  | 1:49:A:LEU:C   | 4                   | 1.36 | 0.58            | 1.02   |
| (1,181) | 1:100:A:LYS:C | 1:101:A:ILE:N  | 1:101:A:ILE:CA | 1:101:A:ILE:C  | 4                   | 1.36 | 0.34            | 1.21   |
| (1,130) | 1:75:A:PHE:N  | 1:75:A:PHE:CA  | 1:75:A:PHE:C   | 1:76:A:ARG:N   | 4                   | 1.28 | 0.13            | 1.31   |
| (1,198) | 1:23:A:ILE:N  | 1:23:A:ILE:CA  | 1:23:A:ILE:CB  | 1:23:A:ILE:CG1 | 4                   | 1.23 | 0.23            | 1.15   |
| (1,219) | 1:75:A:PHE:N  | 1:75:A:PHE:CA  | 1:75:A:PHE:CB  | 1:75:A:PHE:CG  | 4                   | 1.18 | 0.09            | 1.17   |
| (1,86)  | 1:46:A:HIS:N  | 1:46:A:HIS:CA  | 1:46:A:HIS:C   | 1:47:A:ARG:N   | 4                   | 1.07 | 0.11            | 1.01   |
| (1,188) | 1:104:A:LEU:N | 1:104:A:LEU:CA | 1:104:A:LEU:C  | 1:105:A:ALA:N  | 3                   | 2.5  | 1.31            | 1.74   |
| (1,194) | 1:11:A:ASP:N  | 1:11:A:ASP:CA  | 1:11:A:ASP:CB  | 1:11:A:ASP:CG  | 3                   | 2.43 | 0.43            | 2.62   |
| (1,93)  | 1:49:A:LEU:C  | 1:50:A:PHE:N   | 1:50:A:PHE:CA  | 1:50:A:PHE:C   | 3                   | 2.33 | 0.56            | 2.13   |
| (1,132) | 1:76:A:ARG:N  | 1:76:A:ARG:CA  | 1:76:A:ARG:C   | 1:77:A:GLU:N   | 3                   | 1.94 | 0.34            | 2.01   |
| (1,95)  | 1:50:A:PHE:C  | 1:51:A:ASP:N   | 1:51:A:ASP:CA  | 1:51:A:ASP:C   | 3                   | 1.84 | 0.82            | 1.3    |
| (1,10)  | 1:7:A:ARG:N   | 1:7:A:ARG:CA   | 1:7:A:ARG:C    | 1:8:A:GLN:N    | 3                   | 1.79 | 0.28            | 1.82   |
| (1,133) | 1:76:A:ARG:C  | 1:77:A:GLU:N   | 1:77:A:GLU:CA  | 1:77:A:GLU:C   | 3                   | 1.73 | 0.59            | 1.38   |
| (1,102) | 1:61:A:ALA:N  | 1:61:A:ALA:CA  | 1:61:A:ALA:C   | 1:62:A:ALA:N   | 3                   | 1.65 | 0.26            | 1.72   |
| (1,182) | 1:101:A:ILE:N | 1:101:A:ILE:CA | 1:101:A:ILE:C  | 1:102:A:ARG:N  | 3                   | 1.55 | 0.1             | 1.5    |
| (1,221) | 1:80:A:ASP:N  | 1:80:A:ASP:CA  | 1:80:A:ASP:CB  | 1:80:A:ASP:CG  | 3                   | 1.54 | 0.38            | 1.43   |
| (1,189) | 1:104:A:LEU:C | 1:105:A:ALA:N  | 1:105:A:ALA:CA | 1:105:A:ALA:C  | 3                   | 1.52 | 0.24            | 1.39   |
| (1,59)  | 1:32:A:LEU:C  | 1:33:A:GLU:N   | 1:33:A:GLU:CA  | 1:33:A:GLU:C   | 3                   | 1.48 | 0.24            | 1.4    |
| (1,134) | 1:77:A:GLU:N  | 1:77:A:GLU:CA  | 1:77:A:GLU:C   | 1:78:A:ALA:N   | 3                   | 1.42 | 0.28            | 1.42   |
| (1,215) | 1:66:A:ASP:N  | 1:66:A:ASP:CA  | 1:66:A:ASP:CB  | 1:66:A:ASP:CG  | 3                   | 1.41 | 0.44            | 1.2    |
| (1,114) | 1:67:A:GLN:N  | 1:67:A:GLN:CA  | 1:67:A:GLN:C   | 1:68:A:TRP:N   | 3                   | 1.4  | 0.02            | 1.41   |
| (1,117) | 1:68:A:TRP:C  | 1:69:A:VAL:N   | 1:69:A:VAL:CA  | 1:69:A:VAL:C   | 3                   | 1.32 | 0.04            | 1.32   |
| (1,83)  | 1:44:A:GLN:C  | 1:45:A:LYS:N   | 1:45:A:LYS:CA  | 1:45:A:LYS:C   | 3                   | 1.25 | 0.19            | 1.26   |
| (1,162) | 1:91:A:LEU:N  | 1:91:A:LEU:CA  | 1:91:A:LEU:C   | 1:92:A:GLU:N   | 3                   | 1.12 | 0.1             | 1.11   |
| (1,191) | 1:105:A:ALA:C | 1:106:A:GLU:N  | 1:106:A:GLU:CA | 1:106:A:GLU:C  | 2                   | 2.44 | 0.24            | 2.44   |
| (1,201) | 1:26:A:LYS:N  | 1:26:A:LYS:CA  | 1:26:A:LYS:CB  | 1:26:A:LYS:CG  | 2                   | 1.81 | 0.34            | 1.81   |
| (1,63)  | 1:34:A:GLN:C  | 1:35:A:VAL:N   | 1:35:A:VAL:CA  | 1:35:A:VAL:C   | 2                   | 1.68 | 0.36            | 1.68   |
| (1,119) | 1:69:A:VAL:C  | 1:70:A:GLN:N   | 1:70:A:GLN:CA  | 1:70:A:GLN:C   | 2                   | 1.58 | 0.29            | 1.58   |
| (1,214) | 1:55:A:GLU:N  | 1:55:A:GLU:CA  | 1:55:A:GLU:CB  | 1:55:A:GLU:CG  | 2                   | 1.58 | 0.52            | 1.58   |
| (1,112) | 1:66:A:ASP:N  | 1:66:A:ASP:CA  | 1:66:A:ASP:C   | 1:67:A:GLN:N   | 2                   | 1.57 | 0.11            | 1.57   |
| (1,22)  | 1:14:A:VAL:N  | 1:14:A:VAL:CA  | 1:14:A:VAL:C   | 1:15:A:GLN:N   | 2                   | 1.54 | 0.03            | 1.54   |
| (1,97)  | 1:58:A:ASP:C  | 1:59:A:THR:N   | 1:59:A:THR:CA  | 1:59:A:THR:C   | 2                   | 1.52 | 0.33            | 1.52   |
| (1,90)  | 1:48:A:GLN:N  | 1:48:A:GLN:CA  | 1:48:A:GLN:C   | 1:49:A:LEU:N   | 2                   | 1.46 | 0.11            | 1.46   |
| (1,88)  | 1:47:A:ARG:N  | 1:47:A:ARG:CA  | 1:47:A:ARG:C   | 1:48:A:GLN:N   | 2                   | 1.45 | 0.06            | 1.45   |
| (1,126) | 1:73:A:GLN:N  | 1:73:A:GLN:CA  | 1:73:A:GLN:C   | 1:74:A:ARG:N   | 2                   | 1.42 | 0.4             | 1.42   |
| (1,99)  | 1:59:A:THR:C  | 1:60:A:GLU:N   | 1:60:A:GLU:CA  | 1:60:A:GLU:C   | 2                   | 1.4  | 0.21            | 1.4    |
| (1,8)   | 1:6:A:LEU:N   | 1:6:A:LEU:CA   | 1:6:A:LEU:C    | 1:7:A:ARG:N    | 2                   | 1.36 | 0.18            | 1.36   |
| (1,24)  | 1:15:A:GLN:N  | 1:15:A:GLN:CA  | 1:15:A:GLN:C   | 1:16:A:ALA:N   | 2                   | 1.33 | 0.17            | 1.33   |
| (1,206) | 1:39:A:ILE:N  | 1:39:A:ILE:CA  | 1:39:A:ILE:CB  | 1:39:A:ILE:CG1 | 2                   | 1.31 | 0.04            | 1.31   |
| (1,92)  | 1:49:A:LEU:N  | 1:49:A:LEU:CA  | 1:49:A:LEU:C   | 1:50:A:PHE:N   | 2                   | 1.29 | 0.16            | 1.29   |

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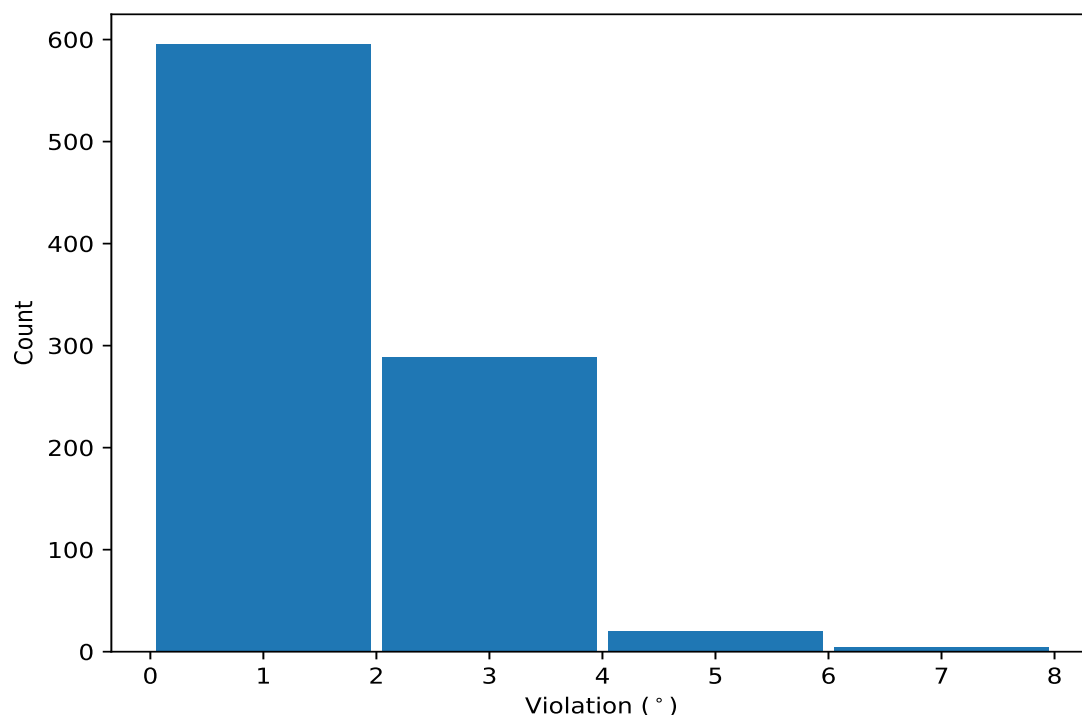
| Key     | Atom-1       | Atom-2        | Atom-3        | Atom-4        | Models <sup>1</sup> | Mean | SD <sup>2</sup> | Median |
|---------|--------------|---------------|---------------|---------------|---------------------|------|-----------------|--------|
| (1,165) | 1:92:A:GLU:C | 1:93:A:GLU:N  | 1:93:A:GLU:CA | 1:93:A:GLU:C  | 2                   | 1.28 | 0.04            | 1.28   |
| (1,124) | 1:72:A:PHE:N | 1:72:A:PHE:CA | 1:72:A:PHE:C  | 1:73:A:GLN:N  | 2                   | 1.27 | 0.09            | 1.27   |
| (1,118) | 1:69:A:VAL:N | 1:69:A:VAL:CA | 1:69:A:VAL:C  | 1:70:A:GLN:N  | 2                   | 1.2  | 0.1             | 1.2    |
| (1,104) | 1:62:A:ALA:N | 1:62:A:ALA:CA | 1:62:A:ALA:C  | 1:63:A:LYS:N  | 2                   | 1.2  | 0.05            | 1.2    |
| (1,62)  | 1:34:A:GLN:N | 1:34:A:GLN:CA | 1:34:A:GLN:C  | 1:35:A:VAL:N  | 2                   | 1.2  | 0.12            | 1.2    |
| (1,218) | 1:72:A:PHE:N | 1:72:A:PHE:CA | 1:72:A:PHE:CB | 1:72:A:PHE:CG | 2                   | 1.16 | 0.01            | 1.16   |

<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 (°) |
|--------|--------------|--------------|---------------|--------------|----------|---------------|
| (1,39) | 1:22:A:GLU:C | 1:23:A:ILE:N | 1:23:A:ILE:CA | 1:23:A:ILE:C | 13       | 7.27          |

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| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,39)  | 1:22:A:GLU:C  | 1:23:A:ILE:N   | 1:23:A:ILE:CA  | 1:23:A:ILE:C  | 3        | 6.39          |
| (1,147) | 1:83:A:ASP:C  | 1:84:A:LYS:N   | 1:84:A:LYS:CA  | 1:84:A:LYS:C  | 3        | 6.37          |
| (1,146) | 1:83:A:ASP:N  | 1:83:A:ASP:CA  | 1:83:A:ASP:C   | 1:84:A:LYS:N  | 17       | 6.23          |
| (1,41)  | 1:23:A:ILE:C  | 1:24:A:PHE:N   | 1:24:A:PHE:CA  | 1:24:A:PHE:C  | 3        | 5.29          |
| (1,57)  | 1:31:A:SER:C  | 1:32:A:LEU:N   | 1:32:A:LEU:CA  | 1:32:A:LEU:C  | 7        | 5.16          |
| (1,137) | 1:78:A:ALA:C  | 1:79:A:ILE:N   | 1:79:A:ILE:CA  | 1:79:A:ILE:C  | 18       | 5.06          |
| (1,147) | 1:83:A:ASP:C  | 1:84:A:LYS:N   | 1:84:A:LYS:CA  | 1:84:A:LYS:C  | 5        | 5.04          |
| (1,7)   | 1:5:A:LYS:C   | 1:6:A:LEU:N    | 1:6:A:LEU:CA   | 1:6:A:LEU:C   | 10       | 5.0           |
| (1,147) | 1:83:A:ASP:C  | 1:84:A:LYS:N   | 1:84:A:LYS:CA  | 1:84:A:LYS:C  | 15       | 4.82          |
| (1,41)  | 1:23:A:ILE:C  | 1:24:A:PHE:N   | 1:24:A:PHE:CA  | 1:24:A:PHE:C  | 19       | 4.67          |
| (1,50)  | 1:28:A:ASP:N  | 1:28:A:ASP:CA  | 1:28:A:ASP:C   | 1:29:A:ASP:N  | 7        | 4.6           |
| (1,147) | 1:83:A:ASP:C  | 1:84:A:LYS:N   | 1:84:A:LYS:CA  | 1:84:A:LYS:C  | 18       | 4.58          |
| (1,50)  | 1:28:A:ASP:N  | 1:28:A:ASP:CA  | 1:28:A:ASP:C   | 1:29:A:ASP:N  | 14       | 4.5           |
| (1,40)  | 1:23:A:ILE:N  | 1:23:A:ILE:CA  | 1:23:A:ILE:C   | 1:24:A:PHE:N  | 9        | 4.39          |
| (1,146) | 1:83:A:ASP:N  | 1:83:A:ASP:CA  | 1:83:A:ASP:C   | 1:84:A:LYS:N  | 4        | 4.36          |
| (1,41)  | 1:23:A:ILE:C  | 1:24:A:PHE:N   | 1:24:A:PHE:CA  | 1:24:A:PHE:C  | 13       | 4.35          |
| (1,188) | 1:104:A:LEU:N | 1:104:A:LEU:CA | 1:104:A:LEU:C  | 1:105:A:ALA:N | 10       | 4.34          |
| (1,202) | 1:28:A:ASP:N  | 1:28:A:ASP:CA  | 1:28:A:ASP:CB  | 1:28:A:ASP:CG | 7        | 4.27          |
| (1,57)  | 1:31:A:SER:C  | 1:32:A:LEU:N   | 1:32:A:LEU:CA  | 1:32:A:LEU:C  | 16       | 4.21          |
| (1,40)  | 1:23:A:ILE:N  | 1:23:A:ILE:CA  | 1:23:A:ILE:C   | 1:24:A:PHE:N  | 16       | 4.18          |
| (1,39)  | 1:22:A:GLU:C  | 1:23:A:ILE:N   | 1:23:A:ILE:CA  | 1:23:A:ILE:C  | 19       | 4.13          |
| (1,7)   | 1:5:A:LYS:C   | 1:6:A:LEU:N    | 1:6:A:LEU:CA   | 1:6:A:LEU:C   | 2        | 4.11          |
| (1,12)  | 1:8:A:GLN:N   | 1:8:A:GLN:CA   | 1:8:A:GLN:C    | 1:9:A:THR:N   | 11       | 4.08          |
| (1,38)  | 1:22:A:GLU:N  | 1:22:A:GLU:CA  | 1:22:A:GLU:C   | 1:23:A:ILE:N  | 10       | 3.99          |
| (1,12)  | 1:8:A:GLN:N   | 1:8:A:GLN:CA   | 1:8:A:GLN:C    | 1:9:A:THR:N   | 2        | 3.97          |
| (1,89)  | 1:47:A:ARG:C  | 1:48:A:GLN:N   | 1:48:A:GLN:CA  | 1:48:A:GLN:C  | 16       | 3.9           |
| (1,40)  | 1:23:A:ILE:N  | 1:23:A:ILE:CA  | 1:23:A:ILE:C   | 1:24:A:PHE:N  | 6        | 3.88          |
| (1,57)  | 1:31:A:SER:C  | 1:32:A:LEU:N   | 1:32:A:LEU:CA  | 1:32:A:LEU:C  | 15       | 3.85          |
| (1,94)  | 1:50:A:PHE:N  | 1:50:A:PHE:CA  | 1:50:A:PHE:C   | 1:51:A:ASP:N  | 14       | 3.84          |
| (1,43)  | 1:24:A:PHE:C  | 1:25:A:ASP:N   | 1:25:A:ASP:CA  | 1:25:A:ASP:C  | 6        | 3.84          |
| (1,12)  | 1:8:A:GLN:N   | 1:8:A:GLN:CA   | 1:8:A:GLN:C    | 1:9:A:THR:N   | 4        | 3.84          |
| (1,51)  | 1:28:A:ASP:C  | 1:29:A:ASP:N   | 1:29:A:ASP:CA  | 1:29:A:ASP:C  | 16       | 3.8           |
| (1,12)  | 1:8:A:GLN:N   | 1:8:A:GLN:CA   | 1:8:A:GLN:C    | 1:9:A:THR:N   | 9        | 3.8           |
| (1,50)  | 1:28:A:ASP:N  | 1:28:A:ASP:CA  | 1:28:A:ASP:C   | 1:29:A:ASP:N  | 13       | 3.73          |
| (1,143) | 1:81:A:LYS:C  | 1:82:A:GLY:N   | 1:82:A:GLY:CA  | 1:82:A:GLY:C  | 11       | 3.72          |
| (1,50)  | 1:28:A:ASP:N  | 1:28:A:ASP:CA  | 1:28:A:ASP:C   | 1:29:A:ASP:N  | 15       | 3.72          |
| (1,39)  | 1:22:A:GLU:C  | 1:23:A:ILE:N   | 1:23:A:ILE:CA  | 1:23:A:ILE:C  | 15       | 3.69          |
| (1,11)  | 1:7:A:ARG:C   | 1:8:A:GLN:N    | 1:8:A:GLN:CA   | 1:8:A:GLN:C   | 19       | 3.67          |
| (1,7)   | 1:5:A:LYS:C   | 1:6:A:LEU:N    | 1:6:A:LEU:CA   | 1:6:A:LEU:C   | 3        | 3.67          |
| (1,152) | 1:86:A:SER:N  | 1:86:A:SER:CA  | 1:86:A:SER:C   | 1:87:A:LEU:N  | 3        | 3.66          |
| (1,51)  | 1:28:A:ASP:C  | 1:29:A:ASP:N   | 1:29:A:ASP:CA  | 1:29:A:ASP:C  | 15       | 3.65          |
| (1,109) | 1:64:A:GLN:C  | 1:65:A:GLY:N   | 1:65:A:GLY:CA  | 1:65:A:GLY:C  | 9        | 3.62          |
| (1,179) | 1:99:A:GLN:C  | 1:100:A:LYS:N  | 1:100:A:LYS:CA | 1:100:A:LYS:C | 19       | 3.61          |
| (1,57)  | 1:31:A:SER:C  | 1:32:A:LEU:N   | 1:32:A:LEU:CA  | 1:32:A:LEU:C  | 3        | 3.61          |
| (1,82)  | 1:44:A:GLN:N  | 1:44:A:GLN:CA  | 1:44:A:GLN:C   | 1:45:A:LYS:N  | 10       | 3.6           |
| (1,38)  | 1:22:A:GLU:N  | 1:22:A:GLU:CA  | 1:22:A:GLU:C   | 1:23:A:ILE:N  | 19       | 3.58          |
| (1,12)  | 1:8:A:GLN:N   | 1:8:A:GLN:CA   | 1:8:A:GLN:C    | 1:9:A:THR:N   | 16       | 3.58          |
| (1,7)   | 1:5:A:LYS:C   | 1:6:A:LEU:N    | 1:6:A:LEU:CA   | 1:6:A:LEU:C   | 7        | 3.58          |
| (1,39)  | 1:22:A:GLU:C  | 1:23:A:ILE:N   | 1:23:A:ILE:CA  | 1:23:A:ILE:C  | 6        | 3.56          |
| (1,57)  | 1:31:A:SER:C  | 1:32:A:LEU:N   | 1:32:A:LEU:CA  | 1:32:A:LEU:C  | 2        | 3.55          |
| (1,156) | 1:88:A:GLU:N  | 1:88:A:GLU:CA  | 1:88:A:GLU:C   | 1:89:A:GLN:N  | 16       | 3.54          |

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| Key     | Atom-1       | Atom-2        | Atom-3        | Atom-4        | Model ID | Violation (°) |
|---------|--------------|---------------|---------------|---------------|----------|---------------|
| (1,57)  | 1:31:A:SER:C | 1:32:A:LEU:N  | 1:32:A:LEU:CA | 1:32:A:LEU:C  | 14       | 3.53          |
| (1,38)  | 1:22:A:GLU:N | 1:22:A:GLU:CA | 1:22:A:GLU:C  | 1:23:A:ILE:N  | 7        | 3.49          |
| (1,153) | 1:86:A:SER:C | 1:87:A:LEU:N  | 1:87:A:LEU:CA | 1:87:A:LEU:C  | 18       | 3.47          |
| (1,40)  | 1:23:A:ILE:N | 1:23:A:ILE:CA | 1:23:A:ILE:C  | 1:24:A:PHE:N  | 7        | 3.47          |
| (1,147) | 1:83:A:ASP:C | 1:84:A:LYS:N  | 1:84:A:LYS:CA | 1:84:A:LYS:C  | 7        | 3.45          |
| (1,216) | 1:68:A:TRP:N | 1:68:A:TRP:CA | 1:68:A:TRP:CB | 1:68:A:TRP:CG | 11       | 3.44          |
| (1,6)   | 1:5:A:LYS:N  | 1:5:A:LYS:CA  | 1:5:A:LYS:C   | 1:6:A:LEU:N   | 20       | 3.42          |
| (1,109) | 1:64:A:GLN:C | 1:65:A:GLY:N  | 1:65:A:GLY:CA | 1:65:A:GLY:C  | 4        | 3.39          |
| (1,38)  | 1:22:A:GLU:N | 1:22:A:GLU:CA | 1:22:A:GLU:C  | 1:23:A:ILE:N  | 6        | 3.38          |
| (1,6)   | 1:5:A:LYS:N  | 1:5:A:LYS:CA  | 1:5:A:LYS:C   | 1:6:A:LEU:N   | 15       | 3.34          |
| (1,109) | 1:64:A:GLN:C | 1:65:A:GLY:N  | 1:65:A:GLY:CA | 1:65:A:GLY:C  | 12       | 3.32          |
| (1,38)  | 1:22:A:GLU:N | 1:22:A:GLU:CA | 1:22:A:GLU:C  | 1:23:A:ILE:N  | 16       | 3.31          |
| (1,57)  | 1:31:A:SER:C | 1:32:A:LEU:N  | 1:32:A:LEU:CA | 1:32:A:LEU:C  | 6        | 3.29          |
| (1,11)  | 1:7:A:ARG:C  | 1:8:A:GLN:N   | 1:8:A:GLN:CA  | 1:8:A:GLN:C   | 14       | 3.25          |
| (1,94)  | 1:50:A:PHE:N | 1:50:A:PHE:CA | 1:50:A:PHE:C  | 1:51:A:ASP:N  | 18       | 3.24          |
| (1,147) | 1:83:A:ASP:C | 1:84:A:LYS:N  | 1:84:A:LYS:CA | 1:84:A:LYS:C  | 9        | 3.21          |
| (1,78)  | 1:42:A:LEU:N | 1:42:A:LEU:CA | 1:42:A:LEU:C  | 1:43:A:ILE:N  | 11       | 3.21          |
| (1,57)  | 1:31:A:SER:C | 1:32:A:LEU:N  | 1:32:A:LEU:CA | 1:32:A:LEU:C  | 1        | 3.2           |
| (1,139) | 1:79:A:ILE:C | 1:80:A:ASP:N  | 1:80:A:ASP:CA | 1:80:A:ASP:C  | 11       | 3.19          |
| (1,19)  | 1:12:A:GLU:C | 1:13:A:LEU:N  | 1:13:A:LEU:CA | 1:13:A:LEU:C  | 16       | 3.19          |
| (1,65)  | 1:35:A:VAL:C | 1:36:A:LEU:N  | 1:36:A:LEU:CA | 1:36:A:LEU:C  | 5        | 3.18          |
| (1,82)  | 1:44:A:GLN:N | 1:44:A:GLN:CA | 1:44:A:GLN:C  | 1:45:A:LYS:N  | 8        | 3.17          |
| (1,57)  | 1:31:A:SER:C | 1:32:A:LEU:N  | 1:32:A:LEU:CA | 1:32:A:LEU:C  | 8        | 3.17          |
| (1,7)   | 1:5:A:LYS:C  | 1:6:A:LEU:N   | 1:6:A:LEU:CA  | 1:6:A:LEU:C   | 5        | 3.17          |
| (1,57)  | 1:31:A:SER:C | 1:32:A:LEU:N  | 1:32:A:LEU:CA | 1:32:A:LEU:C  | 4        | 3.15          |
| (1,7)   | 1:5:A:LYS:C  | 1:6:A:LEU:N   | 1:6:A:LEU:CA  | 1:6:A:LEU:C   | 18       | 3.15          |
| (1,64)  | 1:35:A:VAL:N | 1:35:A:VAL:CA | 1:35:A:VAL:C  | 1:36:A:LEU:N  | 20       | 3.14          |
| (1,153) | 1:86:A:SER:C | 1:87:A:LEU:N  | 1:87:A:LEU:CA | 1:87:A:LEU:C  | 19       | 3.13          |
| (1,43)  | 1:24:A:PHE:C | 1:25:A:ASP:N  | 1:25:A:ASP:CA | 1:25:A:ASP:C  | 11       | 3.13          |
| (1,65)  | 1:35:A:VAL:C | 1:36:A:LEU:N  | 1:36:A:LEU:CA | 1:36:A:LEU:C  | 20       | 3.12          |
| (1,147) | 1:83:A:ASP:C | 1:84:A:LYS:N  | 1:84:A:LYS:CA | 1:84:A:LYS:C  | 20       | 3.1           |
| (1,93)  | 1:49:A:LEU:C | 1:50:A:PHE:N  | 1:50:A:PHE:CA | 1:50:A:PHE:C  | 7        | 3.09          |
| (1,36)  | 1:21:A:ARG:N | 1:21:A:ARG:CA | 1:21:A:ARG:C  | 1:22:A:GLU:N  | 13       | 3.06          |
| (1,147) | 1:83:A:ASP:C | 1:84:A:LYS:N  | 1:84:A:LYS:CA | 1:84:A:LYS:C  | 12       | 3.05          |
| (1,38)  | 1:22:A:GLU:N | 1:22:A:GLU:CA | 1:22:A:GLU:C  | 1:23:A:ILE:N  | 18       | 3.03          |
| (1,146) | 1:83:A:ASP:N | 1:83:A:ASP:CA | 1:83:A:ASP:C  | 1:84:A:LYS:N  | 18       | 3.01          |
| (1,57)  | 1:31:A:SER:C | 1:32:A:LEU:N  | 1:32:A:LEU:CA | 1:32:A:LEU:C  | 19       | 3.0           |
| (1,95)  | 1:50:A:PHE:C | 1:51:A:ASP:N  | 1:51:A:ASP:CA | 1:51:A:ASP:C  | 10       | 2.99          |
| (1,38)  | 1:22:A:GLU:N | 1:22:A:GLU:CA | 1:22:A:GLU:C  | 1:23:A:ILE:N  | 5        | 2.98          |
| (1,152) | 1:86:A:SER:N | 1:86:A:SER:CA | 1:86:A:SER:C  | 1:87:A:LEU:N  | 8        | 2.97          |
| (1,109) | 1:64:A:GLN:C | 1:65:A:GLY:N  | 1:65:A:GLY:CA | 1:65:A:GLY:C  | 15       | 2.97          |
| (1,109) | 1:64:A:GLN:C | 1:65:A:GLY:N  | 1:65:A:GLY:CA | 1:65:A:GLY:C  | 20       | 2.97          |
| (1,65)  | 1:35:A:VAL:C | 1:36:A:LEU:N  | 1:36:A:LEU:CA | 1:36:A:LEU:C  | 15       | 2.97          |
| (1,143) | 1:81:A:LYS:C | 1:82:A:GLY:N  | 1:82:A:GLY:CA | 1:82:A:GLY:C  | 4        | 2.96          |
| (1,57)  | 1:31:A:SER:C | 1:32:A:LEU:N  | 1:32:A:LEU:CA | 1:32:A:LEU:C  | 13       | 2.95          |
| (1,85)  | 1:45:A:LYS:C | 1:46:A:HIS:N  | 1:46:A:HIS:CA | 1:46:A:HIS:C  | 1        | 2.94          |
| (1,57)  | 1:31:A:SER:C | 1:32:A:LEU:N  | 1:32:A:LEU:CA | 1:32:A:LEU:C  | 5        | 2.94          |
| (1,7)   | 1:5:A:LYS:C  | 1:6:A:LEU:N   | 1:6:A:LEU:CA  | 1:6:A:LEU:C   | 1        | 2.94          |
| (1,38)  | 1:22:A:GLU:N | 1:22:A:GLU:CA | 1:22:A:GLU:C  | 1:23:A:ILE:N  | 4        | 2.93          |
| (1,65)  | 1:35:A:VAL:C | 1:36:A:LEU:N  | 1:36:A:LEU:CA | 1:36:A:LEU:C  | 3        | 2.92          |
| (1,137) | 1:78:A:ALA:C | 1:79:A:ILE:N  | 1:79:A:ILE:CA | 1:79:A:ILE:C  | 3        | 2.91          |

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| Key     | Atom-1        | Atom-2        | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|---------------|----------------|---------------|----------|---------------|
| (1,41)  | 1:23:A:ILE:C  | 1:24:A:PHE:N  | 1:24:A:PHE:CA  | 1:24:A:PHE:C  | 2        | 2.91          |
| (1,40)  | 1:23:A:ILE:N  | 1:23:A:ILE:CA | 1:23:A:ILE:C   | 1:24:A:PHE:N  | 1        | 2.91          |
| (1,12)  | 1:8:A:GLN:N   | 1:8:A:GLN:CA  | 1:8:A:GLN:C    | 1:9:A:THR:N   | 7        | 2.9           |
| (1,202) | 1:28:A:ASP:N  | 1:28:A:ASP:CA | 1:28:A:ASP:CB  | 1:28:A:ASP:CG | 2        | 2.88          |
| (1,147) | 1:83:A:ASP:C  | 1:84:A:LYS:N  | 1:84:A:LYS:CA  | 1:84:A:LYS:C  | 8        | 2.88          |
| (1,41)  | 1:23:A:ILE:C  | 1:24:A:PHE:N  | 1:24:A:PHE:CA  | 1:24:A:PHE:C  | 10       | 2.86          |
| (1,154) | 1:87:A:LEU:N  | 1:87:A:LEU:CA | 1:87:A:LEU:C   | 1:88:A:GLU:N  | 16       | 2.85          |
| (1,56)  | 1:31:A:SER:N  | 1:31:A:SER:CA | 1:31:A:SER:C   | 1:32:A:LEU:N  | 7        | 2.85          |
| (1,146) | 1:83:A:ASP:N  | 1:83:A:ASP:CA | 1:83:A:ASP:C   | 1:84:A:LYS:N  | 9        | 2.84          |
| (1,194) | 1:11:A:ASP:N  | 1:11:A:ASP:CA | 1:11:A:ASP:CB  | 1:11:A:ASP:CG | 18       | 2.83          |
| (1,7)   | 1:5:A:LYS:C   | 1:6:A:LEU:N   | 1:6:A:LEU:CA   | 1:6:A:LEU:C   | 13       | 2.83          |
| (1,7)   | 1:5:A:LYS:C   | 1:6:A:LEU:N   | 1:6:A:LEU:CA   | 1:6:A:LEU:C   | 17       | 2.81          |
| (1,137) | 1:78:A:ALA:C  | 1:79:A:ILE:N  | 1:79:A:ILE:CA  | 1:79:A:ILE:C  | 11       | 2.8           |
| (1,152) | 1:86:A:SER:N  | 1:86:A:SER:CA | 1:86:A:SER:C   | 1:87:A:LEU:N  | 6        | 2.79          |
| (1,82)  | 1:44:A:GLN:N  | 1:44:A:GLN:CA | 1:44:A:GLN:C   | 1:45:A:LYS:N  | 17       | 2.79          |
| (1,12)  | 1:8:A:GLN:N   | 1:8:A:GLN:CA  | 1:8:A:GLN:C    | 1:9:A:THR:N   | 8        | 2.79          |
| (1,7)   | 1:5:A:LYS:C   | 1:6:A:LEU:N   | 1:6:A:LEU:CA   | 1:6:A:LEU:C   | 14       | 2.79          |
| (1,183) | 1:101:A:ILE:C | 1:102:A:ARG:N | 1:102:A:ARG:CA | 1:102:A:ARG:C | 8        | 2.77          |
| (1,154) | 1:87:A:LEU:N  | 1:87:A:LEU:CA | 1:87:A:LEU:C   | 1:88:A:GLU:N  | 19       | 2.77          |
| (1,148) | 1:84:A:LYS:N  | 1:84:A:LYS:CA | 1:84:A:LYS:C   | 1:85:A:ASP:N  | 11       | 2.77          |
| (1,158) | 1:89:A:GLN:N  | 1:89:A:GLN:CA | 1:89:A:GLN:C   | 1:90:A:LEU:N  | 12       | 2.76          |
| (1,136) | 1:78:A:ALA:N  | 1:78:A:ALA:CA | 1:78:A:ALA:C   | 1:79:A:ILE:N  | 14       | 2.76          |
| (1,19)  | 1:12:A:GLU:C  | 1:13:A:LEU:N  | 1:13:A:LEU:CA  | 1:13:A:LEU:C  | 11       | 2.76          |
| (1,152) | 1:86:A:SER:N  | 1:86:A:SER:CA | 1:86:A:SER:C   | 1:87:A:LEU:N  | 18       | 2.73          |
| (1,109) | 1:64:A:GLN:C  | 1:65:A:GLY:N  | 1:65:A:GLY:CA  | 1:65:A:GLY:C  | 17       | 2.73          |
| (1,38)  | 1:22:A:GLU:N  | 1:22:A:GLU:CA | 1:22:A:GLU:C   | 1:23:A:ILE:N  | 14       | 2.73          |
| (1,137) | 1:78:A:ALA:C  | 1:79:A:ILE:N  | 1:79:A:ILE:CA  | 1:79:A:ILE:C  | 20       | 2.72          |
| (1,37)  | 1:21:A:ARG:C  | 1:22:A:GLU:N  | 1:22:A:GLU:CA  | 1:22:A:GLU:C  | 10       | 2.71          |
| (1,57)  | 1:31:A:SER:C  | 1:32:A:LEU:N  | 1:32:A:LEU:CA  | 1:32:A:LEU:C  | 11       | 2.7           |
| (1,64)  | 1:35:A:VAL:N  | 1:35:A:VAL:CA | 1:35:A:VAL:C   | 1:36:A:LEU:N  | 5        | 2.69          |
| (1,12)  | 1:8:A:GLN:N   | 1:8:A:GLN:CA  | 1:8:A:GLN:C    | 1:9:A:THR:N   | 13       | 2.69          |
| (1,191) | 1:105:A:ALA:C | 1:106:A:GLU:N | 1:106:A:GLU:CA | 1:106:A:GLU:C | 10       | 2.68          |
| (1,65)  | 1:35:A:VAL:C  | 1:36:A:LEU:N  | 1:36:A:LEU:CA  | 1:36:A:LEU:C  | 6        | 2.67          |
| (1,54)  | 1:30:A:ASP:N  | 1:30:A:ASP:CA | 1:30:A:ASP:C   | 1:31:A:SER:N  | 6        | 2.67          |
| (1,39)  | 1:22:A:GLU:C  | 1:23:A:ILE:N  | 1:23:A:ILE:CA  | 1:23:A:ILE:C  | 2        | 2.67          |
| (1,109) | 1:64:A:GLN:C  | 1:65:A:GLY:N  | 1:65:A:GLY:CA  | 1:65:A:GLY:C  | 6        | 2.66          |
| (1,116) | 1:68:A:TRP:N  | 1:68:A:TRP:CA | 1:68:A:TRP:C   | 1:69:A:VAL:N  | 1        | 2.65          |
| (1,116) | 1:68:A:TRP:N  | 1:68:A:TRP:CA | 1:68:A:TRP:C   | 1:69:A:VAL:N  | 2        | 2.65          |
| (1,6)   | 1:5:A:LYS:N   | 1:5:A:LYS:CA  | 1:5:A:LYS:C    | 1:6:A:LEU:N   | 9        | 2.64          |
| (1,11)  | 1:7:A:ARG:C   | 1:8:A:GLN:N   | 1:8:A:GLN:CA   | 1:8:A:GLN:C   | 12       | 2.63          |
| (1,194) | 1:11:A:ASP:N  | 1:11:A:ASP:CA | 1:11:A:ASP:CB  | 1:11:A:ASP:CG | 15       | 2.62          |
| (1,105) | 1:62:A:ALA:C  | 1:63:A:LYS:N  | 1:63:A:LYS:CA  | 1:63:A:LYS:C  | 16       | 2.61          |
| (1,101) | 1:60:A:GLU:C  | 1:61:A:ALA:N  | 1:61:A:ALA:CA  | 1:61:A:ALA:C  | 6        | 2.61          |
| (1,146) | 1:83:A:ASP:N  | 1:83:A:ASP:CA | 1:83:A:ASP:C   | 1:84:A:LYS:N  | 14       | 2.6           |
| (1,41)  | 1:23:A:ILE:C  | 1:24:A:PHE:N  | 1:24:A:PHE:CA  | 1:24:A:PHE:C  | 7        | 2.59          |
| (1,153) | 1:86:A:SER:C  | 1:87:A:LEU:N  | 1:87:A:LEU:CA  | 1:87:A:LEU:C  | 1        | 2.58          |
| (1,202) | 1:28:A:ASP:N  | 1:28:A:ASP:CA | 1:28:A:ASP:CB  | 1:28:A:ASP:CG | 17       | 2.57          |
| (1,153) | 1:86:A:SER:C  | 1:87:A:LEU:N  | 1:87:A:LEU:CA  | 1:87:A:LEU:C  | 2        | 2.57          |
| (1,57)  | 1:31:A:SER:C  | 1:32:A:LEU:N  | 1:32:A:LEU:CA  | 1:32:A:LEU:C  | 10       | 2.57          |
| (1,23)  | 1:14:A:VAL:C  | 1:15:A:GLN:N  | 1:15:A:GLN:CA  | 1:15:A:GLN:C  | 14       | 2.57          |
| (1,11)  | 1:7:A:ARG:C   | 1:8:A:GLN:N   | 1:8:A:GLN:CA   | 1:8:A:GLN:C   | 8        | 2.57          |

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| Key     | Atom-1       | Atom-2        | Atom-3        | Atom-4        | Model ID | Violation (°) |
|---------|--------------|---------------|---------------|---------------|----------|---------------|
| (1,136) | 1:78:A:ALA:N | 1:78:A:ALA:CA | 1:78:A:ALA:C  | 1:79:A:ILE:N  | 1        | 2.56          |
| (1,133) | 1:76:A:ARG:C | 1:77:A:GLU:N  | 1:77:A:GLU:CA | 1:77:A:GLU:C  | 18       | 2.56          |
| (1,38)  | 1:22:A:GLU:N | 1:22:A:GLU:CA | 1:22:A:GLU:C  | 1:23:A:ILE:N  | 12       | 2.56          |
| (1,177) | 1:98:A:LEU:C | 1:99:A:GLN:N  | 1:99:A:GLN:CA | 1:99:A:GLN:C  | 6        | 2.55          |
| (1,89)  | 1:47:A:ARG:C | 1:48:A:GLN:N  | 1:48:A:GLN:CA | 1:48:A:GLN:C  | 4        | 2.55          |
| (1,54)  | 1:30:A:ASP:N | 1:30:A:ASP:CA | 1:30:A:ASP:C  | 1:31:A:SER:N  | 16       | 2.54          |
| (1,55)  | 1:30:A:ASP:C | 1:31:A:SER:N  | 1:31:A:SER:CA | 1:31:A:SER:C  | 8        | 2.53          |
| (1,40)  | 1:23:A:ILE:N | 1:23:A:ILE:CA | 1:23:A:ILE:C  | 1:24:A:PHE:N  | 20       | 2.53          |
| (1,153) | 1:86:A:SER:C | 1:87:A:LEU:N  | 1:87:A:LEU:CA | 1:87:A:LEU:C  | 5        | 2.52          |
| (1,136) | 1:78:A:ALA:N | 1:78:A:ALA:CA | 1:78:A:ALA:C  | 1:79:A:ILE:N  | 9        | 2.52          |
| (1,177) | 1:98:A:LEU:C | 1:99:A:GLN:N  | 1:99:A:GLN:CA | 1:99:A:GLN:C  | 2        | 2.51          |
| (1,152) | 1:86:A:SER:N | 1:86:A:SER:CA | 1:86:A:SER:C  | 1:87:A:LEU:N  | 19       | 2.51          |
| (1,137) | 1:78:A:ALA:C | 1:79:A:ILE:N  | 1:79:A:ILE:CA | 1:79:A:ILE:C  | 7        | 2.51          |
| (1,116) | 1:68:A:TRP:N | 1:68:A:TRP:CA | 1:68:A:TRP:C  | 1:69:A:VAL:N  | 7        | 2.51          |
| (1,116) | 1:68:A:TRP:N | 1:68:A:TRP:CA | 1:68:A:TRP:C  | 1:69:A:VAL:N  | 17       | 2.51          |
| (1,51)  | 1:28:A:ASP:C | 1:29:A:ASP:N  | 1:29:A:ASP:CA | 1:29:A:ASP:C  | 11       | 2.51          |
| (1,116) | 1:68:A:TRP:N | 1:68:A:TRP:CA | 1:68:A:TRP:C  | 1:69:A:VAL:N  | 11       | 2.5           |
| (1,43)  | 1:24:A:PHE:C | 1:25:A:ASP:N  | 1:25:A:ASP:CA | 1:25:A:ASP:C  | 7        | 2.5           |
| (1,36)  | 1:21:A:ARG:N | 1:21:A:ARG:CA | 1:21:A:ARG:C  | 1:22:A:GLU:N  | 14       | 2.5           |
| (1,143) | 1:81:A:LYS:C | 1:82:A:GLY:N  | 1:82:A:GLY:CA | 1:82:A:GLY:C  | 20       | 2.49          |
| (1,11)  | 1:7:A:ARG:C  | 1:8:A:GLN:N   | 1:8:A:GLN:CA  | 1:8:A:GLN:C   | 2        | 2.48          |
| (1,85)  | 1:45:A:LYS:C | 1:46:A:HIS:N  | 1:46:A:HIS:CA | 1:46:A:HIS:C  | 11       | 2.47          |
| (1,55)  | 1:30:A:ASP:C | 1:31:A:SER:N  | 1:31:A:SER:CA | 1:31:A:SER:C  | 16       | 2.47          |
| (1,116) | 1:68:A:TRP:N | 1:68:A:TRP:CA | 1:68:A:TRP:C  | 1:69:A:VAL:N  | 4        | 2.44          |
| (1,35)  | 1:20:A:LEU:C | 1:21:A:ARG:N  | 1:21:A:ARG:CA | 1:21:A:ARG:C  | 9        | 2.44          |
| (1,135) | 1:77:A:GLU:C | 1:78:A:ALA:N  | 1:78:A:ALA:CA | 1:78:A:ALA:C  | 20       | 2.43          |
| (1,224) | 1:85:A:ASP:N | 1:85:A:ASP:CA | 1:85:A:ASP:CB | 1:85:A:ASP:CG | 20       | 2.42          |
| (1,153) | 1:86:A:SER:C | 1:87:A:LEU:N  | 1:87:A:LEU:CA | 1:87:A:LEU:C  | 7        | 2.42          |
| (1,116) | 1:68:A:TRP:N | 1:68:A:TRP:CA | 1:68:A:TRP:C  | 1:69:A:VAL:N  | 14       | 2.42          |
| (1,146) | 1:83:A:ASP:N | 1:83:A:ASP:CA | 1:83:A:ASP:C  | 1:84:A:LYS:N  | 13       | 2.39          |
| (1,82)  | 1:44:A:GLN:N | 1:44:A:GLN:CA | 1:44:A:GLN:C  | 1:45:A:LYS:N  | 9        | 2.39          |
| (1,19)  | 1:12:A:GLU:C | 1:13:A:LEU:N  | 1:13:A:LEU:CA | 1:13:A:LEU:C  | 14       | 2.39          |
| (1,6)   | 1:5:A:LYS:N  | 1:5:A:LYS:CA  | 1:5:A:LYS:C   | 1:6:A:LEU:N   | 8        | 2.39          |
| (1,116) | 1:68:A:TRP:N | 1:68:A:TRP:CA | 1:68:A:TRP:C  | 1:69:A:VAL:N  | 8        | 2.38          |
| (1,72)  | 1:39:A:ILE:N | 1:39:A:ILE:CA | 1:39:A:ILE:C  | 1:40:A:GLU:N  | 16       | 2.38          |
| (1,12)  | 1:8:A:GLN:N  | 1:8:A:GLN:CA  | 1:8:A:GLN:C   | 1:9:A:THR:N   | 17       | 2.38          |
| (1,216) | 1:68:A:TRP:N | 1:68:A:TRP:CA | 1:68:A:TRP:CB | 1:68:A:TRP:CG | 14       | 2.37          |
| (1,156) | 1:88:A:GLU:N | 1:88:A:GLU:CA | 1:88:A:GLU:C  | 1:89:A:GLN:N  | 9        | 2.37          |
| (1,91)  | 1:48:A:GLN:C | 1:49:A:LEU:N  | 1:49:A:LEU:CA | 1:49:A:LEU:C  | 20       | 2.37          |
| (1,72)  | 1:39:A:ILE:N | 1:39:A:ILE:CA | 1:39:A:ILE:C  | 1:40:A:GLU:N  | 9        | 2.37          |
| (1,57)  | 1:31:A:SER:C | 1:32:A:LEU:N  | 1:32:A:LEU:CA | 1:32:A:LEU:C  | 9        | 2.37          |
| (1,65)  | 1:35:A:VAL:C | 1:36:A:LEU:N  | 1:36:A:LEU:CA | 1:36:A:LEU:C  | 16       | 2.36          |
| (1,56)  | 1:31:A:SER:N | 1:31:A:SER:CA | 1:31:A:SER:C  | 1:32:A:LEU:N  | 4        | 2.36          |
| (1,202) | 1:28:A:ASP:N | 1:28:A:ASP:CA | 1:28:A:ASP:CB | 1:28:A:ASP:CG | 12       | 2.35          |
| (1,177) | 1:98:A:LEU:C | 1:99:A:GLN:N  | 1:99:A:GLN:CA | 1:99:A:GLN:C  | 5        | 2.34          |
| (1,65)  | 1:35:A:VAL:C | 1:36:A:LEU:N  | 1:36:A:LEU:CA | 1:36:A:LEU:C  | 14       | 2.33          |
| (1,40)  | 1:23:A:ILE:N | 1:23:A:ILE:CA | 1:23:A:ILE:C  | 1:24:A:PHE:N  | 19       | 2.33          |
| (1,132) | 1:76:A:ARG:N | 1:76:A:ARG:CA | 1:76:A:ARG:C  | 1:77:A:GLU:N  | 8        | 2.32          |
| (1,54)  | 1:30:A:ASP:N | 1:30:A:ASP:CA | 1:30:A:ASP:C  | 1:31:A:SER:N  | 20       | 2.32          |
| (1,40)  | 1:23:A:ILE:N | 1:23:A:ILE:CA | 1:23:A:ILE:C  | 1:24:A:PHE:N  | 4        | 2.32          |
| (1,73)  | 1:39:A:ILE:C | 1:40:A:GLU:N  | 1:40:A:GLU:CA | 1:40:A:GLU:C  | 20       | 2.3           |

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| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,56)  | 1:31:A:SER:N  | 1:31:A:SER:CA  | 1:31:A:SER:C   | 1:32:A:LEU:N  | 5        | 2.3           |
| (1,38)  | 1:22:A:GLU:N  | 1:22:A:GLU:CA  | 1:22:A:GLU:C   | 1:23:A:ILE:N  | 1        | 2.3           |
| (1,216) | 1:68:A:TRP:N  | 1:68:A:TRP:CA  | 1:68:A:TRP:CB  | 1:68:A:TRP:CG | 2        | 2.29          |
| (1,150) | 1:85:A:ASP:N  | 1:85:A:ASP:CA  | 1:85:A:ASP:C   | 1:86:A:SER:N  | 13       | 2.29          |
| (1,38)  | 1:22:A:GLU:N  | 1:22:A:GLU:CA  | 1:22:A:GLU:C   | 1:23:A:ILE:N  | 13       | 2.29          |
| (1,72)  | 1:39:A:ILE:N  | 1:39:A:ILE:CA  | 1:39:A:ILE:C   | 1:40:A:GLU:N  | 6        | 2.28          |
| (1,38)  | 1:22:A:GLU:N  | 1:22:A:GLU:CA  | 1:22:A:GLU:C   | 1:23:A:ILE:N  | 17       | 2.28          |
| (1,153) | 1:86:A:SER:C  | 1:87:A:LEU:N   | 1:87:A:LEU:CA  | 1:87:A:LEU:C  | 3        | 2.27          |
| (1,152) | 1:86:A:SER:N  | 1:86:A:SER:CA  | 1:86:A:SER:C   | 1:87:A:LEU:N  | 12       | 2.27          |
| (1,216) | 1:68:A:TRP:N  | 1:68:A:TRP:CA  | 1:68:A:TRP:CB  | 1:68:A:TRP:CG | 20       | 2.26          |
| (1,186) | 1:103:A:GLU:N | 1:103:A:GLU:CA | 1:103:A:GLU:C  | 1:104:A:LEU:N | 2        | 2.26          |
| (1,153) | 1:86:A:SER:C  | 1:87:A:LEU:N   | 1:87:A:LEU:CA  | 1:87:A:LEU:C  | 8        | 2.26          |
| (1,32)  | 1:19:A:ARG:N  | 1:19:A:ARG:CA  | 1:19:A:ARG:C   | 1:20:A:LEU:N  | 10       | 2.26          |
| (1,19)  | 1:12:A:GLU:C  | 1:13:A:LEU:N   | 1:13:A:LEU:CA  | 1:13:A:LEU:C  | 7        | 2.25          |
| (1,43)  | 1:24:A:PHE:C  | 1:25:A:ASP:N   | 1:25:A:ASP:CA  | 1:25:A:ASP:C  | 15       | 2.24          |
| (1,11)  | 1:7:A:ARG:C   | 1:8:A:GLN:N    | 1:8:A:GLN:CA   | 1:8:A:GLN:C   | 13       | 2.24          |
| (1,210) | 1:49:A:LEU:N  | 1:49:A:LEU:CA  | 1:49:A:LEU:CB  | 1:49:A:LEU:CG | 18       | 2.23          |
| (1,164) | 1:92:A:GLU:N  | 1:92:A:GLU:CA  | 1:92:A:GLU:C   | 1:93:A:GLU:N  | 7        | 2.23          |
| (1,65)  | 1:35:A:VAL:C  | 1:36:A:LEU:N   | 1:36:A:LEU:CA  | 1:36:A:LEU:C  | 8        | 2.23          |
| (1,54)  | 1:30:A:ASP:N  | 1:30:A:ASP:CA  | 1:30:A:ASP:C   | 1:31:A:SER:N  | 9        | 2.23          |
| (1,41)  | 1:23:A:ILE:C  | 1:24:A:PHE:N   | 1:24:A:PHE:CA  | 1:24:A:PHE:C  | 12       | 2.23          |
| (1,19)  | 1:12:A:GLU:C  | 1:13:A:LEU:N   | 1:13:A:LEU:CA  | 1:13:A:LEU:C  | 15       | 2.23          |
| (1,224) | 1:85:A:ASP:N  | 1:85:A:ASP:CA  | 1:85:A:ASP:CB  | 1:85:A:ASP:CG | 13       | 2.22          |
| (1,170) | 1:95:A:GLU:N  | 1:95:A:GLU:CA  | 1:95:A:GLU:C   | 1:96:A:GLN:N  | 5        | 2.22          |
| (1,110) | 1:65:A:GLY:N  | 1:65:A:GLY:CA  | 1:65:A:GLY:C   | 1:66:A:ASP:N  | 1        | 2.22          |
| (1,78)  | 1:42:A:LEU:N  | 1:42:A:LEU:CA  | 1:42:A:LEU:C   | 1:43:A:ILE:N  | 20       | 2.22          |
| (1,216) | 1:68:A:TRP:N  | 1:68:A:TRP:CA  | 1:68:A:TRP:CB  | 1:68:A:TRP:CG | 7        | 2.21          |
| (1,105) | 1:62:A:ALA:C  | 1:63:A:LYS:N   | 1:63:A:LYS:CA  | 1:63:A:LYS:C  | 19       | 2.21          |
| (1,84)  | 1:45:A:LYS:N  | 1:45:A:LYS:CA  | 1:45:A:LYS:C   | 1:46:A:HIS:N  | 5        | 2.21          |
| (1,191) | 1:105:A:ALA:C | 1:106:A:GLU:N  | 1:106:A:GLU:CA | 1:106:A:GLU:C | 19       | 2.2           |
| (1,152) | 1:86:A:SER:N  | 1:86:A:SER:CA  | 1:86:A:SER:C   | 1:87:A:LEU:N  | 10       | 2.2           |
| (1,84)  | 1:45:A:LYS:N  | 1:45:A:LYS:CA  | 1:45:A:LYS:C   | 1:46:A:HIS:N  | 14       | 2.2           |
| (1,41)  | 1:23:A:ILE:C  | 1:24:A:PHE:N   | 1:24:A:PHE:CA  | 1:24:A:PHE:C  | 6        | 2.2           |
| (1,19)  | 1:12:A:GLU:C  | 1:13:A:LEU:N   | 1:13:A:LEU:CA  | 1:13:A:LEU:C  | 4        | 2.2           |
| (1,179) | 1:99:A:GLN:C  | 1:100:A:LYS:N  | 1:100:A:LYS:CA | 1:100:A:LYS:C | 17       | 2.19          |
| (1,47)  | 1:26:A:LYS:C  | 1:27:A:GLY:N   | 1:27:A:GLY:CA  | 1:27:A:GLY:C  | 11       | 2.18          |
| (1,42)  | 1:24:A:PHE:N  | 1:24:A:PHE:CA  | 1:24:A:PHE:C   | 1:25:A:ASP:N  | 18       | 2.18          |
| (1,12)  | 1:8:A:GLN:N   | 1:8:A:GLN:CA   | 1:8:A:GLN:C    | 1:9:A:THR:N   | 12       | 2.18          |
| (1,154) | 1:87:A:LEU:N  | 1:87:A:LEU:CA  | 1:87:A:LEU:C   | 1:88:A:GLU:N  | 14       | 2.17          |
| (1,136) | 1:78:A:ALA:N  | 1:78:A:ALA:CA  | 1:78:A:ALA:C   | 1:79:A:ILE:N  | 16       | 2.17          |
| (1,65)  | 1:35:A:VAL:C  | 1:36:A:LEU:N   | 1:36:A:LEU:CA  | 1:36:A:LEU:C  | 10       | 2.17          |
| (1,64)  | 1:35:A:VAL:N  | 1:35:A:VAL:CA  | 1:35:A:VAL:C   | 1:36:A:LEU:N  | 8        | 2.17          |
| (1,32)  | 1:19:A:ARG:N  | 1:19:A:ARG:CA  | 1:19:A:ARG:C   | 1:20:A:LEU:N  | 3        | 2.17          |
| (1,177) | 1:98:A:LEU:C  | 1:99:A:GLN:N   | 1:99:A:GLN:CA  | 1:99:A:GLN:C  | 13       | 2.16          |
| (1,147) | 1:83:A:ASP:C  | 1:84:A:LYS:N   | 1:84:A:LYS:CA  | 1:84:A:LYS:C  | 11       | 2.16          |
| (1,136) | 1:78:A:ALA:N  | 1:78:A:ALA:CA  | 1:78:A:ALA:C   | 1:79:A:ILE:N  | 20       | 2.16          |
| (1,109) | 1:64:A:GLN:C  | 1:65:A:GLY:N   | 1:65:A:GLY:CA  | 1:65:A:GLY:C  | 19       | 2.16          |
| (1,201) | 1:26:A:LYS:N  | 1:26:A:LYS:CA  | 1:26:A:LYS:CB  | 1:26:A:LYS:CG | 17       | 2.15          |
| (1,65)  | 1:35:A:VAL:C  | 1:36:A:LEU:N   | 1:36:A:LEU:CA  | 1:36:A:LEU:C  | 13       | 2.15          |
| (1,40)  | 1:23:A:ILE:N  | 1:23:A:ILE:CA  | 1:23:A:ILE:C   | 1:24:A:PHE:N  | 8        | 2.15          |
| (1,137) | 1:78:A:ALA:C  | 1:79:A:ILE:N   | 1:79:A:ILE:CA  | 1:79:A:ILE:C  | 5        | 2.14          |

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| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4         | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|----------------|----------|---------------|
| (1,40)  | 1:23:A:ILE:N  | 1:23:A:ILE:CA  | 1:23:A:ILE:C   | 1:24:A:PHE:N   | 15       | 2.14          |
| (1,19)  | 1:12:A:GLU:C  | 1:13:A:LEU:N   | 1:13:A:LEU:CA  | 1:13:A:LEU:C   | 1        | 2.14          |
| (1,19)  | 1:12:A:GLU:C  | 1:13:A:LEU:N   | 1:13:A:LEU:CA  | 1:13:A:LEU:C   | 12       | 2.14          |
| (1,93)  | 1:49:A:LEU:C  | 1:50:A:PHE:N   | 1:50:A:PHE:CA  | 1:50:A:PHE:C   | 10       | 2.13          |
| (1,73)  | 1:39:A:ILE:C  | 1:40:A:GLU:N   | 1:40:A:GLU:CA  | 1:40:A:GLU:C   | 5        | 2.13          |
| (1,55)  | 1:30:A:ASP:C  | 1:31:A:SER:N   | 1:31:A:SER:CA  | 1:31:A:SER:C   | 6        | 2.13          |
| (1,72)  | 1:39:A:ILE:N  | 1:39:A:ILE:CA  | 1:39:A:ILE:C   | 1:40:A:GLU:N   | 13       | 2.12          |
| (1,57)  | 1:31:A:SER:C  | 1:32:A:LEU:N   | 1:32:A:LEU:CA  | 1:32:A:LEU:C   | 18       | 2.12          |
| (1,214) | 1:55:A:GLU:N  | 1:55:A:GLU:CA  | 1:55:A:GLU:CB  | 1:55:A:GLU:CG  | 6        | 2.11          |
| (1,37)  | 1:21:A:ARG:C  | 1:22:A:GLU:N   | 1:22:A:GLU:CA  | 1:22:A:GLU:C   | 1        | 2.11          |
| (1,12)  | 1:8:A:GLN:N   | 1:8:A:GLN:CA   | 1:8:A:GLN:C    | 1:9:A:THR:N    | 14       | 2.11          |
| (1,10)  | 1:7:A:ARG:N   | 1:7:A:ARG:CA   | 1:7:A:ARG:C    | 1:8:A:GLN:N    | 11       | 2.11          |
| (1,7)   | 1:5:A:LYS:C   | 1:6:A:LEU:N    | 1:6:A:LEU:CA   | 1:6:A:LEU:C    | 19       | 2.11          |
| (1,143) | 1:81:A:LYS:C  | 1:82:A:GLY:N   | 1:82:A:GLY:CA  | 1:82:A:GLY:C   | 17       | 2.1           |
| (1,137) | 1:78:A:ALA:C  | 1:79:A:ILE:N   | 1:79:A:ILE:CA  | 1:79:A:ILE:C   | 8        | 2.1           |
| (1,89)  | 1:47:A:ARG:C  | 1:48:A:GLN:N   | 1:48:A:GLN:CA  | 1:48:A:GLN:C   | 1        | 2.1           |
| (1,11)  | 1:7:A:ARG:C   | 1:8:A:GLN:N    | 1:8:A:GLN:CA   | 1:8:A:GLN:C    | 17       | 2.1           |
| (1,64)  | 1:35:A:VAL:N  | 1:35:A:VAL:CA  | 1:35:A:VAL:C   | 1:36:A:LEU:N   | 13       | 2.09          |
| (1,143) | 1:81:A:LYS:C  | 1:82:A:GLY:N   | 1:82:A:GLY:CA  | 1:82:A:GLY:C   | 9        | 2.08          |
| (1,139) | 1:79:A:ILE:C  | 1:80:A:ASP:N   | 1:80:A:ASP:CA  | 1:80:A:ASP:C   | 18       | 2.08          |
| (1,110) | 1:65:A:GLY:N  | 1:65:A:GLY:CA  | 1:65:A:GLY:C   | 1:66:A:ASP:N   | 13       | 2.08          |
| (1,48)  | 1:27:A:GLY:N  | 1:27:A:GLY:CA  | 1:27:A:GLY:C   | 1:28:A:ASP:N   | 17       | 2.08          |
| (1,72)  | 1:39:A:ILE:N  | 1:39:A:ILE:CA  | 1:39:A:ILE:C   | 1:40:A:GLU:N   | 19       | 2.07          |
| (1,43)  | 1:24:A:PHE:C  | 1:25:A:ASP:N   | 1:25:A:ASP:CA  | 1:25:A:ASP:C   | 20       | 2.07          |
| (1,28)  | 1:17:A:PHE:N  | 1:17:A:PHE:CA  | 1:17:A:PHE:C   | 1:18:A:GLN:N   | 19       | 2.07          |
| (1,25)  | 1:15:A:GLN:C  | 1:16:A:ALA:N   | 1:16:A:ALA:CA  | 1:16:A:ALA:C   | 9        | 2.07          |
| (1,152) | 1:86:A:SER:N  | 1:86:A:SER:CA  | 1:86:A:SER:C   | 1:87:A:LEU:N   | 2        | 2.06          |
| (1,89)  | 1:47:A:ARG:C  | 1:48:A:GLN:N   | 1:48:A:GLN:CA  | 1:48:A:GLN:C   | 9        | 2.06          |
| (1,51)  | 1:28:A:ASP:C  | 1:29:A:ASP:N   | 1:29:A:ASP:CA  | 1:29:A:ASP:C   | 10       | 2.06          |
| (1,228) | 1:104:A:LEU:N | 1:104:A:LEU:CA | 1:104:A:LEU:CB | 1:104:A:LEU:CG | 1        | 2.05          |
| (1,224) | 1:85:A:ASP:N  | 1:85:A:ASP:CA  | 1:85:A:ASP:CB  | 1:85:A:ASP:CG  | 7        | 2.05          |
| (1,221) | 1:80:A:ASP:N  | 1:80:A:ASP:CA  | 1:80:A:ASP:CB  | 1:80:A:ASP:CG  | 14       | 2.05          |
| (1,143) | 1:81:A:LYS:C  | 1:82:A:GLY:N   | 1:82:A:GLY:CA  | 1:82:A:GLY:C   | 7        | 2.05          |
| (1,73)  | 1:39:A:ILE:C  | 1:40:A:GLU:N   | 1:40:A:GLU:CA  | 1:40:A:GLU:C   | 16       | 2.05          |
| (1,28)  | 1:17:A:PHE:N  | 1:17:A:PHE:CA  | 1:17:A:PHE:C   | 1:18:A:GLN:N   | 13       | 2.05          |
| (1,223) | 1:83:A:ASP:N  | 1:83:A:ASP:CA  | 1:83:A:ASP:CB  | 1:83:A:ASP:CG  | 11       | 2.04          |
| (1,158) | 1:89:A:GLN:N  | 1:89:A:GLN:CA  | 1:89:A:GLN:C   | 1:90:A:LEU:N   | 5        | 2.04          |
| (1,154) | 1:87:A:LEU:N  | 1:87:A:LEU:CA  | 1:87:A:LEU:C   | 1:88:A:GLU:N   | 15       | 2.04          |
| (1,98)  | 1:59:A:THR:N  | 1:59:A:THR:CA  | 1:59:A:THR:C   | 1:60:A:GLU:N   | 15       | 2.04          |
| (1,79)  | 1:42:A:LEU:C  | 1:43:A:ILE:N   | 1:43:A:ILE:CA  | 1:43:A:ILE:C   | 20       | 2.04          |
| (1,63)  | 1:34:A:GLN:C  | 1:35:A:VAL:N   | 1:35:A:VAL:CA  | 1:35:A:VAL:C   | 7        | 2.04          |
| (1,154) | 1:87:A:LEU:N  | 1:87:A:LEU:CA  | 1:87:A:LEU:C   | 1:88:A:GLU:N   | 10       | 2.03          |
| (1,108) | 1:64:A:GLN:N  | 1:64:A:GLN:CA  | 1:64:A:GLN:C   | 1:65:A:GLY:N   | 5        | 2.03          |
| (1,56)  | 1:31:A:SER:N  | 1:31:A:SER:CA  | 1:31:A:SER:C   | 1:32:A:LEU:N   | 12       | 2.03          |
| (1,215) | 1:66:A:ASP:N  | 1:66:A:ASP:CA  | 1:66:A:ASP:CB  | 1:66:A:ASP:CG  | 3        | 2.02          |
| (1,54)  | 1:30:A:ASP:N  | 1:30:A:ASP:CA  | 1:30:A:ASP:C   | 1:31:A:SER:N   | 3        | 2.02          |
| (1,37)  | 1:21:A:ARG:C  | 1:22:A:GLU:N   | 1:22:A:GLU:CA  | 1:22:A:GLU:C   | 20       | 2.02          |
| (1,200) | 1:25:A:ASP:N  | 1:25:A:ASP:CA  | 1:25:A:ASP:CB  | 1:25:A:ASP:CG  | 7        | 2.01          |
| (1,132) | 1:76:A:ARG:N  | 1:76:A:ARG:CA  | 1:76:A:ARG:C   | 1:77:A:GLU:N   | 18       | 2.01          |
| (1,61)  | 1:33:A:GLU:C  | 1:34:A:GLN:N   | 1:34:A:GLN:CA  | 1:34:A:GLN:C   | 7        | 2.01          |
| (1,19)  | 1:12:A:GLU:C  | 1:13:A:LEU:N   | 1:13:A:LEU:CA  | 1:13:A:LEU:C   | 17       | 2.01          |

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| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,179) | 1:99:A:GLN:C  | 1:100:A:LYS:N  | 1:100:A:LYS:CA | 1:100:A:LYS:C | 12       | 2.0           |
| (1,108) | 1:64:A:GLN:N  | 1:64:A:GLN:CA  | 1:64:A:GLN:C   | 1:65:A:GLY:N  | 2        | 2.0           |
| (1,89)  | 1:47:A:ARG:C  | 1:48:A:GLN:N   | 1:48:A:GLN:CA  | 1:48:A:GLN:C  | 11       | 2.0           |
| (1,64)  | 1:35:A:VAL:N  | 1:35:A:VAL:CA  | 1:35:A:VAL:C   | 1:36:A:LEU:N  | 14       | 2.0           |
| (1,40)  | 1:23:A:ILE:N  | 1:23:A:ILE:CA  | 1:23:A:ILE:C   | 1:24:A:PHE:N  | 11       | 2.0           |
| (1,11)  | 1:7:A:ARG:C   | 1:8:A:GLN:N    | 1:8:A:GLN:CA   | 1:8:A:GLN:C   | 15       | 2.0           |
| (1,183) | 1:101:A:ILE:C | 1:102:A:ARG:N  | 1:102:A:ARG:CA | 1:102:A:ARG:C | 17       | 1.99          |
| (1,152) | 1:86:A:SER:N  | 1:86:A:SER:CA  | 1:86:A:SER:C   | 1:87:A:LEU:N  | 7        | 1.99          |
| (1,84)  | 1:45:A:LYS:N  | 1:45:A:LYS:CA  | 1:45:A:LYS:C   | 1:46:A:HIS:N  | 16       | 1.99          |
| (1,55)  | 1:30:A:ASP:C  | 1:31:A:SER:N   | 1:31:A:SER:CA  | 1:31:A:SER:C  | 11       | 1.99          |
| (1,186) | 1:103:A:GLU:N | 1:103:A:GLU:CA | 1:103:A:GLU:C  | 1:104:A:LEU:N | 8        | 1.98          |
| (1,152) | 1:86:A:SER:N  | 1:86:A:SER:CA  | 1:86:A:SER:C   | 1:87:A:LEU:N  | 17       | 1.98          |
| (1,40)  | 1:23:A:ILE:N  | 1:23:A:ILE:CA  | 1:23:A:ILE:C   | 1:24:A:PHE:N  | 14       | 1.98          |
| (1,37)  | 1:21:A:ARG:C  | 1:22:A:GLU:N   | 1:22:A:GLU:CA  | 1:22:A:GLU:C  | 9        | 1.98          |
| (1,35)  | 1:20:A:LEU:C  | 1:21:A:ARG:N   | 1:21:A:ARG:CA  | 1:21:A:ARG:C  | 15       | 1.98          |
| (1,33)  | 1:19:A:ARG:C  | 1:20:A:LEU:N   | 1:20:A:LEU:CA  | 1:20:A:LEU:C  | 3        | 1.98          |
| (1,19)  | 1:12:A:GLU:C  | 1:13:A:LEU:N   | 1:13:A:LEU:CA  | 1:13:A:LEU:C  | 5        | 1.97          |
| (1,183) | 1:101:A:ILE:C | 1:102:A:ARG:N  | 1:102:A:ARG:CA | 1:102:A:ARG:C | 15       | 1.96          |
| (1,171) | 1:95:A:GLU:C  | 1:96:A:GLN:N   | 1:96:A:GLN:CA  | 1:96:A:GLN:C  | 9        | 1.96          |
| (1,1)   | 1:2:A:GLU:C   | 1:3:A:PHE:N    | 1:3:A:PHE:CA   | 1:3:A:PHE:C   | 15       | 1.95          |
| (1,210) | 1:49:A:LEU:N  | 1:49:A:LEU:CA  | 1:49:A:LEU:CB  | 1:49:A:LEU:CG | 2        | 1.94          |
| (1,179) | 1:99:A:GLN:C  | 1:100:A:LYS:N  | 1:100:A:LYS:CA | 1:100:A:LYS:C | 2        | 1.94          |
| (1,80)  | 1:43:A:ILE:N  | 1:43:A:ILE:CA  | 1:43:A:ILE:C   | 1:44:A:GLN:N  | 18       | 1.94          |
| (1,35)  | 1:20:A:LEU:C  | 1:21:A:ARG:N   | 1:21:A:ARG:CA  | 1:21:A:ARG:C  | 6        | 1.94          |
| (1,19)  | 1:12:A:GLU:C  | 1:13:A:LEU:N   | 1:13:A:LEU:CA  | 1:13:A:LEU:C  | 13       | 1.94          |
| (1,6)   | 1:5:A:LYS:N   | 1:5:A:LYS:CA   | 1:5:A:LYS:C    | 1:6:A:LEU:N   | 4        | 1.94          |
| (1,181) | 1:100:A:LYS:C | 1:101:A:ILE:N  | 1:101:A:ILE:CA | 1:101:A:ILE:C | 6        | 1.93          |
| (1,157) | 1:88:A:GLU:C  | 1:89:A:GLN:N   | 1:89:A:GLN:CA  | 1:89:A:GLN:C  | 11       | 1.93          |
| (1,102) | 1:61:A:ALA:N  | 1:61:A:ALA:CA  | 1:61:A:ALA:C   | 1:62:A:ALA:N  | 16       | 1.93          |
| (1,64)  | 1:35:A:VAL:N  | 1:35:A:VAL:CA  | 1:35:A:VAL:C   | 1:36:A:LEU:N  | 16       | 1.93          |
| (1,39)  | 1:22:A:GLU:C  | 1:23:A:ILE:N   | 1:23:A:ILE:CA  | 1:23:A:ILE:C  | 16       | 1.93          |
| (1,153) | 1:86:A:SER:C  | 1:87:A:LEU:N   | 1:87:A:LEU:CA  | 1:87:A:LEU:C  | 6        | 1.92          |
| (1,153) | 1:86:A:SER:C  | 1:87:A:LEU:N   | 1:87:A:LEU:CA  | 1:87:A:LEU:C  | 12       | 1.92          |
| (1,152) | 1:86:A:SER:N  | 1:86:A:SER:CA  | 1:86:A:SER:C   | 1:87:A:LEU:N  | 5        | 1.92          |
| (1,19)  | 1:12:A:GLU:C  | 1:13:A:LEU:N   | 1:13:A:LEU:CA  | 1:13:A:LEU:C  | 3        | 1.92          |
| (1,19)  | 1:12:A:GLU:C  | 1:13:A:LEU:N   | 1:13:A:LEU:CA  | 1:13:A:LEU:C  | 8        | 1.92          |
| (1,200) | 1:25:A:ASP:N  | 1:25:A:ASP:CA  | 1:25:A:ASP:CB  | 1:25:A:ASP:CG | 13       | 1.91          |
| (1,155) | 1:87:A:LEU:C  | 1:88:A:GLU:N   | 1:88:A:GLU:CA  | 1:88:A:GLU:C  | 17       | 1.91          |
| (1,109) | 1:64:A:GLN:C  | 1:65:A:GLY:N   | 1:65:A:GLY:CA  | 1:65:A:GLY:C  | 8        | 1.91          |
| (1,80)  | 1:43:A:ILE:N  | 1:43:A:ILE:CA  | 1:43:A:ILE:C   | 1:44:A:GLN:N  | 3        | 1.91          |
| (1,202) | 1:28:A:ASP:N  | 1:28:A:ASP:CA  | 1:28:A:ASP:CB  | 1:28:A:ASP:CG | 19       | 1.9           |
| (1,137) | 1:78:A:ALA:C  | 1:79:A:ILE:N   | 1:79:A:ILE:CA  | 1:79:A:ILE:C  | 12       | 1.89          |
| (1,76)  | 1:41:A:GLU:N  | 1:41:A:GLU:CA  | 1:41:A:GLU:C   | 1:42:A:LEU:N  | 7        | 1.89          |
| (1,152) | 1:86:A:SER:N  | 1:86:A:SER:CA  | 1:86:A:SER:C   | 1:87:A:LEU:N  | 1        | 1.88          |
| (1,73)  | 1:39:A:ILE:C  | 1:40:A:GLU:N   | 1:40:A:GLU:CA  | 1:40:A:GLU:C  | 11       | 1.88          |
| (1,72)  | 1:39:A:ILE:N  | 1:39:A:ILE:CA  | 1:39:A:ILE:C   | 1:40:A:GLU:N  | 3        | 1.88          |
| (1,4)   | 1:4:A:GLU:N   | 1:4:A:GLU:CA   | 1:4:A:GLU:C    | 1:5:A:LYS:N   | 13       | 1.88          |
| (1,186) | 1:103:A:GLU:N | 1:103:A:GLU:CA | 1:103:A:GLU:C  | 1:104:A:LEU:N | 10       | 1.87          |
| (1,119) | 1:69:A:VAL:C  | 1:70:A:GLN:N   | 1:70:A:GLN:CA  | 1:70:A:GLN:C  | 15       | 1.87          |
| (1,28)  | 1:17:A:PHE:N  | 1:17:A:PHE:CA  | 1:17:A:PHE:C   | 1:18:A:GLN:N  | 18       | 1.87          |
| (1,23)  | 1:14:A:VAL:C  | 1:15:A:GLN:N   | 1:15:A:GLN:CA  | 1:15:A:GLN:C  | 7        | 1.87          |

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| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,11)  | 1:7:A:ARG:C   | 1:8:A:GLN:N    | 1:8:A:GLN:CA   | 1:8:A:GLN:C   | 16       | 1.87          |
| (1,89)  | 1:47:A:ARG:C  | 1:48:A:GLN:N   | 1:48:A:GLN:CA  | 1:48:A:GLN:C  | 2        | 1.86          |
| (1,54)  | 1:30:A:ASP:N  | 1:30:A:ASP:CA  | 1:30:A:ASP:C   | 1:31:A:SER:N  | 8        | 1.86          |
| (1,37)  | 1:21:A:ARG:C  | 1:22:A:GLU:N   | 1:22:A:GLU:CA  | 1:22:A:GLU:C  | 11       | 1.86          |
| (1,189) | 1:104:A:LEU:C | 1:105:A:ALA:N  | 1:105:A:ALA:CA | 1:105:A:ALA:C | 15       | 1.85          |
| (1,125) | 1:72:A:PHE:C  | 1:73:A:GLN:N   | 1:73:A:GLN:CA  | 1:73:A:GLN:C  | 20       | 1.85          |
| (1,97)  | 1:58:A:ASP:C  | 1:59:A:THR:N   | 1:59:A:THR:CA  | 1:59:A:THR:C  | 4        | 1.85          |
| (1,94)  | 1:50:A:PHE:N  | 1:50:A:PHE:CA  | 1:50:A:PHE:C   | 1:51:A:ASP:N  | 20       | 1.85          |
| (1,48)  | 1:27:A:GLY:N  | 1:27:A:GLY:CA  | 1:27:A:GLY:C   | 1:28:A:ASP:N  | 18       | 1.85          |
| (1,19)  | 1:12:A:GLU:C  | 1:13:A:LEU:N   | 1:13:A:LEU:CA  | 1:13:A:LEU:C  | 6        | 1.85          |
| (1,202) | 1:28:A:ASP:N  | 1:28:A:ASP:CA  | 1:28:A:ASP:CB  | 1:28:A:ASP:CG | 15       | 1.84          |
| (1,194) | 1:11:A:ASP:N  | 1:11:A:ASP:CA  | 1:11:A:ASP:CB  | 1:11:A:ASP:CG | 20       | 1.84          |
| (1,158) | 1:89:A:GLN:N  | 1:89:A:GLN:CA  | 1:89:A:GLN:C   | 1:90:A:LEU:N  | 1        | 1.84          |
| (1,143) | 1:81:A:LYS:C  | 1:82:A:GLY:N   | 1:82:A:GLY:CA  | 1:82:A:GLY:C  | 14       | 1.84          |
| (1,89)  | 1:47:A:ARG:C  | 1:48:A:GLN:N   | 1:48:A:GLN:CA  | 1:48:A:GLN:C  | 8        | 1.84          |
| (1,73)  | 1:39:A:ILE:C  | 1:40:A:GLU:N   | 1:40:A:GLU:CA  | 1:40:A:GLU:C  | 10       | 1.84          |
| (1,43)  | 1:24:A:PHE:C  | 1:25:A:ASP:N   | 1:25:A:ASP:CA  | 1:25:A:ASP:C  | 10       | 1.84          |
| (1,41)  | 1:23:A:ILE:C  | 1:24:A:PHE:N   | 1:24:A:PHE:CA  | 1:24:A:PHE:C  | 15       | 1.84          |
| (1,19)  | 1:12:A:GLU:C  | 1:13:A:LEU:N   | 1:13:A:LEU:CA  | 1:13:A:LEU:C  | 10       | 1.84          |
| (1,216) | 1:68:A:TRP:N  | 1:68:A:TRP:CA  | 1:68:A:TRP:CB  | 1:68:A:TRP:CG | 8        | 1.83          |
| (1,183) | 1:101:A:ILE:C | 1:102:A:ARG:N  | 1:102:A:ARG:CA | 1:102:A:ARG:C | 14       | 1.83          |
| (1,178) | 1:99:A:GLN:N  | 1:99:A:GLN:CA  | 1:99:A:GLN:C   | 1:100:A:LYS:N | 14       | 1.83          |
| (1,157) | 1:88:A:GLU:C  | 1:89:A:GLN:N   | 1:89:A:GLN:CA  | 1:89:A:GLN:C  | 19       | 1.83          |
| (1,153) | 1:86:A:SER:C  | 1:87:A:LEU:N   | 1:87:A:LEU:CA  | 1:87:A:LEU:C  | 10       | 1.83          |
| (1,150) | 1:85:A:ASP:N  | 1:85:A:ASP:CA  | 1:85:A:ASP:C   | 1:86:A:SER:N  | 4        | 1.83          |
| (1,149) | 1:84:A:LYS:C  | 1:85:A:ASP:N   | 1:85:A:ASP:CA  | 1:85:A:ASP:C  | 8        | 1.83          |
| (1,116) | 1:68:A:TRP:N  | 1:68:A:TRP:CA  | 1:68:A:TRP:C   | 1:69:A:VAL:N  | 12       | 1.83          |
| (1,73)  | 1:39:A:ILE:C  | 1:40:A:GLU:N   | 1:40:A:GLU:CA  | 1:40:A:GLU:C  | 18       | 1.83          |
| (1,11)  | 1:7:A:ARG:C   | 1:8:A:GLN:N    | 1:8:A:GLN:CA   | 1:8:A:GLN:C   | 18       | 1.83          |
| (1,135) | 1:77:A:GLU:C  | 1:78:A:ALA:N   | 1:78:A:ALA:CA  | 1:78:A:ALA:C  | 17       | 1.82          |
| (1,105) | 1:62:A:ALA:C  | 1:63:A:LYS:N   | 1:63:A:LYS:CA  | 1:63:A:LYS:C  | 9        | 1.82          |
| (1,89)  | 1:47:A:ARG:C  | 1:48:A:GLN:N   | 1:48:A:GLN:CA  | 1:48:A:GLN:C  | 17       | 1.82          |
| (1,54)  | 1:30:A:ASP:N  | 1:30:A:ASP:CA  | 1:30:A:ASP:C   | 1:31:A:SER:N  | 5        | 1.82          |
| (1,43)  | 1:24:A:PHE:C  | 1:25:A:ASP:N   | 1:25:A:ASP:CA  | 1:25:A:ASP:C  | 5        | 1.82          |
| (1,23)  | 1:14:A:VAL:C  | 1:15:A:GLN:N   | 1:15:A:GLN:CA  | 1:15:A:GLN:C  | 2        | 1.82          |
| (1,11)  | 1:7:A:ARG:C   | 1:8:A:GLN:N    | 1:8:A:GLN:CA   | 1:8:A:GLN:C   | 5        | 1.82          |
| (1,10)  | 1:7:A:ARG:N   | 1:7:A:ARG:CA   | 1:7:A:ARG:C    | 1:8:A:GLN:N   | 18       | 1.82          |
| (1,186) | 1:103:A:GLU:N | 1:103:A:GLU:CA | 1:103:A:GLU:C  | 1:104:A:LEU:N | 17       | 1.81          |
| (1,177) | 1:98:A:LEU:C  | 1:99:A:GLN:N   | 1:99:A:GLN:CA  | 1:99:A:GLN:C  | 7        | 1.81          |
| (1,171) | 1:95:A:GLU:C  | 1:96:A:GLN:N   | 1:96:A:GLN:CA  | 1:96:A:GLN:C  | 14       | 1.81          |
| (1,137) | 1:78:A:ALA:C  | 1:79:A:ILE:N   | 1:79:A:ILE:CA  | 1:79:A:ILE:C  | 6        | 1.81          |
| (1,126) | 1:73:A:GLN:N  | 1:73:A:GLN:CA  | 1:73:A:GLN:C   | 1:74:A:ARG:N  | 3        | 1.81          |
| (1,109) | 1:64:A:GLN:C  | 1:65:A:GLY:N   | 1:65:A:GLY:CA  | 1:65:A:GLY:C  | 7        | 1.81          |
| (1,59)  | 1:32:A:LEU:C  | 1:33:A:GLU:N   | 1:33:A:GLU:CA  | 1:33:A:GLU:C  | 6        | 1.81          |
| (1,55)  | 1:30:A:ASP:C  | 1:31:A:SER:N   | 1:31:A:SER:CA  | 1:31:A:SER:C  | 3        | 1.81          |
| (1,38)  | 1:22:A:GLU:N  | 1:22:A:GLU:CA  | 1:22:A:GLU:C   | 1:23:A:ILE:N  | 20       | 1.81          |
| (1,137) | 1:78:A:ALA:C  | 1:79:A:ILE:N   | 1:79:A:ILE:CA  | 1:79:A:ILE:C  | 9        | 1.8           |
| (1,105) | 1:62:A:ALA:C  | 1:63:A:LYS:N   | 1:63:A:LYS:CA  | 1:63:A:LYS:C  | 11       | 1.8           |
| (1,54)  | 1:30:A:ASP:N  | 1:30:A:ASP:CA  | 1:30:A:ASP:C   | 1:31:A:SER:N  | 11       | 1.8           |
| (1,51)  | 1:28:A:ASP:C  | 1:29:A:ASP:N   | 1:29:A:ASP:CA  | 1:29:A:ASP:C  | 9        | 1.8           |
| (1,11)  | 1:7:A:ARG:C   | 1:8:A:GLN:N    | 1:8:A:GLN:CA   | 1:8:A:GLN:C   | 7        | 1.8           |

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| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,183) | 1:101:A:ILE:C | 1:102:A:ARG:N  | 1:102:A:ARG:CA | 1:102:A:ARG:C | 4        | 1.79          |
| (1,147) | 1:83:A:ASP:C  | 1:84:A:LYS:N   | 1:84:A:LYS:CA  | 1:84:A:LYS:C  | 14       | 1.79          |
| (1,73)  | 1:39:A:ILE:C  | 1:40:A:GLU:N   | 1:40:A:GLU:CA  | 1:40:A:GLU:C  | 7        | 1.79          |
| (1,40)  | 1:23:A:ILE:N  | 1:23:A:ILE:CA  | 1:23:A:ILE:C   | 1:24:A:PHE:N  | 5        | 1.79          |
| (1,36)  | 1:21:A:ARG:N  | 1:21:A:ARG:CA  | 1:21:A:ARG:C   | 1:22:A:GLU:N  | 19       | 1.79          |
| (1,211) | 1:51:A:ASP:N  | 1:51:A:ASP:CA  | 1:51:A:ASP:CB  | 1:51:A:ASP:CG | 16       | 1.78          |
| (1,153) | 1:86:A:SER:C  | 1:87:A:LEU:N   | 1:87:A:LEU:CA  | 1:87:A:LEU:C  | 4        | 1.78          |
| (1,147) | 1:83:A:ASP:C  | 1:84:A:LYS:N   | 1:84:A:LYS:CA  | 1:84:A:LYS:C  | 2        | 1.78          |
| (1,89)  | 1:47:A:ARG:C  | 1:48:A:GLN:N   | 1:48:A:GLN:CA  | 1:48:A:GLN:C  | 13       | 1.78          |
| (1,75)  | 1:40:A:GLU:C  | 1:41:A:GLU:N   | 1:41:A:GLU:CA  | 1:41:A:GLU:C  | 17       | 1.78          |
| (1,65)  | 1:35:A:VAL:C  | 1:36:A:LEU:N   | 1:36:A:LEU:CA  | 1:36:A:LEU:C  | 17       | 1.78          |
| (1,55)  | 1:30:A:ASP:C  | 1:31:A:SER:N   | 1:31:A:SER:CA  | 1:31:A:SER:C  | 20       | 1.78          |
| (1,41)  | 1:23:A:ILE:C  | 1:24:A:PHE:N   | 1:24:A:PHE:CA  | 1:24:A:PHE:C  | 14       | 1.78          |
| (1,40)  | 1:23:A:ILE:N  | 1:23:A:ILE:CA  | 1:23:A:ILE:C   | 1:24:A:PHE:N  | 17       | 1.78          |
| (1,187) | 1:103:A:GLU:C | 1:104:A:LEU:N  | 1:104:A:LEU:CA | 1:104:A:LEU:C | 10       | 1.77          |
| (1,147) | 1:83:A:ASP:C  | 1:84:A:LYS:N   | 1:84:A:LYS:CA  | 1:84:A:LYS:C  | 13       | 1.77          |
| (1,78)  | 1:42:A:LEU:N  | 1:42:A:LEU:CA  | 1:42:A:LEU:C   | 1:43:A:ILE:N  | 2        | 1.77          |
| (1,65)  | 1:35:A:VAL:C  | 1:36:A:LEU:N   | 1:36:A:LEU:CA  | 1:36:A:LEU:C  | 19       | 1.77          |
| (1,51)  | 1:28:A:ASP:C  | 1:29:A:ASP:N   | 1:29:A:ASP:CA  | 1:29:A:ASP:C  | 18       | 1.77          |
| (1,33)  | 1:19:A:ARG:C  | 1:20:A:LEU:N   | 1:20:A:LEU:CA  | 1:20:A:LEU:C  | 6        | 1.77          |
| (1,23)  | 1:14:A:VAL:C  | 1:15:A:GLN:N   | 1:15:A:GLN:CA  | 1:15:A:GLN:C  | 12       | 1.77          |
| (1,134) | 1:77:A:GLU:N  | 1:77:A:GLU:CA  | 1:77:A:GLU:C   | 1:78:A:ALA:N  | 13       | 1.76          |
| (1,93)  | 1:49:A:LEU:C  | 1:50:A:PHE:N   | 1:50:A:PHE:CA  | 1:50:A:PHE:C  | 11       | 1.76          |
| (1,82)  | 1:44:A:GLN:N  | 1:44:A:GLN:CA  | 1:44:A:GLN:C   | 1:45:A:LYS:N  | 4        | 1.76          |
| (1,51)  | 1:28:A:ASP:C  | 1:29:A:ASP:N   | 1:29:A:ASP:CA  | 1:29:A:ASP:C  | 3        | 1.76          |
| (1,17)  | 1:11:A:ASP:C  | 1:12:A:GLU:N   | 1:12:A:GLU:CA  | 1:12:A:GLU:C  | 14       | 1.76          |
| (1,210) | 1:49:A:LEU:N  | 1:49:A:LEU:CA  | 1:49:A:LEU:CB  | 1:49:A:LEU:CG | 13       | 1.75          |
| (1,143) | 1:81:A:LYS:C  | 1:82:A:GLY:N   | 1:82:A:GLY:CA  | 1:82:A:GLY:C  | 16       | 1.75          |
| (1,89)  | 1:47:A:ARG:C  | 1:48:A:GLN:N   | 1:48:A:GLN:CA  | 1:48:A:GLN:C  | 12       | 1.75          |
| (1,78)  | 1:42:A:LEU:N  | 1:42:A:LEU:CA  | 1:42:A:LEU:C   | 1:43:A:ILE:N  | 9        | 1.75          |
| (1,51)  | 1:28:A:ASP:C  | 1:29:A:ASP:N   | 1:29:A:ASP:CA  | 1:29:A:ASP:C  | 4        | 1.75          |
| (1,43)  | 1:24:A:PHE:C  | 1:25:A:ASP:N   | 1:25:A:ASP:CA  | 1:25:A:ASP:C  | 12       | 1.75          |
| (1,37)  | 1:21:A:ARG:C  | 1:22:A:GLU:N   | 1:22:A:GLU:CA  | 1:22:A:GLU:C  | 5        | 1.75          |
| (1,188) | 1:104:A:LEU:N | 1:104:A:LEU:CA | 1:104:A:LEU:C  | 1:105:A:ALA:N | 7        | 1.74          |
| (1,179) | 1:99:A:GLN:C  | 1:100:A:LYS:N  | 1:100:A:LYS:CA | 1:100:A:LYS:C | 10       | 1.74          |
| (1,157) | 1:88:A:GLU:C  | 1:89:A:GLN:N   | 1:89:A:GLN:CA  | 1:89:A:GLN:C  | 20       | 1.74          |
| (1,156) | 1:88:A:GLU:N  | 1:88:A:GLU:CA  | 1:88:A:GLU:C   | 1:89:A:GLN:N  | 11       | 1.74          |
| (1,152) | 1:86:A:SER:N  | 1:86:A:SER:CA  | 1:86:A:SER:C   | 1:87:A:LEU:N  | 15       | 1.74          |
| (1,136) | 1:78:A:ALA:N  | 1:78:A:ALA:CA  | 1:78:A:ALA:C   | 1:79:A:ILE:N  | 4        | 1.74          |
| (1,101) | 1:60:A:GLU:C  | 1:61:A:ALA:N   | 1:61:A:ALA:CA  | 1:61:A:ALA:C  | 10       | 1.74          |
| (1,89)  | 1:47:A:ARG:C  | 1:48:A:GLN:N   | 1:48:A:GLN:CA  | 1:48:A:GLN:C  | 7        | 1.74          |
| (1,157) | 1:88:A:GLU:C  | 1:89:A:GLN:N   | 1:89:A:GLN:CA  | 1:89:A:GLN:C  | 6        | 1.73          |
| (1,100) | 1:60:A:GLU:N  | 1:60:A:GLU:CA  | 1:60:A:GLU:C   | 1:61:A:ALA:N  | 12       | 1.73          |
| (1,64)  | 1:35:A:VAL:N  | 1:35:A:VAL:CA  | 1:35:A:VAL:C   | 1:36:A:LEU:N  | 15       | 1.73          |
| (1,57)  | 1:31:A:SER:C  | 1:32:A:LEU:N   | 1:32:A:LEU:CA  | 1:32:A:LEU:C  | 12       | 1.73          |
| (1,36)  | 1:21:A:ARG:N  | 1:21:A:ARG:CA  | 1:21:A:ARG:C   | 1:22:A:GLU:N  | 16       | 1.73          |
| (1,179) | 1:99:A:GLN:C  | 1:100:A:LYS:N  | 1:100:A:LYS:CA | 1:100:A:LYS:C | 9        | 1.72          |
| (1,102) | 1:61:A:ALA:N  | 1:61:A:ALA:CA  | 1:61:A:ALA:C   | 1:62:A:ALA:N  | 13       | 1.72          |
| (1,78)  | 1:42:A:LEU:N  | 1:42:A:LEU:CA  | 1:42:A:LEU:C   | 1:43:A:ILE:N  | 13       | 1.72          |
| (1,73)  | 1:39:A:ILE:C  | 1:40:A:GLU:N   | 1:40:A:GLU:CA  | 1:40:A:GLU:C  | 1        | 1.72          |
| (1,23)  | 1:14:A:VAL:C  | 1:15:A:GLN:N   | 1:15:A:GLN:CA  | 1:15:A:GLN:C  | 17       | 1.72          |

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| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,202) | 1:28:A:ASP:N  | 1:28:A:ASP:CA  | 1:28:A:ASP:CB  | 1:28:A:ASP:CG | 11       | 1.71          |
| (1,179) | 1:99:A:GLN:C  | 1:100:A:LYS:N  | 1:100:A:LYS:CA | 1:100:A:LYS:C | 11       | 1.71          |
| (1,84)  | 1:45:A:LYS:N  | 1:45:A:LYS:CA  | 1:45:A:LYS:C   | 1:46:A:HIS:N  | 9        | 1.71          |
| (1,47)  | 1:26:A:LYS:C  | 1:27:A:GLY:N   | 1:27:A:GLY:CA  | 1:27:A:GLY:C  | 12       | 1.71          |
| (1,146) | 1:83:A:ASP:N  | 1:83:A:ASP:CA  | 1:83:A:ASP:C   | 1:84:A:LYS:N  | 3        | 1.7           |
| (1,135) | 1:77:A:GLU:C  | 1:78:A:ALA:N   | 1:78:A:ALA:CA  | 1:78:A:ALA:C  | 16       | 1.7           |
| (1,48)  | 1:27:A:GLY:N  | 1:27:A:GLY:CA  | 1:27:A:GLY:C   | 1:28:A:ASP:N  | 13       | 1.7           |
| (1,47)  | 1:26:A:LYS:C  | 1:27:A:GLY:N   | 1:27:A:GLY:CA  | 1:27:A:GLY:C  | 18       | 1.7           |
| (1,182) | 1:101:A:ILE:N | 1:101:A:ILE:CA | 1:101:A:ILE:C  | 1:102:A:ARG:N | 6        | 1.69          |
| (1,72)  | 1:39:A:ILE:N  | 1:39:A:ILE:CA  | 1:39:A:ILE:C   | 1:40:A:GLU:N  | 2        | 1.69          |
| (1,56)  | 1:31:A:SER:N  | 1:31:A:SER:CA  | 1:31:A:SER:C   | 1:32:A:LEU:N  | 2        | 1.69          |
| (1,42)  | 1:24:A:PHE:N  | 1:24:A:PHE:CA  | 1:24:A:PHE:C   | 1:25:A:ASP:N  | 14       | 1.69          |
| (1,39)  | 1:22:A:GLU:C  | 1:23:A:ILE:N   | 1:23:A:ILE:CA  | 1:23:A:ILE:C  | 8        | 1.69          |
| (1,37)  | 1:21:A:ARG:C  | 1:22:A:GLU:N   | 1:22:A:GLU:CA  | 1:22:A:GLU:C  | 18       | 1.69          |
| (1,17)  | 1:11:A:ASP:C  | 1:12:A:GLU:N   | 1:12:A:GLU:CA  | 1:12:A:GLU:C  | 9        | 1.69          |
| (1,152) | 1:86:A:SER:N  | 1:86:A:SER:CA  | 1:86:A:SER:C   | 1:87:A:LEU:N  | 20       | 1.68          |
| (1,112) | 1:66:A:ASP:N  | 1:66:A:ASP:CA  | 1:66:A:ASP:C   | 1:67:A:GLN:N  | 5        | 1.68          |
| (1,54)  | 1:30:A:ASP:N  | 1:30:A:ASP:CA  | 1:30:A:ASP:C   | 1:31:A:SER:N  | 1        | 1.68          |
| (1,170) | 1:95:A:GLU:N  | 1:95:A:GLU:CA  | 1:95:A:GLU:C   | 1:96:A:GLN:N  | 18       | 1.67          |
| (1,147) | 1:83:A:ASP:C  | 1:84:A:LYS:N   | 1:84:A:LYS:CA  | 1:84:A:LYS:C  | 10       | 1.67          |
| (1,42)  | 1:24:A:PHE:N  | 1:24:A:PHE:CA  | 1:24:A:PHE:C   | 1:25:A:ASP:N  | 6        | 1.67          |
| (1,210) | 1:49:A:LEU:N  | 1:49:A:LEU:CA  | 1:49:A:LEU:CB  | 1:49:A:LEU:CG | 7        | 1.66          |
| (1,175) | 1:97:A:ALA:C  | 1:98:A:LEU:N   | 1:98:A:LEU:CA  | 1:98:A:LEU:C  | 3        | 1.66          |
| (1,116) | 1:68:A:TRP:N  | 1:68:A:TRP:CA  | 1:68:A:TRP:C   | 1:69:A:VAL:N  | 15       | 1.66          |
| (1,89)  | 1:47:A:ARG:C  | 1:48:A:GLN:N   | 1:48:A:GLN:CA  | 1:48:A:GLN:C  | 3        | 1.66          |
| (1,82)  | 1:44:A:GLN:N  | 1:44:A:GLN:CA  | 1:44:A:GLN:C   | 1:45:A:LYS:N  | 5        | 1.66          |
| (1,32)  | 1:19:A:ARG:N  | 1:19:A:ARG:CA  | 1:19:A:ARG:C   | 1:20:A:LEU:N  | 6        | 1.66          |
| (1,85)  | 1:45:A:LYS:C  | 1:46:A:HIS:N   | 1:46:A:HIS:CA  | 1:46:A:HIS:C  | 15       | 1.65          |
| (1,84)  | 1:45:A:LYS:N  | 1:45:A:LYS:CA  | 1:45:A:LYS:C   | 1:46:A:HIS:N  | 4        | 1.65          |
| (1,64)  | 1:35:A:VAL:N  | 1:35:A:VAL:CA  | 1:35:A:VAL:C   | 1:36:A:LEU:N  | 9        | 1.65          |
| (1,58)  | 1:32:A:LEU:N  | 1:32:A:LEU:CA  | 1:32:A:LEU:C   | 1:33:A:GLU:N  | 15       | 1.65          |
| (1,48)  | 1:27:A:GLY:N  | 1:27:A:GLY:CA  | 1:27:A:GLY:C   | 1:28:A:ASP:N  | 14       | 1.65          |
| (1,23)  | 1:14:A:VAL:C  | 1:15:A:GLN:N   | 1:15:A:GLN:CA  | 1:15:A:GLN:C  | 5        | 1.65          |
| (1,210) | 1:49:A:LEU:N  | 1:49:A:LEU:CA  | 1:49:A:LEU:CB  | 1:49:A:LEU:CG | 3        | 1.64          |
| (1,209) | 1:46:A:HIS:N  | 1:46:A:HIS:CA  | 1:46:A:HIS:CB  | 1:46:A:HIS:CG | 20       | 1.64          |
| (1,108) | 1:64:A:GLN:N  | 1:64:A:GLN:CA  | 1:64:A:GLN:C   | 1:65:A:GLY:N  | 3        | 1.64          |
| (1,106) | 1:63:A:LYS:N  | 1:63:A:LYS:CA  | 1:63:A:LYS:C   | 1:64:A:GLN:N  | 16       | 1.64          |
| (1,47)  | 1:26:A:LYS:C  | 1:27:A:GLY:N   | 1:27:A:GLY:CA  | 1:27:A:GLY:C  | 4        | 1.64          |
| (1,6)   | 1:5:A:LYS:N   | 1:5:A:LYS:CA   | 1:5:A:LYS:C    | 1:6:A:LEU:N   | 6        | 1.64          |
| (1,204) | 1:30:A:ASP:N  | 1:30:A:ASP:CA  | 1:30:A:ASP:CB  | 1:30:A:ASP:CG | 2        | 1.63          |
| (1,155) | 1:87:A:LEU:C  | 1:88:A:GLU:N   | 1:88:A:GLU:CA  | 1:88:A:GLU:C  | 12       | 1.63          |
| (1,110) | 1:65:A:GLY:N  | 1:65:A:GLY:CA  | 1:65:A:GLY:C   | 1:66:A:ASP:N  | 18       | 1.63          |
| (1,96)  | 1:51:A:ASP:N  | 1:51:A:ASP:CA  | 1:51:A:ASP:C   | 1:52:A:ASN:N  | 7        | 1.63          |
| (1,47)  | 1:26:A:LYS:C  | 1:27:A:GLY:N   | 1:27:A:GLY:CA  | 1:27:A:GLY:C  | 1        | 1.63          |
| (1,28)  | 1:17:A:PHE:N  | 1:17:A:PHE:CA  | 1:17:A:PHE:C   | 1:18:A:GLN:N  | 16       | 1.63          |
| (1,58)  | 1:32:A:LEU:N  | 1:32:A:LEU:CA  | 1:32:A:LEU:C   | 1:33:A:GLU:N  | 13       | 1.62          |
| (1,57)  | 1:31:A:SER:C  | 1:32:A:LEU:N   | 1:32:A:LEU:CA  | 1:32:A:LEU:C  | 20       | 1.62          |
| (1,28)  | 1:17:A:PHE:N  | 1:17:A:PHE:CA  | 1:17:A:PHE:C   | 1:18:A:GLN:N  | 15       | 1.62          |
| (1,184) | 1:102:A:ARG:N | 1:102:A:ARG:CA | 1:102:A:ARG:C  | 1:103:A:GLU:N | 10       | 1.61          |
| (1,170) | 1:95:A:GLU:N  | 1:95:A:GLU:CA  | 1:95:A:GLU:C   | 1:96:A:GLN:N  | 20       | 1.61          |
| (1,100) | 1:60:A:GLU:N  | 1:60:A:GLU:CA  | 1:60:A:GLU:C   | 1:61:A:ALA:N  | 13       | 1.61          |

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| Key     | Atom-1        | Atom-2         | Atom-3        | Atom-4         | Model ID | Violation (°) |
|---------|---------------|----------------|---------------|----------------|----------|---------------|
| (1,99)  | 1:59:A:THR:C  | 1:60:A:GLU:N   | 1:60:A:GLU:CA | 1:60:A:GLU:C   | 15       | 1.61          |
| (1,37)  | 1:21:A:ARG:C  | 1:22:A:GLU:N   | 1:22:A:GLU:CA | 1:22:A:GLU:C   | 17       | 1.61          |
| (1,32)  | 1:19:A:ARG:N  | 1:19:A:ARG:CA  | 1:19:A:ARG:C  | 1:20:A:LEU:N   | 18       | 1.61          |
| (1,216) | 1:68:A:TRP:N  | 1:68:A:TRP:CA  | 1:68:A:TRP:CB | 1:68:A:TRP:CG  | 10       | 1.6           |
| (1,203) | 1:29:A:ASP:N  | 1:29:A:ASP:CA  | 1:29:A:ASP:CB | 1:29:A:ASP:CG  | 8        | 1.6           |
| (1,170) | 1:95:A:GLU:N  | 1:95:A:GLU:CA  | 1:95:A:GLU:C  | 1:96:A:GLN:N   | 6        | 1.6           |
| (1,154) | 1:87:A:LEU:N  | 1:87:A:LEU:CA  | 1:87:A:LEU:C  | 1:88:A:GLU:N   | 9        | 1.6           |
| (1,84)  | 1:45:A:LYS:N  | 1:45:A:LYS:CA  | 1:45:A:LYS:C  | 1:46:A:HIS:N   | 17       | 1.6           |
| (1,51)  | 1:28:A:ASP:C  | 1:29:A:ASP:N   | 1:29:A:ASP:CA | 1:29:A:ASP:C   | 6        | 1.6           |
| (1,39)  | 1:22:A:GLU:C  | 1:23:A:ILE:N   | 1:23:A:ILE:CA | 1:23:A:ILE:C   | 14       | 1.6           |
| (1,37)  | 1:21:A:ARG:C  | 1:22:A:GLU:N   | 1:22:A:GLU:CA | 1:22:A:GLU:C   | 8        | 1.6           |
| (1,198) | 1:23:A:ILE:N  | 1:23:A:ILE:CA  | 1:23:A:ILE:CB | 1:23:A:ILE:CG1 | 11       | 1.59          |
| (1,58)  | 1:32:A:LEU:N  | 1:32:A:LEU:CA  | 1:32:A:LEU:C  | 1:33:A:GLU:N   | 19       | 1.59          |
| (1,37)  | 1:21:A:ARG:C  | 1:22:A:GLU:N   | 1:22:A:GLU:CA | 1:22:A:GLU:C   | 2        | 1.59          |
| (1,150) | 1:85:A:ASP:N  | 1:85:A:ASP:CA  | 1:85:A:ASP:C  | 1:86:A:SER:N   | 3        | 1.57          |
| (1,90)  | 1:48:A:GLN:N  | 1:48:A:GLN:CA  | 1:48:A:GLN:C  | 1:49:A:LEU:N   | 7        | 1.57          |
| (1,65)  | 1:35:A:VAL:C  | 1:36:A:LEU:N   | 1:36:A:LEU:CA | 1:36:A:LEU:C   | 9        | 1.57          |
| (1,48)  | 1:27:A:GLY:N  | 1:27:A:GLY:CA  | 1:27:A:GLY:C  | 1:28:A:ASP:N   | 6        | 1.57          |
| (1,26)  | 1:16:A:ALA:N  | 1:16:A:ALA:CA  | 1:16:A:ALA:C  | 1:17:A:PHE:N   | 16       | 1.57          |
| (1,19)  | 1:12:A:GLU:C  | 1:13:A:LEU:N   | 1:13:A:LEU:CA | 1:13:A:LEU:C   | 18       | 1.57          |
| (1,19)  | 1:12:A:GLU:C  | 1:13:A:LEU:N   | 1:13:A:LEU:CA | 1:13:A:LEU:C   | 20       | 1.57          |
| (1,137) | 1:78:A:ALA:C  | 1:79:A:ILE:N   | 1:79:A:ILE:CA | 1:79:A:ILE:C   | 1        | 1.56          |
| (1,85)  | 1:45:A:LYS:C  | 1:46:A:HIS:N   | 1:46:A:HIS:CA | 1:46:A:HIS:C   | 16       | 1.56          |
| (1,82)  | 1:44:A:GLN:N  | 1:44:A:GLN:CA  | 1:44:A:GLN:C  | 1:45:A:LYS:N   | 3        | 1.56          |
| (1,32)  | 1:19:A:ARG:N  | 1:19:A:ARG:CA  | 1:19:A:ARG:C  | 1:20:A:LEU:N   | 11       | 1.56          |
| (1,23)  | 1:14:A:VAL:C  | 1:15:A:GLN:N   | 1:15:A:GLN:CA | 1:15:A:GLN:C   | 1        | 1.56          |
| (1,22)  | 1:14:A:VAL:N  | 1:14:A:VAL:CA  | 1:14:A:VAL:C  | 1:15:A:GLN:N   | 9        | 1.56          |
| (1,80)  | 1:43:A:ILE:N  | 1:43:A:ILE:CA  | 1:43:A:ILE:C  | 1:44:A:GLN:N   | 4        | 1.55          |
| (1,78)  | 1:42:A:LEU:N  | 1:42:A:LEU:CA  | 1:42:A:LEU:C  | 1:43:A:ILE:N   | 16       | 1.55          |
| (1,224) | 1:85:A:ASP:N  | 1:85:A:ASP:CA  | 1:85:A:ASP:CB | 1:85:A:ASP:CG  | 11       | 1.54          |
| (1,116) | 1:68:A:TRP:N  | 1:68:A:TRP:CA  | 1:68:A:TRP:C  | 1:69:A:VAL:N   | 5        | 1.54          |
| (1,89)  | 1:47:A:ARG:C  | 1:48:A:GLN:N   | 1:48:A:GLN:CA | 1:48:A:GLN:C   | 15       | 1.54          |
| (1,43)  | 1:24:A:PHE:C  | 1:25:A:ASP:N   | 1:25:A:ASP:CA | 1:25:A:ASP:C   | 13       | 1.54          |
| (1,8)   | 1:6:A:LEU:N   | 1:6:A:LEU:CA   | 1:6:A:LEU:C   | 1:7:A:ARG:N    | 8        | 1.54          |
| (1,49)  | 1:27:A:GLY:C  | 1:28:A:ASP:N   | 1:28:A:ASP:CA | 1:28:A:ASP:C   | 13       | 1.53          |
| (1,170) | 1:95:A:GLU:N  | 1:95:A:GLU:CA  | 1:95:A:GLU:C  | 1:96:A:GLN:N   | 15       | 1.52          |
| (1,157) | 1:88:A:GLU:C  | 1:89:A:GLN:N   | 1:89:A:GLN:CA | 1:89:A:GLN:C   | 2        | 1.52          |
| (1,110) | 1:65:A:GLY:N  | 1:65:A:GLY:CA  | 1:65:A:GLY:C  | 1:66:A:ASP:N   | 16       | 1.52          |
| (1,72)  | 1:39:A:ILE:N  | 1:39:A:ILE:CA  | 1:39:A:ILE:C  | 1:40:A:GLU:N   | 17       | 1.52          |
| (1,152) | 1:86:A:SER:N  | 1:86:A:SER:CA  | 1:86:A:SER:C  | 1:87:A:LEU:N   | 13       | 1.51          |
| (1,88)  | 1:47:A:ARG:N  | 1:47:A:ARG:CA  | 1:47:A:ARG:C  | 1:48:A:GLN:N   | 12       | 1.51          |
| (1,48)  | 1:27:A:GLY:N  | 1:27:A:GLY:CA  | 1:27:A:GLY:C  | 1:28:A:ASP:N   | 19       | 1.51          |
| (1,22)  | 1:14:A:VAL:N  | 1:14:A:VAL:CA  | 1:14:A:VAL:C  | 1:15:A:GLN:N   | 6        | 1.51          |
| (1,216) | 1:68:A:TRP:N  | 1:68:A:TRP:CA  | 1:68:A:TRP:CB | 1:68:A:TRP:CG  | 16       | 1.5           |
| (1,182) | 1:101:A:ILE:N | 1:101:A:ILE:CA | 1:101:A:ILE:C | 1:102:A:ARG:N  | 13       | 1.5           |
| (1,175) | 1:97:A:ALA:C  | 1:98:A:LEU:N   | 1:98:A:LEU:CA | 1:98:A:LEU:C   | 11       | 1.5           |
| (1,143) | 1:81:A:LYS:C  | 1:82:A:GLY:N   | 1:82:A:GLY:CA | 1:82:A:GLY:C   | 6        | 1.5           |
| (1,106) | 1:63:A:LYS:N  | 1:63:A:LYS:CA  | 1:63:A:LYS:C  | 1:64:A:GLN:N   | 14       | 1.5           |
| (1,51)  | 1:28:A:ASP:C  | 1:29:A:ASP:N   | 1:29:A:ASP:CA | 1:29:A:ASP:C   | 13       | 1.5           |
| (1,26)  | 1:16:A:ALA:N  | 1:16:A:ALA:CA  | 1:16:A:ALA:C  | 1:17:A:PHE:N   | 12       | 1.5           |
| (1,26)  | 1:16:A:ALA:N  | 1:16:A:ALA:CA  | 1:16:A:ALA:C  | 1:17:A:PHE:N   | 20       | 1.5           |

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| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4         | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|----------------|----------|---------------|
| (1,24)  | 1:15:A:GLN:N  | 1:15:A:GLN:CA  | 1:15:A:GLN:C   | 1:16:A:ALA:N   | 11       | 1.5           |
| (1,158) | 1:89:A:GLN:N  | 1:89:A:GLN:CA  | 1:89:A:GLN:C   | 1:90:A:LEU:N   | 17       | 1.49          |
| (1,153) | 1:86:A:SER:C  | 1:87:A:LEU:N   | 1:87:A:LEU:CA  | 1:87:A:LEU:C   | 15       | 1.49          |
| (1,132) | 1:76:A:ARG:N  | 1:76:A:ARG:CA  | 1:76:A:ARG:C   | 1:77:A:GLU:N   | 1        | 1.49          |
| (1,73)  | 1:39:A:ILE:C  | 1:40:A:GLU:N   | 1:40:A:GLU:CA  | 1:40:A:GLU:C   | 14       | 1.49          |
| (1,32)  | 1:19:A:ARG:N  | 1:19:A:ARG:CA  | 1:19:A:ARG:C   | 1:20:A:LEU:N   | 9        | 1.49          |
| (1,202) | 1:28:A:ASP:N  | 1:28:A:ASP:CA  | 1:28:A:ASP:CB  | 1:28:A:ASP:CG  | 4        | 1.48          |
| (1,152) | 1:86:A:SER:N  | 1:86:A:SER:CA  | 1:86:A:SER:C   | 1:87:A:LEU:N   | 14       | 1.48          |
| (1,83)  | 1:44:A:GLN:C  | 1:45:A:LYS:N   | 1:45:A:LYS:CA  | 1:45:A:LYS:C   | 7        | 1.48          |
| (1,216) | 1:68:A:TRP:N  | 1:68:A:TRP:CA  | 1:68:A:TRP:CB  | 1:68:A:TRP:CG  | 13       | 1.47          |
| (1,201) | 1:26:A:LYS:N  | 1:26:A:LYS:CA  | 1:26:A:LYS:CB  | 1:26:A:LYS:CG  | 7        | 1.47          |
| (1,216) | 1:68:A:TRP:N  | 1:68:A:TRP:CA  | 1:68:A:TRP:CB  | 1:68:A:TRP:CG  | 6        | 1.46          |
| (1,216) | 1:68:A:TRP:N  | 1:68:A:TRP:CA  | 1:68:A:TRP:CB  | 1:68:A:TRP:CG  | 18       | 1.46          |
| (1,187) | 1:103:A:GLU:C | 1:104:A:LEU:N  | 1:104:A:LEU:CA | 1:104:A:LEU:C  | 19       | 1.46          |
| (1,182) | 1:101:A:ILE:N | 1:101:A:ILE:CA | 1:101:A:ILE:C  | 1:102:A:ARG:N  | 12       | 1.46          |
| (1,170) | 1:95:A:GLU:N  | 1:95:A:GLU:CA  | 1:95:A:GLU:C   | 1:96:A:GLN:N   | 7        | 1.46          |
| (1,137) | 1:78:A:ALA:C  | 1:79:A:ILE:N   | 1:79:A:ILE:CA  | 1:79:A:ILE:C   | 15       | 1.46          |
| (1,112) | 1:66:A:ASP:N  | 1:66:A:ASP:CA  | 1:66:A:ASP:C   | 1:67:A:GLN:N   | 14       | 1.46          |
| (1,105) | 1:62:A:ALA:C  | 1:63:A:LYS:N   | 1:63:A:LYS:CA  | 1:63:A:LYS:C   | 14       | 1.46          |
| (1,78)  | 1:42:A:LEU:N  | 1:42:A:LEU:CA  | 1:42:A:LEU:C   | 1:43:A:ILE:N   | 12       | 1.46          |
| (1,39)  | 1:22:A:GLU:C  | 1:23:A:ILE:N   | 1:23:A:ILE:CA  | 1:23:A:ILE:C   | 7        | 1.46          |
| (1,13)  | 1:8:A:GLN:C   | 1:9:A:THR:N    | 1:9:A:THR:CA   | 1:9:A:THR:C    | 16       | 1.46          |
| (1,11)  | 1:7:A:ARG:C   | 1:8:A:GLN:N    | 1:8:A:GLN:CA   | 1:8:A:GLN:C    | 11       | 1.46          |
| (1,208) | 1:44:A:GLN:N  | 1:44:A:GLN:CA  | 1:44:A:GLN:CB  | 1:44:A:GLN:CG  | 6        | 1.45          |
| (1,100) | 1:60:A:GLU:N  | 1:60:A:GLU:CA  | 1:60:A:GLU:C   | 1:61:A:ALA:N   | 6        | 1.45          |
| (1,92)  | 1:49:A:LEU:N  | 1:49:A:LEU:CA  | 1:49:A:LEU:C   | 1:50:A:PHE:N   | 14       | 1.45          |
| (1,221) | 1:80:A:ASP:N  | 1:80:A:ASP:CA  | 1:80:A:ASP:CB  | 1:80:A:ASP:CG  | 10       | 1.43          |
| (1,114) | 1:67:A:GLN:N  | 1:67:A:GLN:CA  | 1:67:A:GLN:C   | 1:68:A:TRP:N   | 14       | 1.43          |
| (1,82)  | 1:44:A:GLN:N  | 1:44:A:GLN:CA  | 1:44:A:GLN:C   | 1:45:A:LYS:N   | 14       | 1.43          |
| (1,76)  | 1:41:A:GLU:N  | 1:41:A:GLU:CA  | 1:41:A:GLU:C   | 1:42:A:LEU:N   | 3        | 1.43          |
| (1,10)  | 1:7:A:ARG:N   | 1:7:A:ARG:CA   | 1:7:A:ARG:C    | 1:8:A:GLN:N    | 7        | 1.43          |
| (1,224) | 1:85:A:ASP:N  | 1:85:A:ASP:CA  | 1:85:A:ASP:CB  | 1:85:A:ASP:CG  | 6        | 1.42          |
| (1,188) | 1:104:A:LEU:N | 1:104:A:LEU:CA | 1:104:A:LEU:C  | 1:105:A:ALA:N  | 17       | 1.42          |
| (1,153) | 1:86:A:SER:C  | 1:87:A:LEU:N   | 1:87:A:LEU:CA  | 1:87:A:LEU:C   | 13       | 1.42          |
| (1,134) | 1:77:A:GLU:N  | 1:77:A:GLU:CA  | 1:77:A:GLU:C   | 1:78:A:ALA:N   | 19       | 1.42          |
| (1,130) | 1:75:A:PHE:N  | 1:75:A:PHE:CA  | 1:75:A:PHE:C   | 1:76:A:ARG:N   | 8        | 1.42          |
| (1,116) | 1:68:A:TRP:N  | 1:68:A:TRP:CA  | 1:68:A:TRP:C   | 1:69:A:VAL:N   | 6        | 1.42          |
| (1,79)  | 1:42:A:LEU:C  | 1:43:A:ILE:N   | 1:43:A:ILE:CA  | 1:43:A:ILE:C   | 11       | 1.42          |
| (1,72)  | 1:39:A:ILE:N  | 1:39:A:ILE:CA  | 1:39:A:ILE:C   | 1:40:A:GLU:N   | 8        | 1.42          |
| (1,65)  | 1:35:A:VAL:C  | 1:36:A:LEU:N   | 1:36:A:LEU:CA  | 1:36:A:LEU:C   | 18       | 1.42          |
| (1,220) | 1:79:A:ILE:N  | 1:79:A:ILE:CA  | 1:79:A:ILE:CB  | 1:79:A:ILE:CG1 | 5        | 1.41          |
| (1,154) | 1:87:A:LEU:N  | 1:87:A:LEU:CA  | 1:87:A:LEU:C   | 1:88:A:GLU:N   | 6        | 1.41          |
| (1,114) | 1:67:A:GLN:N  | 1:67:A:GLN:CA  | 1:67:A:GLN:C   | 1:68:A:TRP:N   | 11       | 1.41          |
| (1,72)  | 1:39:A:ILE:N  | 1:39:A:ILE:CA  | 1:39:A:ILE:C   | 1:40:A:GLU:N   | 20       | 1.41          |
| (1,58)  | 1:32:A:LEU:N  | 1:32:A:LEU:CA  | 1:32:A:LEU:C   | 1:33:A:GLU:N   | 16       | 1.41          |
| (1,23)  | 1:14:A:VAL:C  | 1:15:A:GLN:N   | 1:15:A:GLN:CA  | 1:15:A:GLN:C   | 4        | 1.41          |
| (1,158) | 1:89:A:GLN:N  | 1:89:A:GLN:CA  | 1:89:A:GLN:C   | 1:90:A:LEU:N   | 18       | 1.4           |
| (1,108) | 1:64:A:GLN:N  | 1:64:A:GLN:CA  | 1:64:A:GLN:C   | 1:65:A:GLY:N   | 14       | 1.4           |
| (1,59)  | 1:32:A:LEU:C  | 1:33:A:GLU:N   | 1:33:A:GLU:CA  | 1:33:A:GLU:C   | 11       | 1.4           |
| (1,51)  | 1:28:A:ASP:C  | 1:29:A:ASP:N   | 1:29:A:ASP:CA  | 1:29:A:ASP:C   | 7        | 1.4           |
| (1,189) | 1:104:A:LEU:C | 1:105:A:ALA:N  | 1:105:A:ALA:CA | 1:105:A:ALA:C  | 12       | 1.39          |

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| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4          | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|-----------------|----------|---------------|
| (1,158) | 1:89:A:GLN:N  | 1:89:A:GLN:CA  | 1:89:A:GLN:C   | 1:90:A:LEU:N    | 6        | 1.39          |
| (1,154) | 1:87:A:LEU:N  | 1:87:A:LEU:CA  | 1:87:A:LEU:C   | 1:88:A:GLU:N    | 13       | 1.39          |
| (1,116) | 1:68:A:TRP:N  | 1:68:A:TRP:CA  | 1:68:A:TRP:C   | 1:69:A:VAL:N    | 20       | 1.39          |
| (1,88)  | 1:47:A:ARG:N  | 1:47:A:ARG:CA  | 1:47:A:ARG:C   | 1:48:A:GLN:N    | 16       | 1.39          |
| (1,51)  | 1:28:A:ASP:C  | 1:29:A:ASP:N   | 1:29:A:ASP:CA  | 1:29:A:ASP:C    | 19       | 1.39          |
| (1,41)  | 1:23:A:ILE:C  | 1:24:A:PHE:N   | 1:24:A:PHE:CA  | 1:24:A:PHE:C    | 5        | 1.39          |
| (1,228) | 1:104:A:LEU:N | 1:104:A:LEU:CA | 1:104:A:LEU:CB | 1:104:A:LEU:CG  | 16       | 1.38          |
| (1,220) | 1:79:A:ILE:N  | 1:79:A:ILE:CA  | 1:79:A:ILE:CB  | 1:79:A:ILE:CG1  | 2        | 1.38          |
| (1,175) | 1:97:A:ALA:C  | 1:98:A:LEU:N   | 1:98:A:LEU:CA  | 1:98:A:LEU:C    | 18       | 1.38          |
| (1,155) | 1:87:A:LEU:C  | 1:88:A:GLU:N   | 1:88:A:GLU:CA  | 1:88:A:GLU:C    | 5        | 1.38          |
| (1,153) | 1:86:A:SER:C  | 1:87:A:LEU:N   | 1:87:A:LEU:CA  | 1:87:A:LEU:C    | 20       | 1.38          |
| (1,133) | 1:76:A:ARG:C  | 1:77:A:GLU:N   | 1:77:A:GLU:CA  | 1:77:A:GLU:C    | 9        | 1.38          |
| (1,130) | 1:75:A:PHE:N  | 1:75:A:PHE:CA  | 1:75:A:PHE:C   | 1:76:A:ARG:N    | 18       | 1.38          |
| (1,117) | 1:68:A:TRP:C  | 1:69:A:VAL:N   | 1:69:A:VAL:CA  | 1:69:A:VAL:C    | 10       | 1.38          |
| (1,72)  | 1:39:A:ILE:N  | 1:39:A:ILE:CA  | 1:39:A:ILE:C   | 1:40:A:GLU:N    | 12       | 1.38          |
| (1,56)  | 1:31:A:SER:N  | 1:31:A:SER:CA  | 1:31:A:SER:C   | 1:32:A:LEU:N    | 10       | 1.38          |
| (1,43)  | 1:24:A:PHE:C  | 1:25:A:ASP:N   | 1:25:A:ASP:CA  | 1:25:A:ASP:C    | 18       | 1.38          |
| (1,19)  | 1:12:A:GLU:C  | 1:13:A:LEU:N   | 1:13:A:LEU:CA  | 1:13:A:LEU:C    | 9        | 1.38          |
| (1,179) | 1:99:A:GLN:C  | 1:100:A:LYS:N  | 1:100:A:LYS:CA | 1:100:A:LYS:C   | 1        | 1.37          |
| (1,114) | 1:67:A:GLN:N  | 1:67:A:GLN:CA  | 1:67:A:GLN:C   | 1:68:A:TRP:N    | 18       | 1.37          |
| (1,113) | 1:66:A:ASP:C  | 1:67:A:GLN:N   | 1:67:A:GLN:CA  | 1:67:A:GLN:C    | 14       | 1.37          |
| (1,100) | 1:60:A:GLU:N  | 1:60:A:GLU:CA  | 1:60:A:GLU:C   | 1:61:A:ALA:N    | 15       | 1.37          |
| (1,84)  | 1:45:A:LYS:N  | 1:45:A:LYS:CA  | 1:45:A:LYS:C   | 1:46:A:HIS:N    | 7        | 1.37          |
| (1,56)  | 1:31:A:SER:N  | 1:31:A:SER:CA  | 1:31:A:SER:C   | 1:32:A:LEU:N    | 15       | 1.37          |
| (1,17)  | 1:11:A:ASP:C  | 1:12:A:GLU:N   | 1:12:A:GLU:CA  | 1:12:A:GLU:C    | 5        | 1.37          |
| (1,193) | 1:9:A:THR:N   | 1:9:A:THR:CA   | 1:9:A:THR:CB   | 1:9:A:THR:OG1   | 6        | 1.36          |
| (1,186) | 1:103:A:GLU:N | 1:103:A:GLU:CA | 1:103:A:GLU:C  | 1:104:A:LEU:N   | 19       | 1.36          |
| (1,64)  | 1:35:A:VAL:N  | 1:35:A:VAL:CA  | 1:35:A:VAL:C   | 1:36:A:LEU:N    | 3        | 1.36          |
| (1,124) | 1:72:A:PHE:N  | 1:72:A:PHE:CA  | 1:72:A:PHE:C   | 1:73:A:GLN:N    | 5        | 1.35          |
| (1,116) | 1:68:A:TRP:N  | 1:68:A:TRP:CA  | 1:68:A:TRP:C   | 1:69:A:VAL:N    | 10       | 1.35          |
| (1,90)  | 1:48:A:GLN:N  | 1:48:A:GLN:CA  | 1:48:A:GLN:C   | 1:49:A:LEU:N    | 8        | 1.35          |
| (1,84)  | 1:45:A:LYS:N  | 1:45:A:LYS:CA  | 1:45:A:LYS:C   | 1:46:A:HIS:N    | 3        | 1.35          |
| (1,65)  | 1:35:A:VAL:C  | 1:36:A:LEU:N   | 1:36:A:LEU:CA  | 1:36:A:LEU:C    | 4        | 1.35          |
| (1,206) | 1:39:A:ILE:N  | 1:39:A:ILE:CA  | 1:39:A:ILE:CB  | 1:39:A:ILE:CG1  | 6        | 1.34          |
| (1,179) | 1:99:A:GLN:C  | 1:100:A:LYS:N  | 1:100:A:LYS:CA | 1:100:A:LYS:C   | 16       | 1.34          |
| (1,105) | 1:62:A:ALA:C  | 1:63:A:LYS:N   | 1:63:A:LYS:CA  | 1:63:A:LYS:C    | 10       | 1.34          |
| (1,101) | 1:60:A:GLU:C  | 1:61:A:ALA:N   | 1:61:A:ALA:CA  | 1:61:A:ALA:C    | 9        | 1.34          |
| (1,78)  | 1:42:A:LEU:N  | 1:42:A:LEU:CA  | 1:42:A:LEU:C   | 1:43:A:ILE:N    | 19       | 1.34          |
| (1,228) | 1:104:A:LEU:N | 1:104:A:LEU:CA | 1:104:A:LEU:CB | 1:104:A:LEU:CG  | 8        | 1.33          |
| (1,227) | 1:101:A:ILE:N | 1:101:A:ILE:CA | 1:101:A:ILE:CB | 1:101:A:ILE:CG1 | 10       | 1.33          |
| (1,227) | 1:101:A:ILE:N | 1:101:A:ILE:CA | 1:101:A:ILE:CB | 1:101:A:ILE:CG1 | 12       | 1.33          |
| (1,210) | 1:49:A:LEU:N  | 1:49:A:LEU:CA  | 1:49:A:LEU:CB  | 1:49:A:LEU:CG   | 4        | 1.33          |
| (1,202) | 1:28:A:ASP:N  | 1:28:A:ASP:CA  | 1:28:A:ASP:CB  | 1:28:A:ASP:CG   | 14       | 1.33          |
| (1,186) | 1:103:A:GLU:N | 1:103:A:GLU:CA | 1:103:A:GLU:C  | 1:104:A:LEU:N   | 3        | 1.33          |
| (1,156) | 1:88:A:GLU:N  | 1:88:A:GLU:CA  | 1:88:A:GLU:C   | 1:89:A:GLN:N    | 7        | 1.33          |
| (1,89)  | 1:47:A:ARG:C  | 1:48:A:GLN:N   | 1:48:A:GLN:CA  | 1:48:A:GLN:C    | 5        | 1.33          |
| (1,42)  | 1:24:A:PHE:N  | 1:24:A:PHE:CA  | 1:24:A:PHE:C   | 1:25:A:ASP:N    | 10       | 1.33          |
| (1,23)  | 1:14:A:VAL:C  | 1:15:A:GLN:N   | 1:15:A:GLN:CA  | 1:15:A:GLN:C    | 11       | 1.33          |
| (1,19)  | 1:12:A:GLU:C  | 1:13:A:LEU:N   | 1:13:A:LEU:CA  | 1:13:A:LEU:C    | 2        | 1.33          |
| (1,223) | 1:83:A:ASP:N  | 1:83:A:ASP:CA  | 1:83:A:ASP:CB  | 1:83:A:ASP:CG   | 20       | 1.32          |
| (1,183) | 1:101:A:ILE:C | 1:102:A:ARG:N  | 1:102:A:ARG:CA | 1:102:A:ARG:C   | 11       | 1.32          |

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| Key     | Atom-1        | Atom-2        | Atom-3         | Atom-4         | Model ID | Violation (°) |
|---------|---------------|---------------|----------------|----------------|----------|---------------|
| (1,175) | 1:97:A:ALA:C  | 1:98:A:LEU:N  | 1:98:A:LEU:CA  | 1:98:A:LEU:C   | 6        | 1.32          |
| (1,165) | 1:92:A:GLU:C  | 1:93:A:GLU:N  | 1:93:A:GLU:CA  | 1:93:A:GLU:C   | 7        | 1.32          |
| (1,155) | 1:87:A:LEU:C  | 1:88:A:GLU:N  | 1:88:A:GLU:CA  | 1:88:A:GLU:C   | 9        | 1.32          |
| (1,117) | 1:68:A:TRP:C  | 1:69:A:VAL:N  | 1:69:A:VAL:CA  | 1:69:A:VAL:C   | 3        | 1.32          |
| (1,82)  | 1:44:A:GLN:N  | 1:44:A:GLN:CA | 1:44:A:GLN:C   | 1:45:A:LYS:N   | 16       | 1.32          |
| (1,65)  | 1:35:A:VAL:C  | 1:36:A:LEU:N  | 1:36:A:LEU:CA  | 1:36:A:LEU:C   | 1        | 1.32          |
| (1,63)  | 1:34:A:GLN:C  | 1:35:A:VAL:N  | 1:35:A:VAL:CA  | 1:35:A:VAL:C   | 6        | 1.32          |
| (1,62)  | 1:34:A:GLN:N  | 1:34:A:GLN:CA | 1:34:A:GLN:C   | 1:35:A:VAL:N   | 15       | 1.32          |
| (1,28)  | 1:17:A:PHE:N  | 1:17:A:PHE:CA | 1:17:A:PHE:C   | 1:18:A:GLN:N   | 2        | 1.32          |
| (1,189) | 1:104:A:LEU:C | 1:105:A:ALA:N | 1:105:A:ALA:CA | 1:105:A:ALA:C  | 7        | 1.31          |
| (1,153) | 1:86:A:SER:C  | 1:87:A:LEU:N  | 1:87:A:LEU:CA  | 1:87:A:LEU:C   | 11       | 1.31          |
| (1,144) | 1:82:A:GLY:N  | 1:82:A:GLY:CA | 1:82:A:GLY:C   | 1:83:A:ASP:N   | 16       | 1.31          |
| (1,118) | 1:69:A:VAL:N  | 1:69:A:VAL:CA | 1:69:A:VAL:C   | 1:70:A:GLN:N   | 5        | 1.31          |
| (1,102) | 1:61:A:ALA:N  | 1:61:A:ALA:CA | 1:61:A:ALA:C   | 1:62:A:ALA:N   | 6        | 1.31          |
| (1,38)  | 1:22:A:GLU:N  | 1:22:A:GLU:CA | 1:22:A:GLU:C   | 1:23:A:ILE:N   | 8        | 1.31          |
| (1,9)   | 1:6:A:LEU:C   | 1:7:A:ARG:N   | 1:7:A:ARG:CA   | 1:7:A:ARG:C    | 18       | 1.31          |
| (1,175) | 1:97:A:ALA:C  | 1:98:A:LEU:N  | 1:98:A:LEU:CA  | 1:98:A:LEU:C   | 19       | 1.3           |
| (1,150) | 1:85:A:ASP:N  | 1:85:A:ASP:CA | 1:85:A:ASP:C   | 1:86:A:SER:N   | 20       | 1.3           |
| (1,146) | 1:83:A:ASP:N  | 1:83:A:ASP:CA | 1:83:A:ASP:C   | 1:84:A:LYS:N   | 7        | 1.3           |
| (1,119) | 1:69:A:VAL:C  | 1:70:A:GLN:N  | 1:70:A:GLN:CA  | 1:70:A:GLN:C   | 1        | 1.3           |
| (1,110) | 1:65:A:GLY:N  | 1:65:A:GLY:CA | 1:65:A:GLY:C   | 1:66:A:ASP:N   | 10       | 1.3           |
| (1,110) | 1:65:A:GLY:N  | 1:65:A:GLY:CA | 1:65:A:GLY:C   | 1:66:A:ASP:N   | 14       | 1.3           |
| (1,95)  | 1:50:A:PHE:C  | 1:51:A:ASP:N  | 1:51:A:ASP:CA  | 1:51:A:ASP:C   | 18       | 1.3           |
| (1,79)  | 1:42:A:LEU:C  | 1:43:A:ILE:N  | 1:43:A:ILE:CA  | 1:43:A:ILE:C   | 15       | 1.3           |
| (1,66)  | 1:36:A:LEU:N  | 1:36:A:LEU:CA | 1:36:A:LEU:C   | 1:37:A:GLU:N   | 4        | 1.3           |
| (1,28)  | 1:17:A:PHE:N  | 1:17:A:PHE:CA | 1:17:A:PHE:C   | 1:18:A:GLN:N   | 20       | 1.3           |
| (1,220) | 1:79:A:ILE:N  | 1:79:A:ILE:CA | 1:79:A:ILE:CB  | 1:79:A:ILE:CG1 | 15       | 1.29          |
| (1,219) | 1:75:A:PHE:N  | 1:75:A:PHE:CA | 1:75:A:PHE:CB  | 1:75:A:PHE:CG  | 5        | 1.29          |
| (1,200) | 1:25:A:ASP:N  | 1:25:A:ASP:CA | 1:25:A:ASP:CB  | 1:25:A:ASP:CG  | 6        | 1.29          |
| (1,171) | 1:95:A:GLU:C  | 1:96:A:GLN:N  | 1:96:A:GLN:CA  | 1:96:A:GLN:C   | 17       | 1.29          |
| (1,155) | 1:87:A:LEU:C  | 1:88:A:GLU:N  | 1:88:A:GLU:CA  | 1:88:A:GLU:C   | 19       | 1.29          |
| (1,143) | 1:81:A:LYS:C  | 1:82:A:GLY:N  | 1:82:A:GLY:CA  | 1:82:A:GLY:C   | 13       | 1.29          |
| (1,135) | 1:77:A:GLU:C  | 1:78:A:ALA:N  | 1:78:A:ALA:CA  | 1:78:A:ALA:C   | 7        | 1.29          |
| (1,110) | 1:65:A:GLY:N  | 1:65:A:GLY:CA | 1:65:A:GLY:C   | 1:66:A:ASP:N   | 2        | 1.29          |
| (1,78)  | 1:42:A:LEU:N  | 1:42:A:LEU:CA | 1:42:A:LEU:C   | 1:43:A:ILE:N   | 5        | 1.29          |
| (1,55)  | 1:30:A:ASP:C  | 1:31:A:SER:N  | 1:31:A:SER:CA  | 1:31:A:SER:C   | 5        | 1.29          |
| (1,36)  | 1:21:A:ARG:N  | 1:21:A:ARG:CA | 1:21:A:ARG:C   | 1:22:A:GLU:N   | 12       | 1.29          |
| (1,33)  | 1:19:A:ARG:C  | 1:20:A:LEU:N  | 1:20:A:LEU:CA  | 1:20:A:LEU:C   | 13       | 1.29          |
| (1,155) | 1:87:A:LEU:C  | 1:88:A:GLU:N  | 1:88:A:GLU:CA  | 1:88:A:GLU:C   | 8        | 1.28          |
| (1,106) | 1:63:A:LYS:N  | 1:63:A:LYS:CA | 1:63:A:LYS:C   | 1:64:A:GLN:N   | 5        | 1.28          |
| (1,12)  | 1:8:A:GLN:N   | 1:8:A:GLN:CA  | 1:8:A:GLN:C    | 1:9:A:THR:N    | 18       | 1.28          |
| (1,206) | 1:39:A:ILE:N  | 1:39:A:ILE:CA | 1:39:A:ILE:CB  | 1:39:A:ILE:CG1 | 20       | 1.27          |
| (1,179) | 1:99:A:GLN:C  | 1:100:A:LYS:N | 1:100:A:LYS:CA | 1:100:A:LYS:C  | 4        | 1.27          |
| (1,117) | 1:68:A:TRP:C  | 1:69:A:VAL:N  | 1:69:A:VAL:CA  | 1:69:A:VAL:C   | 5        | 1.27          |
| (1,82)  | 1:44:A:GLN:N  | 1:44:A:GLN:CA | 1:44:A:GLN:C   | 1:45:A:LYS:N   | 13       | 1.27          |
| (1,60)  | 1:33:A:GLU:N  | 1:33:A:GLU:CA | 1:33:A:GLU:C   | 1:34:A:GLN:N   | 15       | 1.27          |
| (1,38)  | 1:22:A:GLU:N  | 1:22:A:GLU:CA | 1:22:A:GLU:C   | 1:23:A:ILE:N   | 11       | 1.27          |
| (1,28)  | 1:17:A:PHE:N  | 1:17:A:PHE:CA | 1:17:A:PHE:C   | 1:18:A:GLN:N   | 10       | 1.27          |
| (1,12)  | 1:8:A:GLN:N   | 1:8:A:GLN:CA  | 1:8:A:GLN:C    | 1:9:A:THR:N    | 15       | 1.27          |
| (1,198) | 1:23:A:ILE:N  | 1:23:A:ILE:CA | 1:23:A:ILE:CB  | 1:23:A:ILE:CG1 | 4        | 1.26          |
| (1,187) | 1:103:A:GLU:C | 1:104:A:LEU:N | 1:104:A:LEU:CA | 1:104:A:LEU:C  | 2        | 1.26          |

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| Key     | Atom-1        | Atom-2        | Atom-3         | Atom-4         | Model ID | Violation (°) |
|---------|---------------|---------------|----------------|----------------|----------|---------------|
| (1,185) | 1:102:A:ARG:C | 1:103:A:GLU:N | 1:103:A:GLU:CA | 1:103:A:GLU:C  | 11       | 1.26          |
| (1,181) | 1:100:A:LYS:C | 1:101:A:ILE:N | 1:101:A:ILE:CA | 1:101:A:ILE:C  | 19       | 1.26          |
| (1,137) | 1:78:A:ALA:C  | 1:79:A:ILE:N  | 1:79:A:ILE:CA  | 1:79:A:ILE:C   | 16       | 1.26          |
| (1,133) | 1:76:A:ARG:C  | 1:77:A:GLU:N  | 1:77:A:GLU:CA  | 1:77:A:GLU:C   | 3        | 1.26          |
| (1,101) | 1:60:A:GLU:C  | 1:61:A:ALA:N  | 1:61:A:ALA:CA  | 1:61:A:ALA:C   | 14       | 1.26          |
| (1,83)  | 1:44:A:GLN:C  | 1:45:A:LYS:N  | 1:45:A:LYS:CA  | 1:45:A:LYS:C   | 13       | 1.26          |
| (1,76)  | 1:41:A:GLU:N  | 1:41:A:GLU:CA | 1:41:A:GLU:C   | 1:42:A:LEU:N   | 4        | 1.26          |
| (1,165) | 1:92:A:GLU:C  | 1:93:A:GLU:N  | 1:93:A:GLU:CA  | 1:93:A:GLU:C   | 20       | 1.25          |
| (1,162) | 1:91:A:LEU:N  | 1:91:A:LEU:CA | 1:91:A:LEU:C   | 1:92:A:GLU:N   | 9        | 1.25          |
| (1,104) | 1:62:A:ALA:N  | 1:62:A:ALA:CA | 1:62:A:ALA:C   | 1:63:A:LYS:N   | 12       | 1.25          |
| (1,89)  | 1:47:A:ARG:C  | 1:48:A:GLN:N  | 1:48:A:GLN:CA  | 1:48:A:GLN:C   | 6        | 1.25          |
| (1,86)  | 1:46:A:HIS:N  | 1:46:A:HIS:CA | 1:46:A:HIS:C   | 1:47:A:ARG:N   | 16       | 1.25          |
| (1,42)  | 1:24:A:PHE:N  | 1:24:A:PHE:CA | 1:24:A:PHE:C   | 1:25:A:ASP:N   | 7        | 1.25          |
| (1,223) | 1:83:A:ASP:N  | 1:83:A:ASP:CA | 1:83:A:ASP:CB  | 1:83:A:ASP:CG  | 19       | 1.24          |
| (1,219) | 1:75:A:PHE:N  | 1:75:A:PHE:CA | 1:75:A:PHE:CB  | 1:75:A:PHE:CG  | 12       | 1.24          |
| (1,154) | 1:87:A:LEU:N  | 1:87:A:LEU:CA | 1:87:A:LEU:C   | 1:88:A:GLU:N   | 4        | 1.24          |
| (1,130) | 1:75:A:PHE:N  | 1:75:A:PHE:CA | 1:75:A:PHE:C   | 1:76:A:ARG:N   | 10       | 1.24          |
| (1,85)  | 1:45:A:LYS:C  | 1:46:A:HIS:N  | 1:46:A:HIS:CA  | 1:46:A:HIS:C   | 9        | 1.24          |
| (1,78)  | 1:42:A:LEU:N  | 1:42:A:LEU:CA | 1:42:A:LEU:C   | 1:43:A:ILE:N   | 1        | 1.24          |
| (1,59)  | 1:32:A:LEU:C  | 1:33:A:GLU:N  | 1:33:A:GLU:CA  | 1:33:A:GLU:C   | 18       | 1.24          |
| (1,35)  | 1:20:A:LEU:C  | 1:21:A:ARG:N  | 1:21:A:ARG:CA  | 1:21:A:ARG:C   | 18       | 1.24          |
| (1,177) | 1:98:A:LEU:C  | 1:99:A:GLN:N  | 1:99:A:GLN:CA  | 1:99:A:GLN:C   | 11       | 1.23          |
| (1,106) | 1:63:A:LYS:N  | 1:63:A:LYS:CA | 1:63:A:LYS:C   | 1:64:A:GLN:N   | 10       | 1.23          |
| (1,39)  | 1:22:A:GLU:C  | 1:23:A:ILE:N  | 1:23:A:ILE:CA  | 1:23:A:ILE:C   | 12       | 1.23          |
| (1,220) | 1:79:A:ILE:N  | 1:79:A:ILE:CA | 1:79:A:ILE:CB  | 1:79:A:ILE:CG1 | 10       | 1.22          |
| (1,116) | 1:68:A:TRP:N  | 1:68:A:TRP:CA | 1:68:A:TRP:C   | 1:69:A:VAL:N   | 9        | 1.22          |
| (1,95)  | 1:50:A:PHE:C  | 1:51:A:ASP:N  | 1:51:A:ASP:CA  | 1:51:A:ASP:C   | 11       | 1.22          |
| (1,51)  | 1:28:A:ASP:C  | 1:29:A:ASP:N  | 1:29:A:ASP:CA  | 1:29:A:ASP:C   | 17       | 1.22          |
| (1,33)  | 1:19:A:ARG:C  | 1:20:A:LEU:N  | 1:20:A:LEU:CA  | 1:20:A:LEU:C   | 7        | 1.22          |
| (1,139) | 1:79:A:ILE:C  | 1:80:A:ASP:N  | 1:80:A:ASP:CA  | 1:80:A:ASP:C   | 20       | 1.21          |
| (1,136) | 1:78:A:ALA:N  | 1:78:A:ALA:CA | 1:78:A:ALA:C   | 1:79:A:ILE:N   | 7        | 1.21          |
| (1,85)  | 1:45:A:LYS:C  | 1:46:A:HIS:N  | 1:46:A:HIS:CA  | 1:46:A:HIS:C   | 7        | 1.21          |
| (1,215) | 1:66:A:ASP:N  | 1:66:A:ASP:CA | 1:66:A:ASP:CB  | 1:66:A:ASP:CG  | 6        | 1.2           |
| (1,163) | 1:91:A:LEU:C  | 1:92:A:GLU:N  | 1:92:A:GLU:CA  | 1:92:A:GLU:C   | 18       | 1.2           |
| (1,158) | 1:89:A:GLN:N  | 1:89:A:GLN:CA | 1:89:A:GLN:C   | 1:90:A:LEU:N   | 20       | 1.2           |
| (1,139) | 1:79:A:ILE:C  | 1:80:A:ASP:N  | 1:80:A:ASP:CA  | 1:80:A:ASP:C   | 8        | 1.2           |
| (1,99)  | 1:59:A:THR:C  | 1:60:A:GLU:N  | 1:60:A:GLU:CA  | 1:60:A:GLU:C   | 12       | 1.2           |
| (1,97)  | 1:58:A:ASP:C  | 1:59:A:THR:N  | 1:59:A:THR:CA  | 1:59:A:THR:C   | 7        | 1.2           |
| (1,79)  | 1:42:A:LEU:C  | 1:43:A:ILE:N  | 1:43:A:ILE:CA  | 1:43:A:ILE:C   | 10       | 1.2           |
| (1,65)  | 1:35:A:VAL:C  | 1:36:A:LEU:N  | 1:36:A:LEU:CA  | 1:36:A:LEU:C   | 7        | 1.2           |
| (1,32)  | 1:19:A:ARG:N  | 1:19:A:ARG:CA | 1:19:A:ARG:C   | 1:20:A:LEU:N   | 15       | 1.2           |
| (1,3)   | 1:3:A:PHE:C   | 1:4:A:GLU:N   | 1:4:A:GLU:CA   | 1:4:A:GLU:C    | 6        | 1.2           |
| (1,220) | 1:79:A:ILE:N  | 1:79:A:ILE:CA | 1:79:A:ILE:CB  | 1:79:A:ILE:CG1 | 13       | 1.19          |
| (1,153) | 1:86:A:SER:C  | 1:87:A:LEU:N  | 1:87:A:LEU:CA  | 1:87:A:LEU:C   | 14       | 1.19          |
| (1,76)  | 1:41:A:GLU:N  | 1:41:A:GLU:CA | 1:41:A:GLU:C   | 1:42:A:LEU:N   | 11       | 1.19          |
| (1,73)  | 1:39:A:ILE:C  | 1:40:A:GLU:N  | 1:40:A:GLU:CA  | 1:40:A:GLU:C   | 9        | 1.19          |
| (1,35)  | 1:20:A:LEU:C  | 1:21:A:ARG:N  | 1:21:A:ARG:CA  | 1:21:A:ARG:C   | 12       | 1.19          |
| (1,33)  | 1:19:A:ARG:C  | 1:20:A:LEU:N  | 1:20:A:LEU:CA  | 1:20:A:LEU:C   | 15       | 1.19          |
| (1,32)  | 1:19:A:ARG:N  | 1:19:A:ARG:CA | 1:19:A:ARG:C   | 1:20:A:LEU:N   | 7        | 1.19          |
| (1,223) | 1:83:A:ASP:N  | 1:83:A:ASP:CA | 1:83:A:ASP:CB  | 1:83:A:ASP:CG  | 2        | 1.18          |
| (1,177) | 1:98:A:LEU:C  | 1:99:A:GLN:N  | 1:99:A:GLN:CA  | 1:99:A:GLN:C   | 10       | 1.18          |

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| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4          | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|-----------------|----------|---------------|
| (1,175) | 1:97:A:ALA:C  | 1:98:A:LEU:N   | 1:98:A:LEU:CA  | 1:98:A:LEU:C    | 4        | 1.18          |
| (1,124) | 1:72:A:PHE:N  | 1:72:A:PHE:CA  | 1:72:A:PHE:C   | 1:73:A:GLN:N    | 20       | 1.18          |
| (1,105) | 1:62:A:ALA:C  | 1:63:A:LYS:N   | 1:63:A:LYS:CA  | 1:63:A:LYS:C    | 1        | 1.18          |
| (1,73)  | 1:39:A:ILE:C  | 1:40:A:GLU:N   | 1:40:A:GLU:CA  | 1:40:A:GLU:C    | 2        | 1.18          |
| (1,47)  | 1:26:A:LYS:C  | 1:27:A:GLY:N   | 1:27:A:GLY:CA  | 1:27:A:GLY:C    | 20       | 1.18          |
| (1,41)  | 1:23:A:ILE:C  | 1:24:A:PHE:N   | 1:24:A:PHE:CA  | 1:24:A:PHE:C    | 20       | 1.18          |
| (1,12)  | 1:8:A:GLN:N   | 1:8:A:GLN:CA   | 1:8:A:GLN:C    | 1:9:A:THR:N     | 3        | 1.18          |
| (1,8)   | 1:6:A:LEU:N   | 1:6:A:LEU:CA   | 1:6:A:LEU:C    | 1:7:A:ARG:N     | 12       | 1.18          |
| (1,227) | 1:101:A:ILE:N | 1:101:A:ILE:CA | 1:101:A:ILE:CB | 1:101:A:ILE:CG1 | 14       | 1.17          |
| (1,227) | 1:101:A:ILE:N | 1:101:A:ILE:CA | 1:101:A:ILE:CB | 1:101:A:ILE:CG1 | 17       | 1.17          |
| (1,218) | 1:72:A:PHE:N  | 1:72:A:PHE:CA  | 1:72:A:PHE:CB  | 1:72:A:PHE:CG   | 12       | 1.17          |
| (1,186) | 1:103:A:GLU:N | 1:103:A:GLU:CA | 1:103:A:GLU:C  | 1:104:A:LEU:N   | 12       | 1.17          |
| (1,181) | 1:100:A:LYS:C | 1:101:A:ILE:N  | 1:101:A:ILE:CA | 1:101:A:ILE:C   | 10       | 1.17          |
| (1,143) | 1:81:A:LYS:C  | 1:82:A:GLY:N   | 1:82:A:GLY:CA  | 1:82:A:GLY:C    | 18       | 1.17          |
| (1,76)  | 1:41:A:GLU:N  | 1:41:A:GLU:CA  | 1:41:A:GLU:C   | 1:42:A:LEU:N    | 18       | 1.17          |
| (1,218) | 1:72:A:PHE:N  | 1:72:A:PHE:CA  | 1:72:A:PHE:CB  | 1:72:A:PHE:CG   | 15       | 1.16          |
| (1,200) | 1:25:A:ASP:N  | 1:25:A:ASP:CA  | 1:25:A:ASP:CB  | 1:25:A:ASP:CG   | 19       | 1.16          |
| (1,171) | 1:95:A:GLU:C  | 1:96:A:GLN:N   | 1:96:A:GLN:CA  | 1:96:A:GLN:C    | 12       | 1.16          |
| (1,80)  | 1:43:A:ILE:N  | 1:43:A:ILE:CA  | 1:43:A:ILE:C   | 1:44:A:GLN:N    | 5        | 1.16          |
| (1,24)  | 1:15:A:GLN:N  | 1:15:A:GLN:CA  | 1:15:A:GLN:C   | 1:16:A:ALA:N    | 6        | 1.16          |
| (1,227) | 1:101:A:ILE:N | 1:101:A:ILE:CA | 1:101:A:ILE:CB | 1:101:A:ILE:CG1 | 3        | 1.15          |
| (1,202) | 1:28:A:ASP:N  | 1:28:A:ASP:CA  | 1:28:A:ASP:CB  | 1:28:A:ASP:CG   | 16       | 1.15          |
| (1,158) | 1:89:A:GLN:N  | 1:89:A:GLN:CA  | 1:89:A:GLN:C   | 1:90:A:LEU:N    | 10       | 1.15          |
| (1,157) | 1:88:A:GLU:C  | 1:89:A:GLN:N   | 1:89:A:GLN:CA  | 1:89:A:GLN:C    | 16       | 1.15          |
| (1,140) | 1:80:A:ASP:N  | 1:80:A:ASP:CA  | 1:80:A:ASP:C   | 1:81:A:LYS:N    | 19       | 1.15          |
| (1,104) | 1:62:A:ALA:N  | 1:62:A:ALA:CA  | 1:62:A:ALA:C   | 1:63:A:LYS:N    | 15       | 1.15          |
| (1,38)  | 1:22:A:GLU:N  | 1:22:A:GLU:CA  | 1:22:A:GLU:C   | 1:23:A:ILE:N    | 9        | 1.15          |
| (1,17)  | 1:11:A:ASP:C  | 1:12:A:GLU:N   | 1:12:A:GLU:CA  | 1:12:A:GLU:C    | 2        | 1.15          |
| (1,17)  | 1:11:A:ASP:C  | 1:12:A:GLU:N   | 1:12:A:GLU:CA  | 1:12:A:GLU:C    | 13       | 1.15          |
| (1,221) | 1:80:A:ASP:N  | 1:80:A:ASP:CA  | 1:80:A:ASP:CB  | 1:80:A:ASP:CG   | 17       | 1.14          |
| (1,220) | 1:79:A:ILE:N  | 1:79:A:ILE:CA  | 1:79:A:ILE:CB  | 1:79:A:ILE:CG1  | 19       | 1.14          |
| (1,170) | 1:95:A:GLU:N  | 1:95:A:GLU:CA  | 1:95:A:GLU:C   | 1:96:A:GLN:N    | 2        | 1.14          |
| (1,85)  | 1:45:A:LYS:C  | 1:46:A:HIS:N   | 1:46:A:HIS:CA  | 1:46:A:HIS:C    | 19       | 1.14          |
| (1,78)  | 1:42:A:LEU:N  | 1:42:A:LEU:CA  | 1:42:A:LEU:C   | 1:43:A:ILE:N    | 10       | 1.14          |
| (1,51)  | 1:28:A:ASP:C  | 1:29:A:ASP:N   | 1:29:A:ASP:CA  | 1:29:A:ASP:C    | 5        | 1.14          |
| (1,48)  | 1:27:A:GLY:N  | 1:27:A:GLY:CA  | 1:27:A:GLY:C   | 1:28:A:ASP:N    | 7        | 1.14          |
| (1,48)  | 1:27:A:GLY:N  | 1:27:A:GLY:CA  | 1:27:A:GLY:C   | 1:28:A:ASP:N    | 11       | 1.14          |
| (1,35)  | 1:20:A:LEU:C  | 1:21:A:ARG:N   | 1:21:A:ARG:CA  | 1:21:A:ARG:C    | 7        | 1.14          |
| (1,28)  | 1:17:A:PHE:N  | 1:17:A:PHE:CA  | 1:17:A:PHE:C   | 1:18:A:GLN:N    | 5        | 1.14          |
| (1,23)  | 1:14:A:VAL:C  | 1:15:A:GLN:N   | 1:15:A:GLN:CA  | 1:15:A:GLN:C    | 10       | 1.14          |
| (1,175) | 1:97:A:ALA:C  | 1:98:A:LEU:N   | 1:98:A:LEU:CA  | 1:98:A:LEU:C    | 13       | 1.13          |
| (1,108) | 1:64:A:GLN:N  | 1:64:A:GLN:CA  | 1:64:A:GLN:C   | 1:65:A:GLY:N    | 1        | 1.13          |
| (1,101) | 1:60:A:GLU:C  | 1:61:A:ALA:N   | 1:61:A:ALA:CA  | 1:61:A:ALA:C    | 8        | 1.13          |
| (1,92)  | 1:49:A:LEU:N  | 1:49:A:LEU:CA  | 1:49:A:LEU:C   | 1:50:A:PHE:N    | 18       | 1.13          |
| (1,85)  | 1:45:A:LYS:C  | 1:46:A:HIS:N   | 1:46:A:HIS:CA  | 1:46:A:HIS:C    | 10       | 1.13          |
| (1,85)  | 1:45:A:LYS:C  | 1:46:A:HIS:N   | 1:46:A:HIS:CA  | 1:46:A:HIS:C    | 13       | 1.13          |
| (1,47)  | 1:26:A:LYS:C  | 1:27:A:GLY:N   | 1:27:A:GLY:CA  | 1:27:A:GLY:C    | 5        | 1.13          |
| (1,220) | 1:79:A:ILE:N  | 1:79:A:ILE:CA  | 1:79:A:ILE:CB  | 1:79:A:ILE:CG1  | 4        | 1.12          |
| (1,216) | 1:68:A:TRP:N  | 1:68:A:TRP:CA  | 1:68:A:TRP:CB  | 1:68:A:TRP:CG   | 9        | 1.12          |
| (1,105) | 1:62:A:ALA:C  | 1:63:A:LYS:N   | 1:63:A:LYS:CA  | 1:63:A:LYS:C    | 20       | 1.12          |
| (1,55)  | 1:30:A:ASP:C  | 1:31:A:SER:N   | 1:31:A:SER:CA  | 1:31:A:SER:C    | 18       | 1.12          |

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| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4         | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|----------------|----------|---------------|
| (1,216) | 1:68:A:TRP:N  | 1:68:A:TRP:CA  | 1:68:A:TRP:CB  | 1:68:A:TRP:CG  | 3        | 1.11          |
| (1,210) | 1:49:A:LEU:N  | 1:49:A:LEU:CA  | 1:49:A:LEU:CB  | 1:49:A:LEU:CG  | 17       | 1.11          |
| (1,177) | 1:98:A:LEU:C  | 1:99:A:GLN:N   | 1:99:A:GLN:CA  | 1:99:A:GLN:C   | 1        | 1.11          |
| (1,177) | 1:98:A:LEU:C  | 1:99:A:GLN:N   | 1:99:A:GLN:CA  | 1:99:A:GLN:C   | 20       | 1.11          |
| (1,162) | 1:91:A:LEU:N  | 1:91:A:LEU:CA  | 1:91:A:LEU:C   | 1:92:A:GLU:N   | 10       | 1.11          |
| (1,158) | 1:89:A:GLN:N  | 1:89:A:GLN:CA  | 1:89:A:GLN:C   | 1:90:A:LEU:N   | 13       | 1.11          |
| (1,121) | 1:70:A:GLN:C  | 1:71:A:LEU:N   | 1:71:A:LEU:CA  | 1:71:A:LEU:C   | 8        | 1.11          |
| (1,56)  | 1:31:A:SER:N  | 1:31:A:SER:CA  | 1:31:A:SER:C   | 1:32:A:LEU:N   | 8        | 1.11          |
| (1,32)  | 1:19:A:ARG:N  | 1:19:A:ARG:CA  | 1:19:A:ARG:C   | 1:20:A:LEU:N   | 17       | 1.11          |
| (1,219) | 1:75:A:PHE:N  | 1:75:A:PHE:CA  | 1:75:A:PHE:CB  | 1:75:A:PHE:CG  | 16       | 1.1           |
| (1,186) | 1:103:A:GLU:N | 1:103:A:GLU:CA | 1:103:A:GLU:C  | 1:104:A:LEU:N  | 9        | 1.1           |
| (1,171) | 1:95:A:GLU:C  | 1:96:A:GLN:N   | 1:96:A:GLN:CA  | 1:96:A:GLN:C   | 16       | 1.1           |
| (1,129) | 1:74:A:ARG:C  | 1:75:A:PHE:N   | 1:75:A:PHE:CA  | 1:75:A:PHE:C   | 1        | 1.1           |
| (1,118) | 1:69:A:VAL:N  | 1:69:A:VAL:CA  | 1:69:A:VAL:C   | 1:70:A:GLN:N   | 8        | 1.1           |
| (1,94)  | 1:50:A:PHE:N  | 1:50:A:PHE:CA  | 1:50:A:PHE:C   | 1:51:A:ASP:N   | 13       | 1.1           |
| (1,70)  | 1:38:A:GLU:N  | 1:38:A:GLU:CA  | 1:38:A:GLU:C   | 1:39:A:ILE:N   | 16       | 1.1           |
| (1,33)  | 1:19:A:ARG:C  | 1:20:A:LEU:N   | 1:20:A:LEU:CA  | 1:20:A:LEU:C   | 8        | 1.1           |
| (1,23)  | 1:14:A:VAL:C  | 1:15:A:GLN:N   | 1:15:A:GLN:CA  | 1:15:A:GLN:C   | 13       | 1.1           |
| (1,158) | 1:89:A:GLN:N  | 1:89:A:GLN:CA  | 1:89:A:GLN:C   | 1:90:A:LEU:N   | 11       | 1.09          |
| (1,120) | 1:70:A:GLN:N  | 1:70:A:GLN:CA  | 1:70:A:GLN:C   | 1:71:A:LEU:N   | 20       | 1.09          |
| (1,64)  | 1:35:A:VAL:N  | 1:35:A:VAL:CA  | 1:35:A:VAL:C   | 1:36:A:LEU:N   | 17       | 1.09          |
| (1,54)  | 1:30:A:ASP:N  | 1:30:A:ASP:CA  | 1:30:A:ASP:C   | 1:31:A:SER:N   | 19       | 1.09          |
| (1,213) | 1:54:A:GLN:N  | 1:54:A:GLN:CA  | 1:54:A:GLN:CB  | 1:54:A:GLN:CG  | 19       | 1.08          |
| (1,154) | 1:87:A:LEU:N  | 1:87:A:LEU:CA  | 1:87:A:LEU:C   | 1:88:A:GLU:N   | 3        | 1.08          |
| (1,130) | 1:75:A:PHE:N  | 1:75:A:PHE:CA  | 1:75:A:PHE:C   | 1:76:A:ARG:N   | 9        | 1.08          |
| (1,106) | 1:63:A:LYS:N  | 1:63:A:LYS:CA  | 1:63:A:LYS:C   | 1:64:A:GLN:N   | 13       | 1.08          |
| (1,85)  | 1:45:A:LYS:C  | 1:46:A:HIS:N   | 1:46:A:HIS:CA  | 1:46:A:HIS:C   | 2        | 1.08          |
| (1,57)  | 1:31:A:SER:C  | 1:32:A:LEU:N   | 1:32:A:LEU:CA  | 1:32:A:LEU:C   | 17       | 1.08          |
| (1,47)  | 1:26:A:LYS:C  | 1:27:A:GLY:N   | 1:27:A:GLY:CA  | 1:27:A:GLY:C   | 8        | 1.08          |
| (1,43)  | 1:24:A:PHE:C  | 1:25:A:ASP:N   | 1:25:A:ASP:CA  | 1:25:A:ASP:C   | 8        | 1.08          |
| (1,219) | 1:75:A:PHE:N  | 1:75:A:PHE:CA  | 1:75:A:PHE:CB  | 1:75:A:PHE:CG  | 17       | 1.07          |
| (1,181) | 1:100:A:LYS:C | 1:101:A:ILE:N  | 1:101:A:ILE:CA | 1:101:A:ILE:C  | 8        | 1.07          |
| (1,161) | 1:90:A:LEU:C  | 1:91:A:LEU:N   | 1:91:A:LEU:CA  | 1:91:A:LEU:C   | 11       | 1.07          |
| (1,152) | 1:86:A:SER:N  | 1:86:A:SER:CA  | 1:86:A:SER:C   | 1:87:A:LEU:N   | 4        | 1.07          |
| (1,146) | 1:83:A:ASP:N  | 1:83:A:ASP:CA  | 1:83:A:ASP:C   | 1:84:A:LYS:N   | 1        | 1.07          |
| (1,134) | 1:77:A:GLU:N  | 1:77:A:GLU:CA  | 1:77:A:GLU:C   | 1:78:A:ALA:N   | 17       | 1.07          |
| (1,62)  | 1:34:A:GLN:N  | 1:34:A:GLN:CA  | 1:34:A:GLN:C   | 1:35:A:VAL:N   | 17       | 1.07          |
| (1,51)  | 1:28:A:ASP:C  | 1:29:A:ASP:N   | 1:29:A:ASP:CA  | 1:29:A:ASP:C   | 8        | 1.07          |
| (1,214) | 1:55:A:GLU:N  | 1:55:A:GLU:CA  | 1:55:A:GLU:CB  | 1:55:A:GLU:CG  | 18       | 1.06          |
| (1,202) | 1:28:A:ASP:N  | 1:28:A:ASP:CA  | 1:28:A:ASP:CB  | 1:28:A:ASP:CG  | 13       | 1.06          |
| (1,150) | 1:85:A:ASP:N  | 1:85:A:ASP:CA  | 1:85:A:ASP:C   | 1:86:A:SER:N   | 7        | 1.06          |
| (1,147) | 1:83:A:ASP:C  | 1:84:A:LYS:N   | 1:84:A:LYS:CA  | 1:84:A:LYS:C   | 17       | 1.06          |
| (1,100) | 1:60:A:GLU:N  | 1:60:A:GLU:CA  | 1:60:A:GLU:C   | 1:61:A:ALA:N   | 9        | 1.06          |
| (1,101) | 1:60:A:GLU:C  | 1:61:A:ALA:N   | 1:61:A:ALA:CA  | 1:61:A:ALA:C   | 13       | 1.05          |
| (1,78)  | 1:42:A:LEU:N  | 1:42:A:LEU:CA  | 1:42:A:LEU:C   | 1:43:A:ILE:N   | 3        | 1.05          |
| (1,64)  | 1:35:A:VAL:N  | 1:35:A:VAL:CA  | 1:35:A:VAL:C   | 1:36:A:LEU:N   | 19       | 1.05          |
| (1,58)  | 1:32:A:LEU:N  | 1:32:A:LEU:CA  | 1:32:A:LEU:C   | 1:33:A:GLU:N   | 20       | 1.05          |
| (1,198) | 1:23:A:ILE:N  | 1:23:A:ILE:CA  | 1:23:A:ILE:CB  | 1:23:A:ILE:CG1 | 20       | 1.04          |
| (1,79)  | 1:42:A:LEU:C  | 1:43:A:ILE:N   | 1:43:A:ILE:CA  | 1:43:A:ILE:C   | 6        | 1.04          |
| (1,26)  | 1:16:A:ALA:N  | 1:16:A:ALA:CA  | 1:16:A:ALA:C   | 1:17:A:PHE:N   | 13       | 1.04          |
| (1,26)  | 1:16:A:ALA:N  | 1:16:A:ALA:CA  | 1:16:A:ALA:C   | 1:17:A:PHE:N   | 18       | 1.04          |

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| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4          | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|-----------------|----------|---------------|
| (1,23)  | 1:14:A:VAL:C  | 1:15:A:GLN:N   | 1:15:A:GLN:CA  | 1:15:A:GLN:C    | 8        | 1.04          |
| (1,220) | 1:79:A:ILE:N  | 1:79:A:ILE:CA  | 1:79:A:ILE:CB  | 1:79:A:ILE:CG1  | 17       | 1.03          |
| (1,187) | 1:103:A:GLU:C | 1:104:A:LEU:N  | 1:104:A:LEU:CA | 1:104:A:LEU:C   | 4        | 1.03          |
| (1,173) | 1:96:A:GLN:C  | 1:97:A:ALA:N   | 1:97:A:ALA:CA  | 1:97:A:ALA:C    | 19       | 1.03          |
| (1,156) | 1:88:A:GLU:N  | 1:88:A:GLU:CA  | 1:88:A:GLU:C   | 1:89:A:GLN:N    | 12       | 1.03          |
| (1,135) | 1:77:A:GLU:C  | 1:78:A:ALA:N   | 1:78:A:ALA:CA  | 1:78:A:ALA:C    | 1        | 1.03          |
| (1,91)  | 1:48:A:GLN:C  | 1:49:A:LEU:N   | 1:49:A:LEU:CA  | 1:49:A:LEU:C    | 19       | 1.03          |
| (1,73)  | 1:39:A:ILE:C  | 1:40:A:GLU:N   | 1:40:A:GLU:CA  | 1:40:A:GLU:C    | 17       | 1.03          |
| (1,72)  | 1:39:A:ILE:N  | 1:39:A:ILE:CA  | 1:39:A:ILE:C   | 1:40:A:GLU:N    | 4        | 1.03          |
| (1,23)  | 1:14:A:VAL:C  | 1:15:A:GLN:N   | 1:15:A:GLN:CA  | 1:15:A:GLN:C    | 3        | 1.03          |
| (1,223) | 1:83:A:ASP:N  | 1:83:A:ASP:CA  | 1:83:A:ASP:CB  | 1:83:A:ASP:CG   | 7        | 1.02          |
| (1,215) | 1:66:A:ASP:N  | 1:66:A:ASP:CA  | 1:66:A:ASP:CB  | 1:66:A:ASP:CG   | 17       | 1.02          |
| (1,183) | 1:101:A:ILE:C | 1:102:A:ARG:N  | 1:102:A:ARG:CA | 1:102:A:ARG:C   | 6        | 1.02          |
| (1,126) | 1:73:A:GLN:N  | 1:73:A:GLN:CA  | 1:73:A:GLN:C   | 1:74:A:ARG:N    | 20       | 1.02          |
| (1,91)  | 1:48:A:GLN:C  | 1:49:A:LEU:N   | 1:49:A:LEU:CA  | 1:49:A:LEU:C    | 7        | 1.02          |
| (1,91)  | 1:48:A:GLN:C  | 1:49:A:LEU:N   | 1:49:A:LEU:CA  | 1:49:A:LEU:C    | 11       | 1.02          |
| (1,34)  | 1:20:A:LEU:N  | 1:20:A:LEU:CA  | 1:20:A:LEU:C   | 1:21:A:ARG:N    | 12       | 1.02          |
| (1,26)  | 1:16:A:ALA:N  | 1:16:A:ALA:CA  | 1:16:A:ALA:C   | 1:17:A:PHE:N    | 2        | 1.02          |
| (1,228) | 1:104:A:LEU:N | 1:104:A:LEU:CA | 1:104:A:LEU:CB | 1:104:A:LEU:CG  | 6        | 1.01          |
| (1,228) | 1:104:A:LEU:N | 1:104:A:LEU:CA | 1:104:A:LEU:CB | 1:104:A:LEU:CG  | 14       | 1.01          |
| (1,202) | 1:28:A:ASP:N  | 1:28:A:ASP:CA  | 1:28:A:ASP:CB  | 1:28:A:ASP:CG   | 10       | 1.01          |
| (1,198) | 1:23:A:ILE:N  | 1:23:A:ILE:CA  | 1:23:A:ILE:CB  | 1:23:A:ILE:CG1  | 3        | 1.01          |
| (1,152) | 1:86:A:SER:N  | 1:86:A:SER:CA  | 1:86:A:SER:C   | 1:87:A:LEU:N    | 11       | 1.01          |
| (1,111) | 1:65:A:GLY:C  | 1:66:A:ASP:N   | 1:66:A:ASP:CA  | 1:66:A:ASP:C    | 20       | 1.01          |
| (1,108) | 1:64:A:GLN:N  | 1:64:A:GLN:CA  | 1:64:A:GLN:C   | 1:65:A:GLY:N    | 16       | 1.01          |
| (1,86)  | 1:46:A:HIS:N  | 1:46:A:HIS:CA  | 1:46:A:HIS:C   | 1:47:A:ARG:N    | 2        | 1.01          |
| (1,86)  | 1:46:A:HIS:N  | 1:46:A:HIS:CA  | 1:46:A:HIS:C   | 1:47:A:ARG:N    | 19       | 1.01          |
| (1,83)  | 1:44:A:GLN:C  | 1:45:A:LYS:N   | 1:45:A:LYS:CA  | 1:45:A:LYS:C    | 4        | 1.01          |
| (1,72)  | 1:39:A:ILE:N  | 1:39:A:ILE:CA  | 1:39:A:ILE:C   | 1:40:A:GLU:N    | 15       | 1.01          |
| (1,48)  | 1:27:A:GLY:N  | 1:27:A:GLY:CA  | 1:27:A:GLY:C   | 1:28:A:ASP:N    | 16       | 1.01          |
| (1,40)  | 1:23:A:ILE:N  | 1:23:A:ILE:CA  | 1:23:A:ILE:C   | 1:24:A:PHE:N    | 2        | 1.01          |
| (1,7)   | 1:5:A:LYS:C   | 1:6:A:LEU:N    | 1:6:A:LEU:CA   | 1:6:A:LEU:C     | 12       | 1.01          |
| (1,227) | 1:101:A:ILE:N | 1:101:A:ILE:CA | 1:101:A:ILE:CB | 1:101:A:ILE:CG1 | 19       | 1.0           |
| (1,183) | 1:101:A:ILE:C | 1:102:A:ARG:N  | 1:102:A:ARG:CA | 1:102:A:ARG:C   | 1        | 1.0           |
| (1,177) | 1:98:A:LEU:C  | 1:99:A:GLN:N   | 1:99:A:GLN:CA  | 1:99:A:GLN:C    | 12       | 1.0           |
| (1,162) | 1:91:A:LEU:N  | 1:91:A:LEU:CA  | 1:91:A:LEU:C   | 1:92:A:GLU:N    | 17       | 1.0           |
| (1,86)  | 1:46:A:HIS:N  | 1:46:A:HIS:CA  | 1:46:A:HIS:C   | 1:47:A:ARG:N    | 6        | 1.0           |
| (1,85)  | 1:45:A:LYS:C  | 1:46:A:HIS:N   | 1:46:A:HIS:CA  | 1:46:A:HIS:C    | 4        | 1.0           |
| (1,55)  | 1:30:A:ASP:C  | 1:31:A:SER:N   | 1:31:A:SER:CA  | 1:31:A:SER:C    | 19       | 1.0           |
| (1,31)  | 1:18:A:GLN:C  | 1:19:A:ARG:N   | 1:19:A:ARG:CA  | 1:19:A:ARG:C    | 8        | 1.0           |