



# Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2026 – 08:52 AM UTC

PDB ID : 9KON / pdb\_00009kon  
BMRB ID : 36714  
Title : Solid-state NMR Structure of VsSemiSWEET in Lipid Bilayers  
Authors : Zhang, Y.; Yang, J.  
Deposited on : 2024-11-20

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

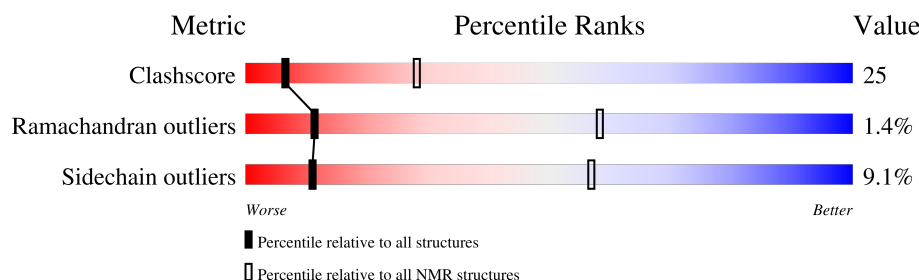
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLID-STATE NMR*

The overall completeness of chemical shifts assignment is 18%.

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     | 80     |                  |
| 1   | B     | 80     |                  |

## 2 Ensemble composition and analysis

This entry contains 10 models. Model 8 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

| Well-defined (core) protein residues |                          |                   |              |
|--------------------------------------|--------------------------|-------------------|--------------|
| Well-defined core                    | Residue range (total)    | Backbone RMSD (Å) | Medoid model |
| 1                                    | A:1-A:80, B:1-B:80 (160) | 1.42              | 8            |

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

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

The models can be grouped into 3 clusters and 1 single-model cluster was found.

| Cluster number        | Models     |
|-----------------------|------------|
| 1                     | 3, 4, 5, 6 |
| 2                     | 1, 2, 7    |
| 3                     | 8, 9       |
| Single-model clusters | 10         |

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

There is only 1 type of molecule in this entry. The entry contains 2548 atoms, of which 1286 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Sugar transporter SemiSWEET.

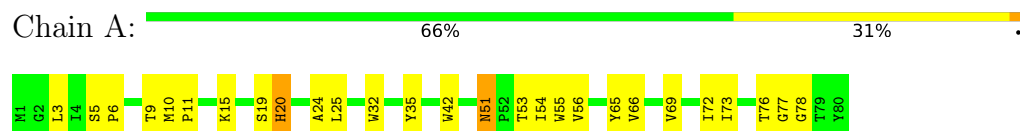
| Mol | Chain | Residues | Atoms |     |     |    |     |   | Trace |
|-----|-------|----------|-------|-----|-----|----|-----|---|-------|
| 1   | A     | 80       | Total | C   | H   | N  | O   | S | 0     |
|     |       |          | 1274  | 425 | 643 | 96 | 105 | 5 |       |
| 1   | B     | 80       | Total | C   | H   | N  | O   | S | 0     |
|     |       |          | 1274  | 425 | 643 | 96 | 105 | 5 |       |

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

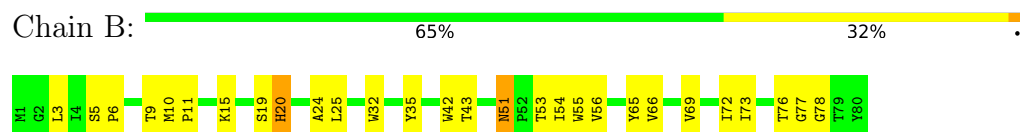
### 4.1 Average score per residue in the NMR ensemble

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: Sugar transporter SemiSWEET



- Molecule 1: Sugar transporter SemiSWEET

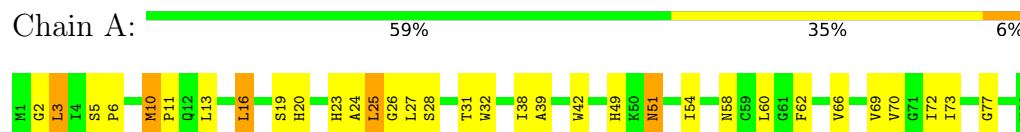


### 4.2 Scores per residue for each member of the ensemble

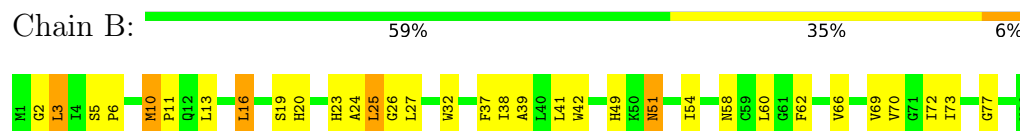
Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1

- Molecule 1: Sugar transporter SemiSWEET

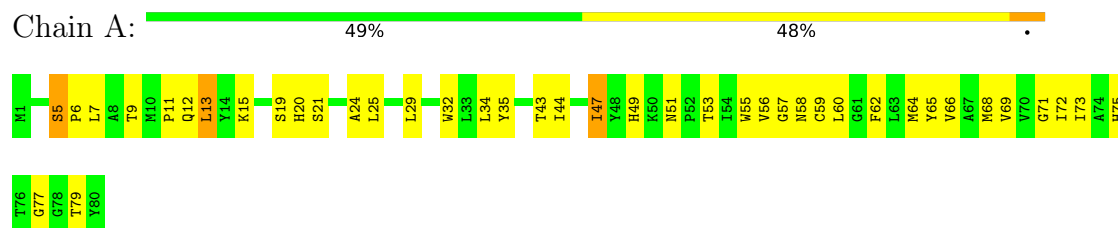


- Molecule 1: Sugar transporter SemiSWEET

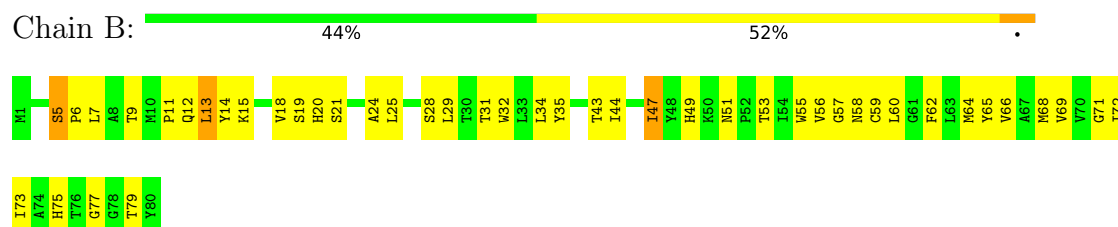


### 4.2.2 Score per residue for model 2

- Molecule 1: Sugar transporter SemiSWEET

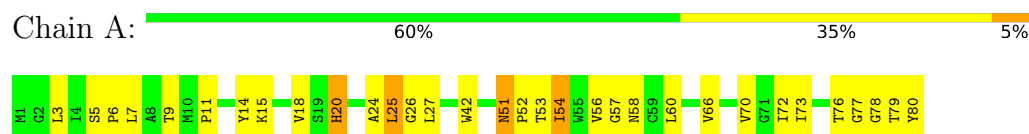


- Molecule 1: Sugar transporter SemiSWEET

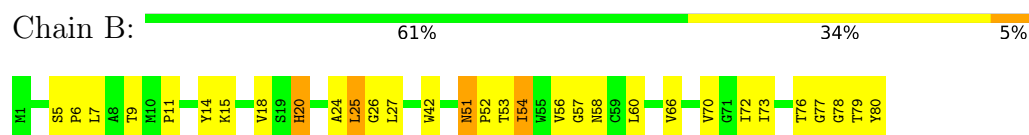


### 4.2.3 Score per residue for model 3

- Molecule 1: Sugar transporter SemiSWEET

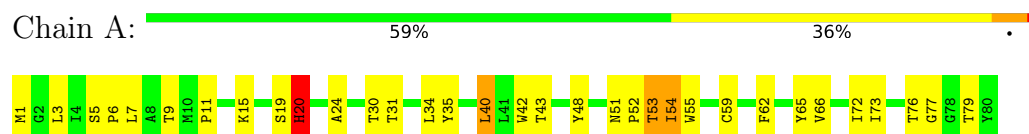


- Molecule 1: Sugar transporter SemiSWEET

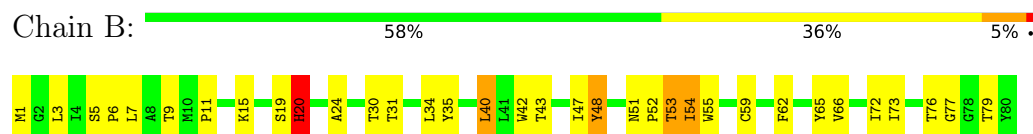


### 4.2.4 Score per residue for model 4

- Molecule 1: Sugar transporter SemiSWEET

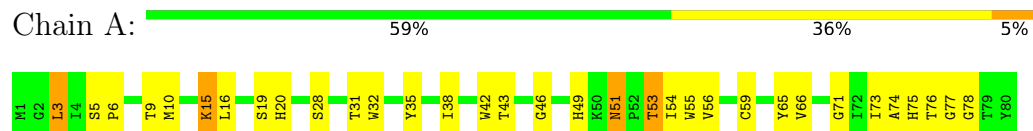


- Molecule 1: Sugar transporter SemiSWEET

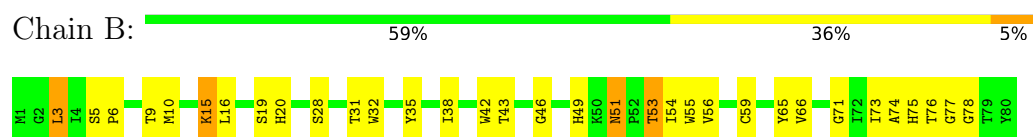


#### 4.2.5 Score per residue for model 5

- Molecule 1: Sugar transporter SemiSWEET

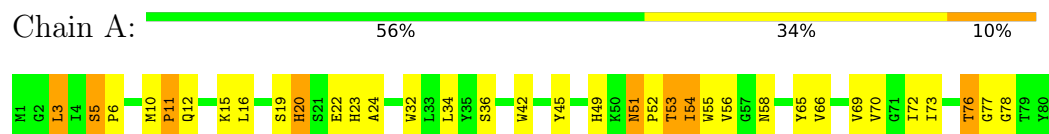


- Molecule 1: Sugar transporter SemiSWEET

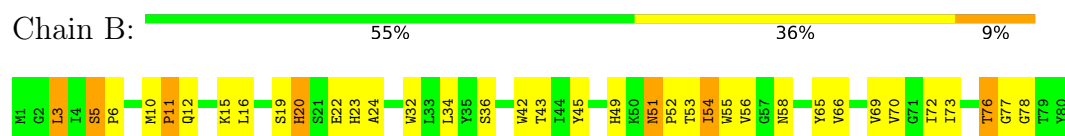


#### 4.2.6 Score per residue for model 6

- Molecule 1: Sugar transporter SemiSWEET

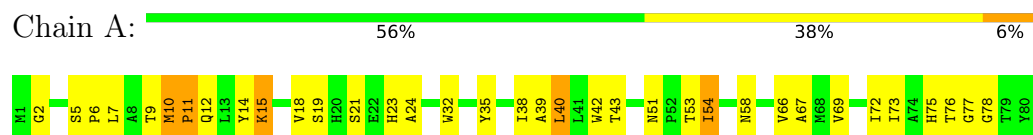


- Molecule 1: Sugar transporter SemiSWEET

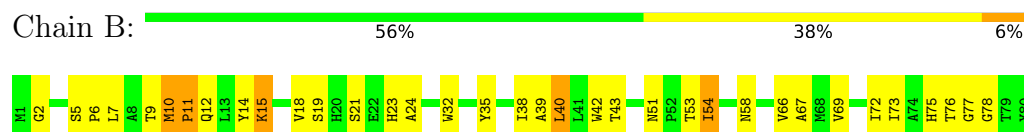


#### 4.2.7 Score per residue for model 7

- Molecule 1: Sugar transporter SemiSWEET

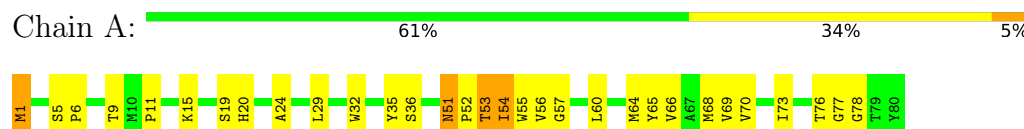


- Molecule 1: Sugar transporter SemiSWEET

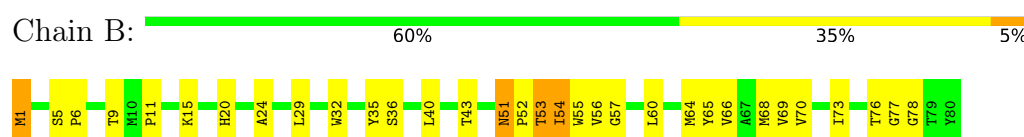


#### 4.2.8 Score per residue for model 8 (medoid)

- Molecule 1: Sugar transporter SemiSWEET

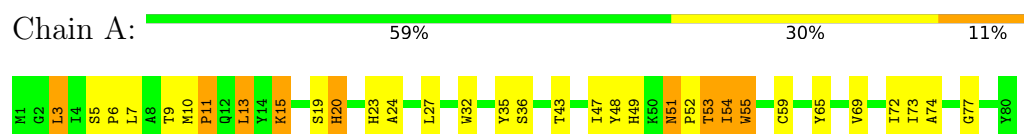


- Molecule 1: Sugar transporter SemiSWEET

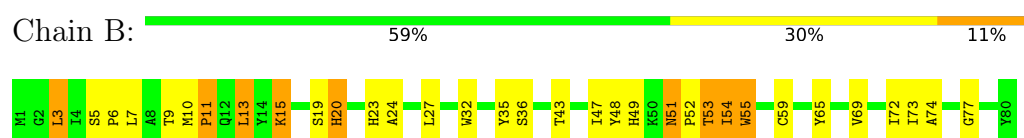


#### 4.2.9 Score per residue for model 9

- Molecule 1: Sugar transporter SemiSWEET

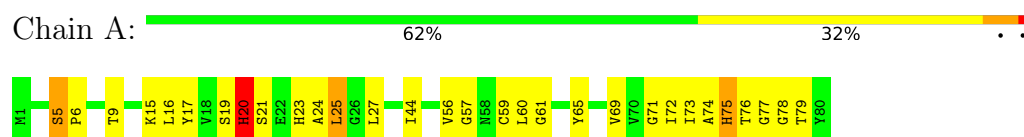


- Molecule 1: Sugar transporter SemiSWEET



#### 4.2.10 Score per residue for model 10

- Molecule 1: Sugar transporter SemiSWEET



- Molecule 1: Sugar transporter SemiSWEET

Chain B:  64% 31% . .



## 5 Refinement protocol and experimental data overview

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

Of the 1024 calculated structures, 10 were deposited, based on the following criterion: *structures with the lowest energy*.

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

| Software name | Classification        | Version |
|---------------|-----------------------|---------|
| X-PLOR NIH    | structure calculation | 2.47    |

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                       | 394            |
| Number of shifts mapped to atoms             | 394            |
| Number of unparsed shifts                    | 0              |
| Number of shifts with mapping errors         | 0              |
| Number of shifts with mapping warnings       | 0              |
| Assignment completeness (well-defined parts) | 18%            |

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

## 6 Model quality [i](#)

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

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes |
|-----|-------|-------|----------|----------|---------|
| 1   | A     | 631   | 643      | 643      | 33±5    |
| 1   | B     | 631   | 643      | 643      | 33±5    |
| All | All   | 12620 | 12860    | 12860    | 640     |

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 25.

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

| Atom-1         | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|----------------|-----------------|----------|-------------|--------|-------|
|                |                 |          |             | Worst  | Total |
| 1:A:32:TRP:CD1 | 1:A:36:SER:HG   | 0.72     | 2.02        | 6      | 2     |
| 1:B:20:HIS:O   | 1:B:24:ALA:HB2  | 0.71     | 1.85        | 2      | 6     |
| 1:A:20:HIS:O   | 1:A:24:ALA:HB2  | 0.71     | 1.85        | 2      | 6     |
| 1:B:20:HIS:C   | 1:B:24:ALA:HB2  | 0.70     | 2.11        | 4      | 1     |
| 1:A:20:HIS:C   | 1:A:24:ALA:HB2  | 0.70     | 2.11        | 4      | 1     |
| 1:A:16:LEU:C   | 1:A:16:LEU:HD13 | 0.70     | 2.12        | 5      | 1     |
| 1:B:16:LEU:C   | 1:B:16:LEU:HD13 | 0.69     | 2.12        | 5      | 1     |
| 1:B:32:TRP:CD1 | 1:B:36:SER:HG   | 0.68     | 2.06        | 6      | 2     |
| 1:B:5:SER:N    | 1:B:6:PRO:CD    | 0.67     | 2.57        | 7      | 10    |
| 1:A:5:SER:N    | 1:A:6:PRO:CD    | 0.67     | 2.57        | 7      | 10    |
| 1:A:23:HIS:CD2 | 1:B:20:HIS:ND1  | 0.64     | 2.66        | 10     | 1     |
| 1:A:6:PRO:O    | 1:A:9:THR:HG22  | 0.63     | 1.93        | 5      | 6     |
| 1:A:55:TRP:CZ3 | 1:B:42:TRP:CZ3  | 0.62     | 2.87        | 5      | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:B:35:TYR:CD2  | 1:B:65:TYR:CD2  | 0.62     | 2.87        | 8      | 2     |
| 1:A:54:ILE:N    | 1:A:54:ILE:HD13 | 0.62     | 2.10        | 7      | 1     |
| 1:A:35:TYR:CD2  | 1:A:65:TYR:CD2  | 0.62     | 2.87        | 8      | 2     |
| 1:A:42:TRP:CZ3  | 1:B:55:TRP:CZ3  | 0.62     | 2.88        | 5      | 1     |
| 1:B:6:PRO:O     | 1:B:9:THR:HG22  | 0.62     | 1.93        | 5      | 6     |
| 1:B:35:TYR:CE2  | 1:B:65:TYR:CG   | 0.62     | 2.87        | 5      | 3     |
| 1:B:54:ILE:HD13 | 1:B:54:ILE:N    | 0.61     | 2.10        | 7      | 1     |
| 1:A:35:TYR:CE2  | 1:A:65:TYR:CG   | 0.61     | 2.87        | 5      | 3     |
| 1:A:44:ILE:HD12 | 1:A:44:ILE:N    | 0.61     | 2.10        | 10     | 1     |
| 1:B:73:ILE:O    | 1:B:77:GLY:N    | 0.61     | 2.34        | 5      | 10    |
| 1:A:35:TYR:CD2  | 1:A:65:TYR:CE2  | 0.60     | 2.88        | 4      | 3     |
| 1:A:73:ILE:O    | 1:A:77:GLY:N    | 0.60     | 2.34        | 5      | 10    |
| 1:B:35:TYR:CD2  | 1:B:65:TYR:CE2  | 0.60     | 2.89        | 4      | 3     |
| 1:B:44:ILE:HD12 | 1:B:44:ILE:N    | 0.60     | 2.10        | 10     | 1     |
| 1:A:59:CYS:SG   | 1:A:60:LEU:N    | 0.60     | 2.75        | 10     | 1     |
| 1:B:20:HIS:CD2  | 1:B:23:HIS:ND1  | 0.60     | 2.70        | 6      | 1     |
| 1:A:20:HIS:CD2  | 1:A:23:HIS:ND1  | 0.60     | 2.70        | 6      | 1     |
| 1:B:56:VAL:HG13 | 1:B:57:GLY:N    | 0.59     | 2.12        | 2      | 3     |
| 1:A:20:HIS:ND1  | 1:B:23:HIS:CD2  | 0.59     | 2.71        | 10     | 2     |
| 1:A:23:HIS:CD2  | 1:B:20:HIS:HD1  | 0.59     | 2.16        | 10     | 1     |
| 1:B:59:CYS:SG   | 1:B:60:LEU:N    | 0.59     | 2.75        | 10     | 1     |
| 1:A:55:TRP:CZ3  | 1:B:42:TRP:CE3  | 0.59     | 2.90        | 5      | 1     |
| 1:B:32:TRP:CD1  | 1:B:69:VAL:HG11 | 0.59     | 2.33        | 7      | 2     |
| 1:A:66:VAL:O    | 1:A:70:VAL:HG22 | 0.59     | 1.97        | 1      | 2     |
| 1:B:66:VAL:O    | 1:B:70:VAL:HG22 | 0.58     | 1.97        | 1      | 2     |
| 1:A:32:TRP:CD1  | 1:A:69:VAL:HG11 | 0.58     | 2.33        | 7      | 2     |
| 1:A:56:VAL:HG13 | 1:A:57:GLY:N    | 0.58     | 2.12        | 2      | 3     |
| 1:A:5:SER:N     | 1:A:6:PRO:HD2   | 0.58     | 2.14        | 2      | 3     |
| 1:A:42:TRP:CE3  | 1:B:55:TRP:CZ3  | 0.58     | 2.91        | 5      | 1     |
| 1:B:55:TRP:C    | 1:B:55:TRP:CD1  | 0.58     | 2.82        | 9      | 2     |
| 1:B:5:SER:N     | 1:B:6:PRO:HD2   | 0.58     | 2.14        | 10     | 3     |
| 1:A:55:TRP:C    | 1:A:55:TRP:CD1  | 0.57     | 2.82        | 9      | 2     |
| 1:B:71:GLY:O    | 1:B:75:HIS:CG   | 0.57     | 2.56        | 10     | 2     |
| 1:B:71:GLY:O    | 1:B:75:HIS:ND1  | 0.57     | 2.37        | 2      | 2     |
| 1:A:71:GLY:O    | 1:A:75:HIS:CG   | 0.57     | 2.56        | 10     | 2     |
| 1:A:38:ILE:CG2  | 1:A:42:TRP:CZ2  | 0.57     | 2.87        | 7      | 1     |
| 1:A:71:GLY:O    | 1:A:75:HIS:ND1  | 0.57     | 2.38        | 2      | 2     |
| 1:B:38:ILE:CG2  | 1:B:42:TRP:CZ2  | 0.57     | 2.87        | 7      | 1     |
| 1:B:6:PRO:O     | 1:B:9:THR:HG23  | 0.57     | 2.00        | 8      | 1     |
| 1:A:6:PRO:O     | 1:A:9:THR:HG23  | 0.56     | 2.00        | 8      | 1     |
| 1:B:20:HIS:CD2  | 1:B:23:HIS:HD1  | 0.56     | 2.18        | 6      | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:32:TRP:CE2  | 1:A:69:VAL:HG21 | 0.56     | 2.35        | 6      | 1     |
| 1:B:1:MET:SD    | 1:B:1:MET:N     | 0.56     | 2.75        | 8      | 1     |
| 1:A:20:HIS:CD2  | 1:A:23:HIS:HD1  | 0.55     | 2.18        | 6      | 1     |
| 1:B:32:TRP:CE2  | 1:B:69:VAL:HG21 | 0.55     | 2.35        | 6      | 1     |
| 1:A:32:TRP:NE1  | 1:A:36:SER:OG   | 0.55     | 2.40        | 6      | 3     |
| 1:B:32:TRP:NE1  | 1:B:36:SER:OG   | 0.55     | 2.40        | 6      | 3     |
| 1:A:20:HIS:HD1  | 1:B:23:HIS:CD2  | 0.54     | 2.20        | 10     | 1     |
| 1:A:56:VAL:HG23 | 1:A:57:GLY:N    | 0.54     | 2.17        | 10     | 1     |
| 1:B:56:VAL:HG23 | 1:B:57:GLY:N    | 0.54     | 2.17        | 10     | 1     |
| 1:B:55:TRP:CD1  | 1:B:56:VAL:N    | 0.54     | 2.76        | 6      | 1     |
| 1:A:55:TRP:CD1  | 1:A:56:VAL:N    | 0.54     | 2.76        | 6      | 1     |
| 1:B:62:PHE:O    | 1:B:66:VAL:HG23 | 0.54     | 2.03        | 1      | 3     |
| 1:B:25:LEU:HD13 | 1:B:68:MET:CE   | 0.54     | 2.33        | 2      | 1     |
| 1:A:49:HIS:ND1  | 1:A:51:ASN:OD1  | 0.54     | 2.40        | 5      | 1     |
| 1:A:43:THR:CG2  | 1:A:59:CYS:SG   | 0.54     | 2.96        | 9      | 2     |
| 1:A:19:SER:O    | 1:A:20:HIS:CG   | 0.54     | 2.61        | 2      | 2     |
| 1:A:25:LEU:HD13 | 1:A:68:MET:CE   | 0.54     | 2.33        | 2      | 1     |
| 1:B:43:THR:CG2  | 1:B:59:CYS:SG   | 0.54     | 2.96        | 9      | 2     |
| 1:A:64:MET:SD   | 1:A:68:MET:SD   | 0.54     | 3.06        | 8      | 1     |
| 1:B:64:MET:SD   | 1:B:68:MET:SD   | 0.54     | 3.06        | 8      | 1     |
| 1:A:62:PHE:O    | 1:A:66:VAL:HG23 | 0.53     | 2.03        | 1      | 3     |
| 1:B:19:SER:O    | 1:B:20:HIS:CG   | 0.53     | 2.61        | 2      | 2     |
| 1:A:23:HIS:CE1  | 1:B:19:SER:O    | 0.53     | 2.61        | 10     | 1     |
| 1:B:19:SER:O    | 1:B:20:HIS:ND1  | 0.53     | 2.42        | 10     | 1     |
| 1:A:52:PRO:O    | 1:A:54:ILE:N    | 0.53     | 2.42        | 4      | 5     |
| 1:A:23:HIS:ND1  | 1:B:19:SER:OG   | 0.52     | 2.41        | 9      | 2     |
| 1:A:26:GLY:H    | 1:A:72:ILE:CD1  | 0.52     | 2.17        | 1      | 1     |
| 1:B:52:PRO:C    | 1:B:54:ILE:N    | 0.52     | 2.65        | 4      | 5     |
| 1:A:22:GLU:O    | 1:A:72:ILE:HD11 | 0.52     | 2.04        | 6      | 1     |
| 1:A:19:SER:O    | 1:A:20:HIS:ND1  | 0.52     | 2.42        | 10     | 1     |
| 1:B:49:HIS:O    | 1:B:51:ASN:ND2  | 0.52     | 2.42        | 2      | 1     |
| 1:B:3:LEU:HD12  | 1:B:3:LEU:N     | 0.52     | 2.18        | 4      | 1     |
| 1:A:42:TRP:CE3  | 1:A:58:ASN:CG   | 0.52     | 2.88        | 6      | 1     |
| 1:B:42:TRP:CE3  | 1:B:58:ASN:CG   | 0.52     | 2.87        | 6      | 1     |
| 1:B:40:LEU:O    | 1:B:40:LEU:HD13 | 0.52     | 2.05        | 7      | 1     |
| 1:B:56:VAL:CG2  | 1:B:57:GLY:N    | 0.52     | 2.72        | 10     | 1     |
| 1:B:25:LEU:H    | 1:B:72:ILE:HD12 | 0.52     | 1.65        | 3      | 2     |
| 1:A:24:ALA:HB3  | 1:A:72:ILE:CG2  | 0.52     | 2.35        | 2      | 1     |
| 1:B:24:ALA:HB3  | 1:B:72:ILE:CG2  | 0.52     | 2.34        | 2      | 1     |
| 1:A:3:LEU:HD12  | 1:A:3:LEU:N     | 0.52     | 2.18        | 4      | 1     |
| 1:A:19:SER:O    | 1:B:23:HIS:CE1  | 0.52     | 2.62        | 10     | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:56:VAL:CG2  | 1:A:57:GLY:N    | 0.52     | 2.72        | 10     | 1     |
| 1:B:52:PRO:O    | 1:B:54:ILE:N    | 0.52     | 2.43        | 4      | 5     |
| 1:B:21:SER:OG   | 1:B:75:HIS:CD2  | 0.52     | 2.63        | 7      | 1     |
| 1:B:42:TRP:CZ3  | 1:B:58:ASN:ND2  | 0.52     | 2.78        | 3      | 1     |
| 1:B:40:LEU:HD23 | 1:B:40:LEU:O    | 0.52     | 2.05        | 4      | 1     |
| 1:A:25:LEU:H    | 1:A:72:ILE:HD12 | 0.52     | 1.65        | 3      | 2     |
| 1:B:26:GLY:H    | 1:B:72:ILE:CD1  | 0.52     | 2.17        | 1      | 1     |
| 1:A:49:HIS:O    | 1:A:51:ASN:ND2  | 0.52     | 2.42        | 2      | 1     |
| 1:B:22:GLU:O    | 1:B:72:ILE:HD11 | 0.52     | 2.04        | 6      | 1     |
| 1:A:40:LEU:HD13 | 1:A:40:LEU:O    | 0.52     | 2.05        | 7      | 1     |
| 1:A:60:LEU:CD2  | 1:A:60:LEU:N    | 0.52     | 2.73        | 1      | 2     |
| 1:A:52:PRO:C    | 1:A:54:ILE:N    | 0.52     | 2.68        | 9      | 5     |
| 1:A:52:PRO:C    | 1:A:54:ILE:H    | 0.52     | 2.13        | 4      | 5     |
| 1:A:72:ILE:HG23 | 1:A:73:ILE:N    | 0.52     | 2.20        | 10     | 3     |
| 1:A:60:LEU:N    | 1:A:60:LEU:HD22 | 0.52     | 2.20        | 1      | 2     |
| 1:A:1:MET:SD    | 1:A:1:MET:N     | 0.52     | 2.75        | 8      | 2     |
| 1:B:52:PRO:C    | 1:B:54:ILE:H    | 0.51     | 2.14        | 4      | 5     |
| 1:A:21:SER:OG   | 1:A:75:HIS:CD2  | 0.51     | 2.62        | 7      | 1     |
| 1:A:40:LEU:HD23 | 1:A:40:LEU:O    | 0.51     | 2.04        | 4      | 1     |
| 1:B:73:ILE:HG23 | 1:B:74:ALA:N    | 0.51     | 2.20        | 10     | 2     |
| 1:A:42:TRP:CZ3  | 1:A:58:ASN:ND2  | 0.51     | 2.78        | 3      | 1     |
| 1:A:15:LYS:NZ   | 1:A:19:SER:OG   | 0.51     | 2.43        | 5      | 1     |
| 1:B:38:ILE:O    | 1:B:42:TRP:CD1  | 0.51     | 2.63        | 5      | 2     |
| 1:B:60:LEU:N    | 1:B:60:LEU:CD2  | 0.51     | 2.73        | 1      | 3     |
| 1:A:60:LEU:HD22 | 1:A:60:LEU:N    | 0.51     | 2.20        | 2      | 1     |
| 1:B:72:ILE:HG23 | 1:B:73:ILE:N    | 0.51     | 2.20        | 10     | 3     |
| 1:A:73:ILE:CG2  | 1:A:74:ALA:N    | 0.51     | 2.73        | 10     | 3     |
| 1:A:73:ILE:HG23 | 1:A:74:ALA:N    | 0.51     | 2.20        | 10     | 3     |
| 1:B:15:LYS:NZ   | 1:B:19:SER:OG   | 0.51     | 2.43        | 5      | 1     |
| 1:B:54:ILE:N    | 1:B:54:ILE:CD1  | 0.51     | 2.73        | 7      | 1     |
| 1:A:38:ILE:O    | 1:A:42:TRP:CD1  | 0.51     | 2.63        | 5      | 2     |
| 1:B:73:ILE:CG2  | 1:B:74:ALA:N    | 0.51     | 2.73        | 10     | 3     |
| 1:A:54:ILE:N    | 1:A:54:ILE:CD1  | 0.51     | 2.73        | 7      | 1     |
| 1:A:76:THR:HG22 | 1:A:76:THR:O    | 0.51     | 2.06        | 10     | 1     |
| 1:B:1:MET:N     | 1:B:1:MET:SD    | 0.51     | 2.84        | 4      | 1     |
| 1:B:60:LEU:N    | 1:B:60:LEU:HD22 | 0.50     | 2.20        | 1      | 3     |
| 1:A:30:THR:HG23 | 1:A:31:THR:N    | 0.50     | 2.22        | 4      | 1     |
| 1:A:60:LEU:N    | 1:A:60:LEU:CD2  | 0.50     | 2.74        | 2      | 1     |
| 1:B:7:LEU:HD22  | 1:B:7:LEU:N     | 0.50     | 2.21        | 3      | 1     |
| 1:A:35:TYR:CE2  | 1:A:65:TYR:CD2  | 0.50     | 3.00        | 8      | 2     |
| 1:B:6:PRO:O     | 1:B:9:THR:CG2   | 0.50     | 2.60        | 4      | 7     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:6:PRO:O     | 1:A:9:THR:CG2   | 0.50     | 2.60        | 4      | 7     |
| 1:B:49:HIS:ND1  | 1:B:51:ASN:OD1  | 0.50     | 2.40        | 5      | 1     |
| 1:A:35:TYR:OH   | 1:B:12:GLN:NE2  | 0.50     | 2.45        | 7      | 1     |
| 1:A:76:THR:C    | 1:A:78:GLY:H    | 0.50     | 2.15        | 7      | 6     |
| 1:B:76:THR:HG22 | 1:B:76:THR:O    | 0.50     | 2.06        | 10     | 1     |
| 1:A:7:LEU:N     | 1:A:7:LEU:HD22  | 0.50     | 2.21        | 3      | 1     |
| 1:B:29:LEU:HD12 | 1:B:29:LEU:N    | 0.50     | 2.22        | 8      | 1     |
| 1:B:32:TRP:CD1  | 1:B:36:SER:OG   | 0.49     | 2.64        | 6      | 1     |
| 1:A:3:LEU:O     | 1:A:3:LEU:HD23  | 0.49     | 2.07        | 1      | 3     |
| 1:A:19:SER:OG   | 1:B:23:HIS:ND1  | 0.49     | 2.45        | 1      | 2     |
| 1:B:56:VAL:CG1  | 1:B:57:GLY:N    | 0.49     | 2.75        | 2      | 3     |
| 1:A:12:GLN:NE2  | 1:B:35:TYR:OH   | 0.49     | 2.45        | 7      | 1     |
| 1:B:3:LEU:HD23  | 1:B:3:LEU:O     | 0.49     | 2.07        | 1      | 3     |
| 1:B:35:TYR:CE2  | 1:B:65:TYR:CD2  | 0.49     | 3.00        | 8      | 2     |
| 1:A:29:LEU:HD12 | 1:A:29:LEU:N    | 0.49     | 2.22        | 8      | 1     |
| 1:A:47:ILE:HG23 | 1:A:48:TYR:N    | 0.49     | 2.22        | 9      | 1     |
| 1:A:64:MET:SD   | 1:A:64:MET:C    | 0.49     | 2.96        | 8      | 1     |
| 1:A:65:TYR:O    | 1:A:69:VAL:HG23 | 0.49     | 2.08        | 2      | 2     |
| 1:B:16:LEU:C    | 1:B:16:LEU:CD1  | 0.49     | 2.84        | 5      | 1     |
| 1:B:64:MET:SD   | 1:B:64:MET:C    | 0.49     | 2.96        | 8      | 1     |
| 1:A:56:VAL:CG1  | 1:A:57:GLY:N    | 0.49     | 2.75        | 2      | 3     |
| 1:B:65:TYR:O    | 1:B:69:VAL:HG22 | 0.49     | 2.08        | 6      | 1     |
| 1:A:7:LEU:N     | 1:A:7:LEU:CD2   | 0.48     | 2.76        | 3      | 1     |
| 1:A:14:TYR:O    | 1:A:18:VAL:HG23 | 0.48     | 2.09        | 3      | 2     |
| 1:A:44:ILE:N    | 1:A:44:ILE:CD1  | 0.48     | 2.76        | 10     | 1     |
| 1:A:11:PRO:O    | 1:A:15:LYS:CB   | 0.48     | 2.62        | 4      | 6     |
| 1:B:14:TYR:O    | 1:B:18:VAL:HG23 | 0.48     | 2.09        | 3      | 3     |
| 1:B:76:THR:C    | 1:B:78:GLY:H    | 0.48     | 2.16        | 8      | 6     |
| 1:A:65:TYR:O    | 1:A:69:VAL:HG22 | 0.48     | 2.08        | 6      | 1     |
| 1:B:65:TYR:O    | 1:B:69:VAL:HG23 | 0.48     | 2.08        | 2      | 2     |
| 1:A:42:TRP:CD2  | 1:A:58:ASN:OD1  | 0.48     | 2.67        | 3      | 1     |
| 1:B:7:LEU:N     | 1:B:7:LEU:CD2   | 0.48     | 2.76        | 3      | 1     |
| 1:B:30:THR:HG23 | 1:B:31:THR:N    | 0.48     | 2.22        | 4      | 1     |
| 1:A:39:ALA:O    | 1:A:58:ASN:ND2  | 0.48     | 2.47        | 7      | 2     |
| 1:B:7:LEU:HD12  | 1:B:7:LEU:N     | 0.48     | 2.23        | 7      | 2     |
| 1:A:51:ASN:O    | 1:A:52:PRO:C    | 0.48     | 2.57        | 4      | 5     |
| 1:B:32:TRP:CE3  | 1:B:73:ILE:CD1  | 0.48     | 2.97        | 6      | 1     |
| 1:B:11:PRO:O    | 1:B:15:LYS:CB   | 0.48     | 2.62        | 4      | 6     |
| 1:A:32:TRP:CD1  | 1:A:36:SER:OG   | 0.48     | 2.64        | 6      | 1     |
| 1:A:32:TRP:CE3  | 1:A:73:ILE:CD1  | 0.48     | 2.97        | 6      | 1     |
| 1:B:44:ILE:N    | 1:B:44:ILE:CD1  | 0.47     | 2.76        | 10     | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:34:LEU:CD2  | 1:A:34:LEU:N    | 0.47     | 2.77        | 2      | 1     |
| 1:A:76:THR:C    | 1:A:78:GLY:N    | 0.47     | 2.72        | 7      | 5     |
| 1:A:7:LEU:HD12  | 1:A:7:LEU:N     | 0.47     | 2.23        | 7      | 3     |
| 1:B:42:TRP:CH2  | 1:B:58:ASN:ND2  | 0.47     | 2.82        | 3      | 1     |
| 1:B:47:ILE:HG23 | 1:B:48:TYR:N    | 0.47     | 2.22        | 9      | 2     |
| 1:A:3:LEU:H     | 1:A:3:LEU:HD23  | 0.47     | 1.69        | 5      | 1     |
| 1:B:21:SER:O    | 1:B:75:HIS:ND1  | 0.47     | 2.47        | 2      | 1     |
| 1:B:3:LEU:H     | 1:B:3:LEU:HD23  | 0.47     | 1.69        | 5      | 1     |
| 1:A:66:VAL:CG1  | 1:A:67:ALA:N    | 0.47     | 2.77        | 7      | 1     |
| 1:B:34:LEU:CD2  | 1:B:34:LEU:N    | 0.47     | 2.77        | 2      | 2     |
| 1:A:21:SER:O    | 1:A:75:HIS:ND1  | 0.47     | 2.47        | 2      | 1     |
| 1:B:39:ALA:O    | 1:B:58:ASN:ND2  | 0.47     | 2.47        | 7      | 2     |
| 1:A:12:GLN:OE1  | 1:A:64:MET:SD   | 0.47     | 2.73        | 2      | 1     |
| 1:B:42:TRP:CD2  | 1:B:58:ASN:OD1  | 0.47     | 2.67        | 3      | 1     |
| 1:B:51:ASN:O    | 1:B:52:PRO:C    | 0.47     | 2.57        | 4      | 5     |
| 1:A:54:ILE:CD1  | 1:A:54:ILE:H    | 0.47     | 2.22        | 7      | 1     |
| 1:B:66:VAL:CG1  | 1:B:67:ALA:N    | 0.47     | 2.77        | 7      | 1     |
| 1:A:42:TRP:CH2  | 1:A:58:ASN:ND2  | 0.47     | 2.82        | 3      | 1     |
| 1:B:76:THR:C    | 1:B:78:GLY:N    | 0.47     | 2.72        | 7      | 5     |
| 1:B:53:THR:O    | 1:B:56:VAL:N    | 0.47     | 2.47        | 5      | 1     |
| 1:A:66:VAL:O    | 1:A:70:VAL:HG23 | 0.47     | 2.10        | 6      | 2     |
| 1:B:62:PHE:CD2  | 1:B:62:PHE:C    | 0.47     | 2.93        | 4      | 1     |
| 1:B:12:GLN:OE1  | 1:B:64:MET:SD   | 0.46     | 2.73        | 2      | 1     |
| 1:B:30:THR:CG2  | 1:B:31:THR:N    | 0.46     | 2.79        | 4      | 1     |
| 1:B:54:ILE:CD1  | 1:B:54:ILE:H    | 0.46     | 2.22        | 7      | 1     |
| 1:A:62:PHE:C    | 1:A:62:PHE:CD2  | 0.46     | 2.93        | 4      | 1     |
| 1:A:16:LEU:C    | 1:A:16:LEU:CD1  | 0.46     | 2.84        | 5      | 1     |
| 1:A:7:LEU:C     | 1:A:9:THR:H     | 0.46     | 2.19        | 7      | 4     |
| 1:B:24:ALA:CB   | 1:B:72:ILE:HG21 | 0.46     | 2.41        | 7      | 1     |
| 1:B:66:VAL:O    | 1:B:70:VAL:HG23 | 0.46     | 2.10        | 6      | 2     |
| 1:A:30:THR:CG2  | 1:A:31:THR:N    | 0.46     | 2.78        | 4      | 1     |
| 1:A:51:ASN:ND2  | 1:A:52:PRO:O    | 0.46     | 2.49        | 8      | 1     |
| 1:A:5:SER:N     | 1:A:6:PRO:HD3   | 0.46     | 2.26        | 5      | 7     |
| 1:A:69:VAL:O    | 1:A:73:ILE:HG22 | 0.46     | 2.11        | 10     | 2     |
| 1:A:35:TYR:CD1  | 1:A:65:TYR:OH   | 0.46     | 2.62        | 2      | 1     |
| 1:A:24:ALA:CB   | 1:A:72:ILE:HG21 | 0.46     | 2.41        | 7      | 1     |
| 1:B:45:TYR:CD2  | 1:B:49:HIS:NE2  | 0.46     | 2.84        | 6      | 1     |
| 1:B:56:VAL:O    | 1:B:59:CYS:SG   | 0.46     | 2.70        | 10     | 1     |
| 1:A:45:TYR:CD2  | 1:A:49:HIS:NE2  | 0.45     | 2.84        | 6      | 1     |
| 1:B:51:ASN:ND2  | 1:B:52:PRO:O    | 0.45     | 2.49        | 8      | 1     |
| 1:A:23:HIS:O    | 1:B:23:HIS:O    | 0.45     | 2.35        | 1      | 2     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:B:2:GLY:O     | 1:B:6:PRO:HD3   | 0.45     | 2.11        | 7      | 2     |
| 1:A:34:LEU:N    | 1:A:34:LEU:HD22 | 0.45     | 2.25        | 2      | 2     |
| 1:B:35:TYR:CD1  | 1:B:65:TYR:OH   | 0.45     | 2.62        | 2      | 1     |
| 1:B:35:TYR:CG   | 1:B:65:TYR:CZ   | 0.45     | 3.05        | 2      | 1     |
| 1:A:35:TYR:CZ   | 1:A:65:TYR:CE1  | 0.45     | 3.04        | 5      | 1     |
| 1:B:32:TRP:CD1  | 1:B:32:TRP:C    | 0.45     | 2.93        | 1      | 1     |
| 1:A:35:TYR:CG   | 1:A:65:TYR:CZ   | 0.45     | 3.05        | 2      | 1     |
| 1:B:34:LEU:N    | 1:B:34:LEU:HD22 | 0.45     | 2.25        | 2      | 2     |
| 1:B:69:VAL:O    | 1:B:73:ILE:HG22 | 0.45     | 2.10        | 10     | 2     |
| 1:B:51:ASN:OD1  | 1:B:51:ASN:O    | 0.45     | 2.35        | 2      | 2     |
| 1:A:3:LEU:N     | 1:A:3:LEU:CD1   | 0.45     | 2.80        | 4      | 1     |
| 1:A:38:ILE:CG2  | 1:A:42:TRP:HE1  | 0.45     | 2.25        | 5      | 1     |
| 1:A:56:VAL:O    | 1:A:59:CYS:SG   | 0.45     | 2.70        | 10     | 1     |
| 1:B:35:TYR:CZ   | 1:B:65:TYR:CE1  | 0.45     | 3.04        | 5      | 1     |
| 1:B:5:SER:N     | 1:B:6:PRO:HD3   | 0.45     | 2.26        | 5      | 6     |
| 1:B:3:LEU:N     | 1:B:3:LEU:CD1   | 0.45     | 2.80        | 4      | 1     |
| 1:A:66:VAL:HG13 | 1:A:67:ALA:N    | 0.45     | 2.26        | 7      | 1     |
| 1:A:2:GLY:O     | 1:A:6:PRO:HD3   | 0.45     | 2.11        | 7      | 2     |
| 1:B:38:ILE:CG2  | 1:B:42:TRP:HE1  | 0.45     | 2.25        | 5      | 1     |
| 1:B:66:VAL:HG13 | 1:B:67:ALA:N    | 0.45     | 2.26        | 7      | 1     |
| 1:B:42:TRP:CE3  | 1:B:58:ASN:OD1  | 0.45     | 2.70        | 6      | 1     |
| 1:B:49:HIS:N    | 1:B:49:HIS:ND1  | 0.45     | 2.65        | 6      | 1     |
| 1:A:49:HIS:ND1  | 1:A:49:HIS:O    | 0.44     | 2.51        | 5      | 1     |
| 1:A:42:TRP:CE3  | 1:A:58:ASN:OD1  | 0.44     | 2.70        | 6      | 1     |
| 1:B:58:ASN:O    | 1:B:58:ASN:ND2  | 0.44     | 2.50        | 6      | 1     |
| 1:A:16:LEU:HG   | 1:A:24:ALA:HB1  | 0.44     | 1.88        | 10     | 2     |
| 1:A:51:ASN:O    | 1:A:51:ASN:OD1  | 0.44     | 2.35        | 2      | 2     |
| 1:A:42:TRP:CE2  | 1:A:58:ASN:OD1  | 0.44     | 2.70        | 3      | 1     |
| 1:A:13:LEU:O    | 1:A:13:LEU:HD13 | 0.44     | 2.12        | 2      | 2     |
| 1:B:35:TYR:CZ   | 1:B:65:TYR:CD1  | 0.44     | 3.04        | 5      | 1     |
| 1:B:43:THR:HG21 | 1:B:59:CYS:SG   | 0.44     | 2.52        | 5      | 1     |
| 1:B:35:TYR:CE1  | 1:B:65:TYR:OH   | 0.44     | 2.63        | 2      | 1     |
| 1:A:43:THR:HG21 | 1:A:59:CYS:SG   | 0.44     | 2.52        | 5      | 1     |
| 1:B:7:LEU:C     | 1:B:9:THR:H     | 0.44     | 2.19        | 7      | 4     |
| 1:A:15:LYS:O    | 1:A:19:SER:CB   | 0.44     | 2.65        | 6      | 4     |
| 1:A:53:THR:O    | 1:A:56:VAL:N    | 0.44     | 2.47        | 5      | 1     |
| 1:B:49:HIS:ND1  | 1:B:49:HIS:O    | 0.44     | 2.51        | 5      | 1     |
| 1:B:32:TRP:NE1  | 1:B:69:VAL:HG21 | 0.44     | 2.27        | 6      | 1     |
| 1:A:32:TRP:CD1  | 1:A:32:TRP:C    | 0.44     | 2.93        | 1      | 2     |
| 1:B:42:TRP:CE2  | 1:B:58:ASN:OD1  | 0.44     | 2.70        | 3      | 1     |
| 1:A:35:TYR:CE2  | 1:A:65:TYR:CD1  | 0.44     | 3.06        | 5      | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:35:TYR:CZ   | 1:A:65:TYR:CD1  | 0.44     | 3.04        | 5      | 1     |
| 1:B:34:LEU:HD12 | 1:B:34:LEU:N    | 0.44     | 2.28        | 6      | 1     |
| 1:A:54:ILE:O    | 1:A:58:ASN:N    | 0.43     | 2.49        | 1      | 1     |
| 1:B:13:LEU:HD13 | 1:B:13:LEU:O    | 0.43     | 2.13        | 2      | 2     |
| 1:A:15:LYS:O    | 1:A:19:SER:OG   | 0.43     | 2.36        | 6      | 2     |
| 1:B:15:LYS:O    | 1:B:19:SER:CB   | 0.43     | 2.66        | 6      | 3     |
| 1:A:49:HIS:ND1  | 1:A:51:ASN:ND2  | 0.43     | 2.66        | 9      | 1     |
| 1:B:49:HIS:ND1  | 1:B:51:ASN:ND2  | 0.43     | 2.66        | 9      | 1     |
| 1:A:62:PHE:O    | 1:A:66:VAL:CG2  | 0.43     | 2.66        | 1      | 1     |
| 1:A:29:LEU:N    | 1:A:79:THR:OG1  | 0.43     | 2.51        | 2      | 1     |
| 1:B:53:THR:O    | 1:B:56:VAL:HG12 | 0.43     | 2.13        | 2      | 1     |
| 1:B:72:ILE:CG2  | 1:B:73:ILE:N    | 0.43     | 2.81        | 3      | 1     |
| 1:B:35:TYR:CE2  | 1:B:65:TYR:CD1  | 0.43     | 3.06        | 5      | 1     |
| 1:B:66:VAL:O    | 1:B:70:VAL:HG13 | 0.43     | 2.14        | 8      | 1     |
| 1:B:49:HIS:O    | 1:B:51:ASN:CG   | 0.43     | 2.61        | 2      | 1     |
| 1:A:72:ILE:CG2  | 1:A:73:ILE:N    | 0.43     | 2.82        | 3      | 1     |
| 1:B:62:PHE:O    | 1:B:66:VAL:CG2  | 0.43     | 2.66        | 1      | 1     |
| 1:A:44:ILE:O    | 1:A:47:ILE:HG22 | 0.43     | 2.13        | 2      | 1     |
| 1:A:58:ASN:O    | 1:A:58:ASN:ND2  | 0.43     | 2.50        | 6      | 1     |
| 1:A:73:ILE:O    | 1:A:77:GLY:CA   | 0.43     | 2.66        | 10     | 1     |
| 1:B:73:ILE:O    | 1:B:77:GLY:CA   | 0.43     | 2.67        | 10     | 1     |
| 1:A:35:TYR:CE1  | 1:A:65:TYR:OH   | 0.43     | 2.63        | 2      | 1     |
| 1:A:43:THR:OG1  | 1:A:58:ASN:ND2  | 0.43     | 2.51        | 2      | 1     |
| 1:B:29:LEU:N    | 1:B:79:THR:OG1  | 0.43     | 2.51        | 2      | 1     |
| 1:A:7:LEU:C     | 1:A:9:THR:N     | 0.43     | 2.77        | 7      | 2     |
| 1:A:32:TRP:NE1  | 1:A:69:VAL:HG21 | 0.43     | 2.27        | 6      | 1     |
| 1:A:28:SER:O    | 1:A:31:THR:OG1  | 0.43     | 2.35        | 1      | 2     |
| 1:B:24:ALA:HB3  | 1:B:72:ILE:HG22 | 0.43     | 1.90        | 2      | 1     |
| 1:B:16:LEU:HG   | 1:B:24:ALA:HB1  | 0.43     | 1.89        | 10     | 2     |
| 1:B:43:THR:HG1  | 1:B:58:ASN:CG   | 0.43     | 2.21        | 6      | 1     |
| 1:B:69:VAL:HG23 | 1:B:70:VAL:N    | 0.43     | 2.29        | 6      | 1     |
| 1:A:66:VAL:O    | 1:A:70:VAL:HG13 | 0.43     | 2.14        | 8      | 1     |
| 1:A:49:HIS:O    | 1:A:51:ASN:OD1  | 0.43     | 2.36        | 1      | 1     |
| 1:A:26:GLY:O    | 1:A:27:LEU:HD12 | 0.43     | 2.13        | 3      | 1     |
| 1:A:32:TRP:CH2  | 1:A:66:VAL:HG23 | 0.43     | 2.48        | 5      | 1     |
| 1:B:32:TRP:CH2  | 1:B:66:VAL:HG23 | 0.43     | 2.48        | 5      | 1     |
| 1:B:11:PRO:O    | 1:B:15:LYS:N    | 0.43     | 2.44        | 4      | 2     |
| 1:B:15:LYS:O    | 1:B:19:SER:OG   | 0.43     | 2.36        | 6      | 2     |
| 1:B:54:ILE:O    | 1:B:58:ASN:N    | 0.42     | 2.49        | 1      | 1     |
| 1:A:53:THR:O    | 1:A:56:VAL:HG12 | 0.42     | 2.14        | 2      | 1     |
| 1:B:44:ILE:CD1  | 1:B:44:ILE:H    | 0.42     | 2.27        | 10     | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:49:HIS:O    | 1:A:51:ASN:CG   | 0.42     | 2.61        | 2      | 1     |
| 1:B:44:ILE:O    | 1:B:47:ILE:HG22 | 0.42     | 2.13        | 2      | 1     |
| 1:B:47:ILE:CG2  | 1:B:48:TYR:N    | 0.42     | 2.82        | 9      | 1     |
| 1:B:25:LEU:C    | 1:B:27:LEU:N    | 0.42     | 2.76        | 10     | 1     |
| 1:B:49:HIS:O    | 1:B:51:ASN:OD1  | 0.42     | 2.37        | 1      | 1     |
| 1:B:28:SER:O    | 1:B:31:THR:OG1  | 0.42     | 2.36        | 2      | 2     |
| 1:B:25:LEU:C    | 1:B:27:LEU:H    | 0.42     | 2.23        | 10     | 1     |
| 1:B:61:GLY:O    | 1:B:65:TYR:CD1  | 0.42     | 2.72        | 10     | 1     |
| 1:A:24:ALA:HB3  | 1:A:72:ILE:HG22 | 0.42     | 1.90        | 2      | 1     |
| 1:B:43:THR:OG1  | 1:B:58:ASN:ND2  | 0.42     | 2.51        | 2      | 1     |
| 1:B:26:GLY:O    | 1:B:27:LEU:HD12 | 0.42     | 2.13        | 3      | 1     |
| 1:A:47:ILE:CG2  | 1:A:48:TYR:N    | 0.42     | 2.82        | 9      | 1     |
| 1:A:44:ILE:CD1  | 1:A:44:ILE:H    | 0.42     | 2.27        | 10     | 1     |
| 1:B:49:HIS:O    | 1:B:49:HIS:CG   | 0.42     | 2.72        | 5      | 1     |
| 1:A:25:LEU:C    | 1:A:27:LEU:H    | 0.42     | 2.23        | 10     | 1     |
| 1:A:44:ILE:HD12 | 1:A:44:ILE:H    | 0.42     | 1.74        | 10     | 1     |
| 1:B:6:PRO:O     | 1:B:9:THR:OG1   | 0.42     | 2.34        | 8      | 2     |
| 1:A:34:LEU:N    | 1:A:34:LEU:CD2  | 0.42     | 2.81        | 4      | 1     |
| 1:B:65:TYR:O    | 1:B:69:VAL:HG13 | 0.42     | 2.14        | 6      | 1     |
| 1:A:61:GLY:O    | 1:A:65:TYR:CD1  | 0.42     | 2.72        | 10     | 1     |
| 1:A:79:THR:O    | 1:A:80:TYR:O    | 0.42     | 2.38        | 3      | 1     |
| 1:B:7:LEU:N     | 1:B:7:LEU:CD1   | 0.42     | 2.82        | 7      | 1     |
| 1:B:40:LEU:O    | 1:B:43:THR:OG1  | 0.42     | 2.36        | 8      | 1     |
| 1:B:35:TYR:CB   | 1:B:65:TYR:CE2  | 0.42     | 3.03        | 2      | 1     |
| 1:A:11:PRO:O    | 1:A:15:LYS:N    | 0.42     | 2.44        | 4      | 1     |
| 1:A:7:LEU:N     | 1:A:7:LEU:CD1   | 0.42     | 2.82        | 7      | 1     |
| 1:B:55:TRP:CH2  | 1:B:59:CYS:SG   | 0.41     | 3.13        | 2      | 1     |
| 1:B:7:LEU:C     | 1:B:9:THR:N     | 0.41     | 2.78        | 4      | 2     |
| 1:B:53:THR:C    | 1:B:55:TRP:N    | 0.41     | 2.78        | 8      | 2     |
| 1:B:15:LYS:O    | 1:B:19:SER:N    | 0.41     | 2.45        | 5      | 2     |
| 1:A:34:LEU:HD12 | 1:A:34:LEU:N    | 0.41     | 2.28        | 6      | 1     |
| 1:A:60:LEU:N    | 1:A:60:LEU:HD12 | 0.41     | 2.30        | 8      | 1     |
| 1:A:35:TYR:CD2  | 1:A:35:TYR:C    | 0.41     | 2.98        | 4      | 1     |
| 1:A:65:TYR:O    | 1:A:69:VAL:HG13 | 0.41     | 2.14        | 6      | 1     |
| 1:A:69:VAL:HG23 | 1:A:70:VAL:N    | 0.41     | 2.28        | 6      | 1     |
| 1:B:20:HIS:O    | 1:B:24:ALA:CB   | 0.41     | 2.65        | 2      | 1     |
| 1:A:53:THR:C    | 1:A:55:TRP:N    | 0.41     | 2.78        | 8      | 3     |
| 1:B:35:TYR:CD2  | 1:B:35:TYR:C    | 0.41     | 2.98        | 4      | 1     |
| 1:B:38:ILE:HG22 | 1:B:42:TRP:HE1  | 0.41     | 1.75        | 5      | 1     |
| 1:B:46:GLY:HA3  | 1:B:55:TRP:CD1  | 0.41     | 2.50        | 5      | 1     |
| 1:A:55:TRP:CZ2  | 1:A:59:CYS:SG   | 0.41     | 3.14        | 2      | 1     |

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| Atom-1         | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|----------------|-----------------|----------|-------------|--------|-------|
|                |                 |          |             | Worst  | Total |
| 1:A:49:HIS:ND1 | 1:A:49:HIS:N    | 0.41     | 2.65        | 6      | 1     |
| 1:B:10:MET:N   | 1:B:11:PRO:CD   | 0.41     | 2.84        | 1      | 2     |
| 1:A:55:TRP:CH2 | 1:A:59:CYS:SG   | 0.41     | 3.13        | 2      | 1     |
| 1:B:79:THR:O   | 1:B:80:TYR:O    | 0.41     | 2.38        | 3      | 1     |
| 1:B:32:TRP:NE1 | 1:B:36:SER:HG   | 0.41     | 2.13        | 8      | 1     |
| 1:A:17:TYR:CD2 | 1:A:17:TYR:C    | 0.41     | 2.99        | 10     | 1     |
| 1:A:25:LEU:C   | 1:A:27:LEU:N    | 0.41     | 2.77        | 10     | 1     |
| 1:A:20:HIS:O   | 1:A:24:ALA:CB   | 0.41     | 2.65        | 2      | 2     |
| 1:A:46:GLY:HA3 | 1:A:55:TRP:CD1  | 0.41     | 2.50        | 5      | 1     |
| 1:B:60:LEU:N   | 1:B:60:LEU:HD12 | 0.41     | 2.30        | 8      | 1     |
| 1:A:49:HIS:O   | 1:A:49:HIS:CG   | 0.41     | 2.72        | 5      | 1     |
| 1:A:32:TRP:NE1 | 1:A:36:SER:HG   | 0.41     | 2.13        | 8      | 1     |
| 1:B:35:TYR:CG  | 1:B:65:TYR:CE2  | 0.41     | 3.09        | 5      | 1     |
| 1:A:12:GLN:O   | 1:A:16:LEU:CB   | 0.41     | 2.69        | 6      | 1     |
| 1:A:15:LYS:O   | 1:A:19:SER:N    | 0.41     | 2.48        | 10     | 1     |
| 1:A:10:MET:N   | 1:A:11:PRO:CD   | 0.41     | 2.84        | 1      | 2     |
| 1:A:42:TRP:CD1 | 1:A:42:TRP:O    | 0.41     | 2.74        | 3      | 1     |
| 1:B:17:TYR:CD2 | 1:B:17:TYR:C    | 0.41     | 2.99        | 10     | 1     |
| 1:A:35:TYR:CB  | 1:A:65:TYR:CE2  | 0.40     | 3.03        | 2      | 1     |
| 1:B:55:TRP:CZ2 | 1:B:59:CYS:SG   | 0.40     | 3.14        | 2      | 1     |
| 1:B:3:LEU:H    | 1:B:3:LEU:CD2   | 0.40     | 2.29        | 5      | 1     |
| 1:A:43:THR:OG1 | 1:A:58:ASN:CG   | 0.40     | 2.64        | 7      | 1     |
| 1:A:3:LEU:O    | 1:A:6:PRO:HD2   | 0.40     | 2.17        | 3      | 1     |
| 1:B:34:LEU:N   | 1:B:34:LEU:CD1  | 0.40     | 2.84        | 6      | 1     |
| 1:B:7:LEU:N    | 1:B:7:LEU:HD12  | 0.40     | 2.30        | 4      | 1     |
| 1:B:43:THR:OG1 | 1:B:58:ASN:CG   | 0.40     | 2.64        | 7      | 1     |
| 1:B:37:PHE:O   | 1:B:41:LEU:N    | 0.40     | 2.51        | 1      | 1     |
| 1:A:35:TYR:CG  | 1:A:65:TYR:CE2  | 0.40     | 3.09        | 5      | 1     |
| 1:B:12:GLN:O   | 1:B:16:LEU:CB   | 0.40     | 2.69        | 6      | 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     | 78/80 (98%) | 72±2 (93±2%) | 4±2 (6±2%) | 1±1 (1±1%) | 11 58       |

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| Mol | Chain | Analysed        | Favoured     | Allowed    | Outliers   | Percentiles |    |
|-----|-------|-----------------|--------------|------------|------------|-------------|----|
| 1   | B     | 78/80 (98%)     | 72±2 (93±2%) | 4±2 (6±2%) | 1±1 (1±1%) | 11          | 58 |
| All | All   | 1560/1600 (98%) | 1450 (93%)   | 88 (6%)    | 22 (1%)    | 11          | 58 |

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

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 53  | THR  | 5              |
| 1   | B     | 53  | THR  | 5              |
| 1   | A     | 20  | HIS  | 3              |
| 1   | B     | 20  | HIS  | 3              |
| 1   | A     | 11  | PRO  | 3              |
| 1   | B     | 11  | PRO  | 3              |

### 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     | 67/67 (100%)     | 61±2 (91±3%) | 6±2 (9±3%) | 11          | 57 |
| 1   | B     | 67/67 (100%)     | 61±2 (91±3%) | 6±2 (9±3%) | 11          | 57 |
| All | All   | 1340/1340 (100%) | 1218 (91%)   | 122 (9%)   | 11          | 57 |

All 48 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     | 54  | ILE  | 7              |
| 1   | B     | 54  | ILE  | 7              |
| 1   | A     | 20  | HIS  | 6              |
| 1   | A     | 51  | ASN  | 6              |
| 1   | B     | 20  | HIS  | 6              |
| 1   | B     | 51  | ASN  | 6              |
| 1   | A     | 10  | MET  | 5              |
| 1   | B     | 10  | MET  | 5              |
| 1   | A     | 3   | LEU  | 4              |
| 1   | B     | 3   | LEU  | 4              |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 13  | LEU  | 3              |
| 1   | A     | 25  | LEU  | 3              |
| 1   | B     | 13  | LEU  | 3              |
| 1   | B     | 25  | LEU  | 3              |
| 1   | A     | 5   | SER  | 3              |
| 1   | B     | 5   | SER  | 3              |
| 1   | A     | 15  | LYS  | 3              |
| 1   | A     | 53  | THR  | 3              |
| 1   | B     | 15  | LYS  | 3              |
| 1   | B     | 53  | THR  | 3              |
| 1   | A     | 27  | LEU  | 2              |
| 1   | B     | 27  | LEU  | 2              |
| 1   | A     | 40  | LEU  | 2              |
| 1   | A     | 76  | THR  | 2              |
| 1   | A     | 79  | THR  | 2              |
| 1   | B     | 40  | LEU  | 2              |
| 1   | B     | 76  | THR  | 2              |
| 1   | B     | 79  | THR  | 2              |
| 1   | A     | 16  | LEU  | 1              |
| 1   | B     | 16  | LEU  | 1              |
| 1   | A     | 32  | TRP  | 1              |
| 1   | A     | 47  | ILE  | 1              |
| 1   | B     | 32  | TRP  | 1              |
| 1   | B     | 47  | ILE  | 1              |
| 1   | A     | 42  | TRP  | 1              |
| 1   | A     | 48  | TYR  | 1              |
| 1   | A     | 72  | ILE  | 1              |
| 1   | B     | 42  | TRP  | 1              |
| 1   | B     | 48  | TYR  | 1              |
| 1   | B     | 72  | ILE  | 1              |
| 1   | A     | 1   | MET  | 1              |
| 1   | B     | 1   | MET  | 1              |
| 1   | A     | 55  | TRP  | 1              |
| 1   | B     | 55  | TRP  | 1              |
| 1   | A     | 21  | SER  | 1              |
| 1   | A     | 75  | HIS  | 1              |
| 1   | B     | 21  | SER  | 1              |
| 1   | B     | 75  | HIS  | 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](#)

There are no ligands in this entry.

## 6.7 Other polymers [i](#)

There are no such molecules in this entry.

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

There are no chain breaks in this entry.

## 7 Chemical shift validation [i](#)

The completeness of assignment taking into account all chemical shift lists is 18% for the well-defined parts and 18% for the entire structure.

### 7.1 Chemical shift list 1

File name: working\_cs.cif

Chemical shift list name: *assigned\_chemical\_shifts\_1*

#### 7.1.1 Bookkeeping [i](#)

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                  | 394 |
| Number of shifts mapped to atoms        | 394 |
| Number of unparsed shifts               | 0   |
| Number of shifts with mapping errors    | 0   |
| Number of shifts with mapping warnings  | 0   |
| Number of shift outliers (ShiftChecker) | 0   |

#### 7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

| Nucleus                | # values | Correction $\pm$ precision, ppm | Suggested action           |
|------------------------|----------|---------------------------------|----------------------------|
| $^{13}\text{C}_\alpha$ | 80       | $-1.30 \pm 0.18$                | Should be checked          |
| $^{13}\text{C}_\beta$  | 72       | $0.37 \pm 0.27$                 | None needed ( $< 0.5$ ppm) |
| $^{13}\text{C}'$       | 80       | $-0.73 \pm 0.19$                | Should be applied          |
| $^{15}\text{N}$        | 79       | $0.86 \pm 0.31$                 | Should be applied          |

#### 7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 18%, i.e. 391 atoms were assigned a chemical shift out of a possible 2222. 0 out of 36 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total          | $^1\text{H}$ | $^{13}\text{C}$ | $^{15}\text{N}$ |
|-----------|----------------|--------------|-----------------|-----------------|
| Backbone  | 236/804 (29%)  | 0/330 (0%)   | 160/320 (50%)   | 76/154 (49%)    |
| Sidechain | 155/1124 (14%) | 0/764 (0%)   | 151/350 (43%)   | 4/10 (40%)      |

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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 | 0/294 (0%)     | 0/144 (0%)           | 0/136 (0%)            | 0/14 (0%)             |
| Overall  | 391/2222 (18%) | 0/1238 (0%)          | 311/806 (39%)         | 80/178 (45%)          |

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 18%, i.e. 391 atoms were assigned a chemical shift out of a possible 2222. 0 out of 36 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  | 236/804 (29%)  | 0/330 (0%)           | 160/320 (50%)         | 76/154 (49%)          |
| Sidechain | 155/1124 (14%) | 0/764 (0%)           | 151/350 (43%)         | 4/10 (40%)            |
| Aromatic  | 0/294 (0%)     | 0/144 (0%)           | 0/136 (0%)            | 0/14 (0%)             |
| Overall   | 391/2222 (18%) | 0/1238 (0%)          | 311/806 (39%)         | 80/178 (45%)          |

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

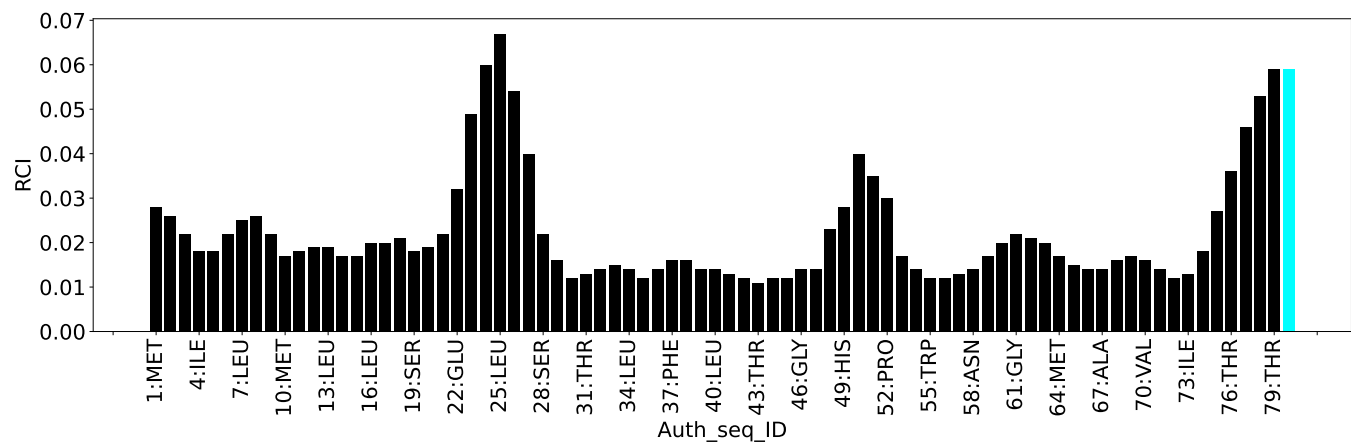
#### 7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

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

Random coil index (RCI) for chain A:



## 8 NMR restraints analysis

### 8.1 Conformationally restricting restraints

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

| Description                                              | Value |
|----------------------------------------------------------|-------|
| Total distance restraints                                | 918   |
| Intra-residue ( $ i-j =0$ )                              | 356   |
| Sequential ( $ i-j =1$ )                                 | 164   |
| Medium range ( $ i-j >1$ and $ i-j <5$ )                 | 256   |
| Long range ( $ i-j \geq 5$ )                             | 142   |
| Inter-chain                                              | 0     |
| Hydrogen bond restraints                                 | 0     |
| Disulfide bond restraints                                | 0     |
| Total dihedral-angle restraints                          | 312   |
| Number of unmapped restraints                            | 0     |
| Number of restraints per residue                         | 7.7   |
| Number of long range restraints per residue <sup>1</sup> | 0.9   |

<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)  | 1.2                                    | 0.2     |
| 0.2-0.5 (Medium) | 3.8                                    | 0.5     |
| >0.5 (Large)     | 13.6                                   | 4.32    |

### 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)   | 73.7                                   | 10.0    |
| 10.0-20.0 (Medium) | 8.5                                    | 19.48   |
| >20.0 (Large)      | 6.0                                    | 159.89  |

## 9 Distance violation analysis ⓘ

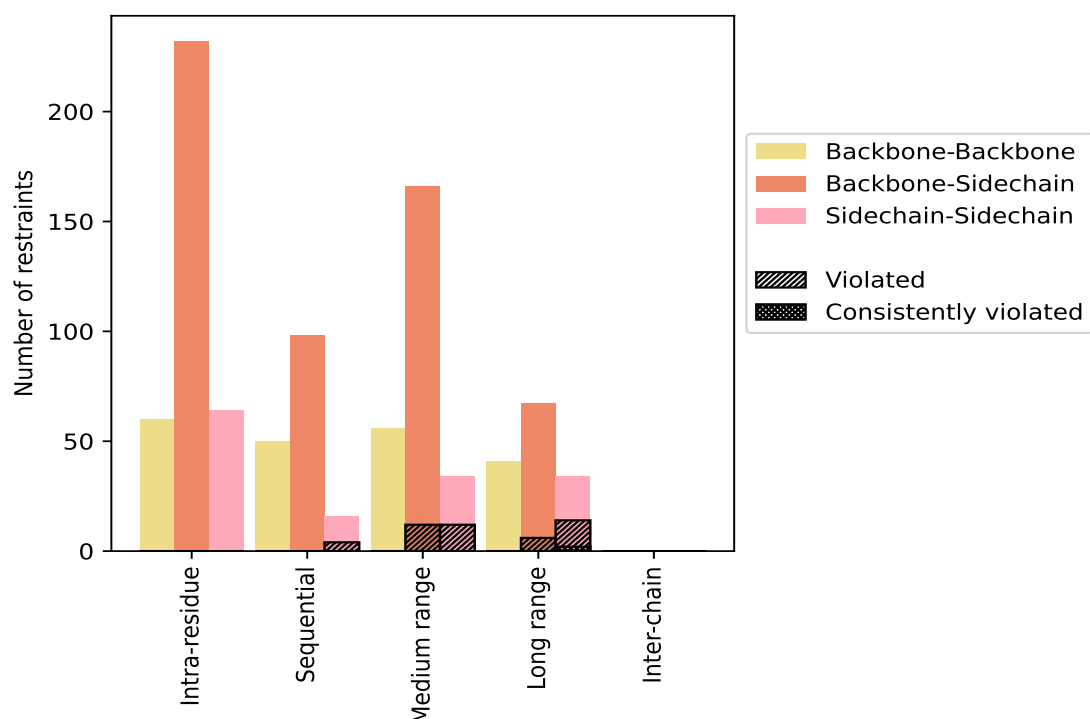
### 9.1 Summary of distance violations ⓘ

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="#">356</a> | <a href="#">38.8</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                                          | 60                  | 6.5                   | 0                     | 0.0                  | 0.0                 | 0                                  | 0.0                 | 0.0                 |
| Backbone-Sidechain                                         | 232                 | 25.3                  | 0                     | 0.0                  | 0.0                 | 0                                  | 0.0                 | 0.0                 |
| Sidechain-Sidechain                                        | 64                  | 7.0                   | 0                     | 0.0                  | 0.0                 | 0                                  | 0.0                 | 0.0                 |
| <a href="#">Sequential ( i-j =1)</a>                       | <a href="#">164</a> | <a href="#">17.9</a>  | <a href="#">4</a>     | <a href="#">2.4</a>  | <a href="#">0.4</a> | <a href="#">0</a>                  | <a href="#">0.0</a> | <a href="#">0.0</a> |
| Backbone-Backbone                                          | 50                  | 5.4                   | 0                     | 0.0                  | 0.0                 | 0                                  | 0.0                 | 0.0                 |
| Backbone-Sidechain                                         | 98                  | 10.7                  | 0                     | 0.0                  | 0.0                 | 0                                  | 0.0                 | 0.0                 |
| Sidechain-Sidechain                                        | 16                  | 1.7                   | 4                     | 25.0                 | 0.4                 | 0                                  | 0.0                 | 0.0                 |
| <a href="#">Medium range ( i-j &gt;1 &amp;  i-j &lt;5)</a> | <a href="#">256</a> | <a href="#">27.9</a>  | <a href="#">24</a>    | <a href="#">9.4</a>  | <a href="#">2.6</a> | <a href="#">0</a>                  | <a href="#">0.0</a> | <a href="#">0.0</a> |
| Backbone-Backbone                                          | 56                  | 6.1                   | 0                     | 0.0                  | 0.0                 | 0                                  | 0.0                 | 0.0                 |
| Backbone-Sidechain                                         | 166                 | 18.1                  | 12                    | 7.2                  | 1.3                 | 0                                  | 0.0                 | 0.0                 |
| Sidechain-Sidechain                                        | 34                  | 3.7                   | 12                    | 35.3                 | 1.3                 | 0                                  | 0.0                 | 0.0                 |
| <a href="#">Long range ( i-j ≥5)</a>                       | <a href="#">142</a> | <a href="#">15.5</a>  | <a href="#">20</a>    | <a href="#">14.1</a> | <a href="#">2.2</a> | <a href="#">2</a>                  | <a href="#">1.4</a> | <a href="#">0.2</a> |
| Backbone-Backbone                                          | 41                  | 4.5                   | 0                     | 0.0                  | 0.0                 | 0                                  | 0.0                 | 0.0                 |
| Backbone-Sidechain                                         | 67                  | 7.3                   | 6                     | 9.0                  | 0.7                 | 0                                  | 0.0                 | 0.0                 |
| Sidechain-Sidechain                                        | 34                  | 3.7                   | 14                    | 41.2                 | 1.5                 | 2                                  | 5.9                 | 0.2                 |
| <a href="#">Inter-chain</a>                                | <a href="#">0</a>   | <a href="#">0.0</a>   | <a href="#">0</a>     | <a href="#">0.0</a>  | <a href="#">0.0</a> | <a href="#">0</a>                  | <a href="#">0.0</a> | <a href="#">0.0</a> |
| Backbone-Backbone                                          | 0                   | 0.0                   | 0                     | 0.0                  | 0.0                 | 0                                  | 0.0                 | 0.0                 |
| Backbone-Sidechain                                         | 0                   | 0.0                   | 0                     | 0.0                  | 0.0                 | 0                                  | 0.0                 | 0.0                 |
| Sidechain-Sidechain                                        | 0                   | 0.0                   | 0                     | 0.0                  | 0.0                 | 0                                  | 0.0                 | 0.0                 |
| <a href="#">Hydrogen bond</a>                              | <a href="#">0</a>   | <a href="#">0.0</a>   | <a href="#">0</a>     | <a href="#">0.0</a>  | <a href="#">0.0</a> | <a href="#">0</a>                  | <a href="#">0.0</a> | <a href="#">0.0</a> |
| <a href="#">Disulfide bond</a>                             | <a href="#">0</a>   | <a href="#">0.0</a>   | <a href="#">0</a>     | <a href="#">0.0</a>  | <a href="#">0.0</a> | <a href="#">0</a>                  | <a href="#">0.0</a> | <a href="#">0.0</a> |
| <a href="#">Total</a>                                      | <a href="#">918</a> | <a href="#">100.0</a> | <a href="#">48</a>    | <a href="#">5.2</a>  | <a href="#">5.2</a> | <a href="#">2</a>                  | <a href="#">0.2</a> | <a href="#">0.2</a> |
| Backbone-Backbone                                          | 207                 | 22.5                  | 0                     | 0.0                  | 0.0                 | 0                                  | 0.0                 | 0.0                 |
| Backbone-Sidechain                                         | 563                 | 61.3                  | 18                    | 3.2                  | 2.0                 | 0                                  | 0.0                 | 0.0                 |
| Sidechain-Sidechain                                        | 148                 | 16.1                  | 30                    | 20.3                 | 3.3                 | 2                                  | 1.4                 | 0.2                 |

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

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



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

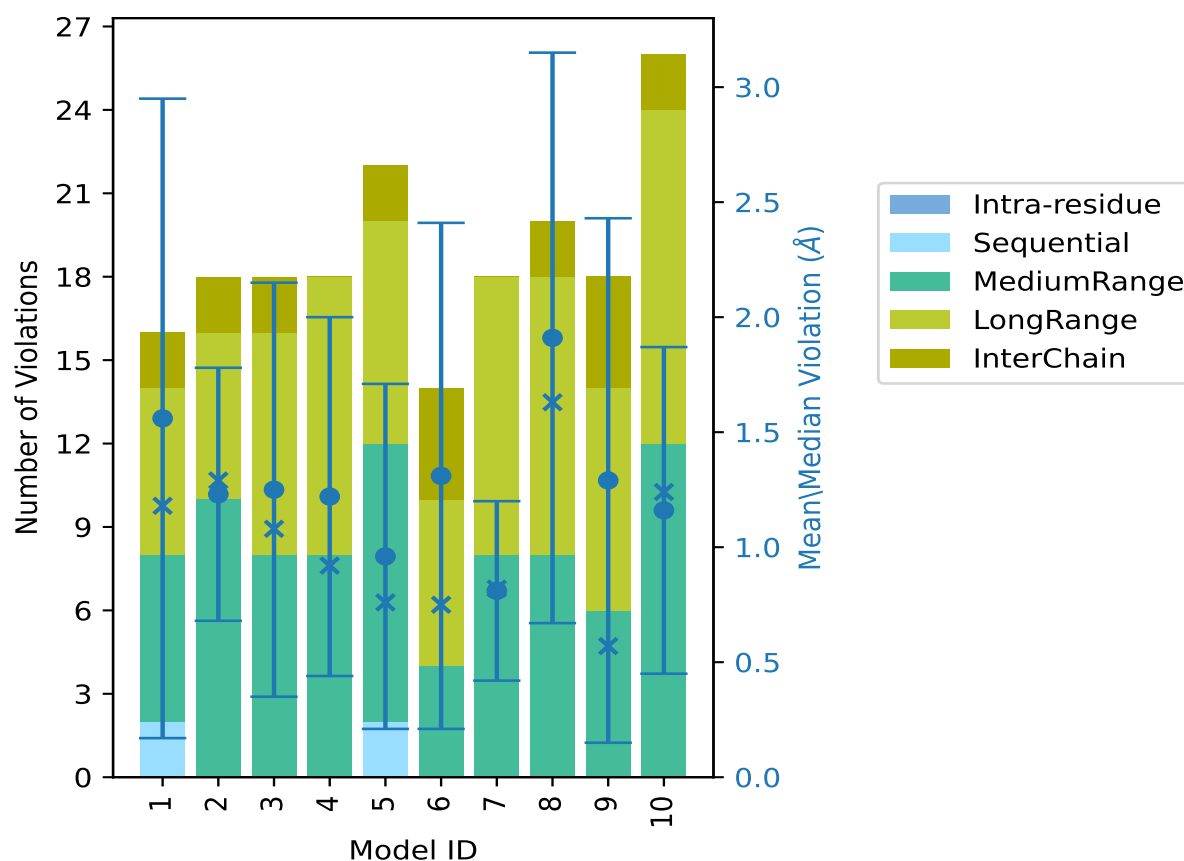
## 9.2 Distance violation statistics for each model [i](#)

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

| Model ID | Number of violations |                 |                 |                 |                 |       | Mean (Å) | Max (Å) | SD <sup>6</sup> (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
|          | IR <sup>1</sup>      | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total |          |         |                     |            |
| 1        | 0                    | 2               | 6               | 6               | 2               | 16    | 1.56     | 3.73    | 1.39                | 1.18       |
| 2        | 0                    | 0               | 10              | 6               | 2               | 18    | 1.23     | 1.75    | 0.55                | 1.29       |
| 3        | 0                    | 0               | 8               | 8               | 2               | 18    | 1.25     | 3.12    | 0.9                 | 1.08       |
| 4        | 0                    | 0               | 8               | 10              | 0               | 18    | 1.22     | 2.75    | 0.78                | 0.92       |
| 5        | 0                    | 2               | 10              | 8               | 2               | 22    | 0.96     | 2.84    | 0.75                | 0.76       |
| 6        | 0                    | 0               | 4               | 6               | 4               | 14    | 1.31     | 3.19    | 1.1                 | 0.75       |
| 7        | 0                    | 0               | 8               | 10              | 0               | 18    | 0.81     | 1.38    | 0.39                | 0.82       |
| 8        | 0                    | 0               | 8               | 10              | 2               | 20    | 1.91     | 4.32    | 1.24                | 1.63       |
| 9        | 0                    | 0               | 6               | 8               | 4               | 18    | 1.29     | 2.88    | 1.14                | 0.57       |
| 10       | 0                    | 0               | 12              | 12              | 2               | 26    | 1.16     | 2.5     | 0.71                | 1.24       |

<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 [i](#)



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 [i](#)

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, 870(IR:356, SQ:160, MR:232, LR:122, IC:0) restraints are not violated in the ensemble.

| Number of violated restraints |                 |                 |                 |                 |       | Fraction of the ensemble |      |
|-------------------------------|-----------------|-----------------|-----------------|-----------------|-------|--------------------------|------|
| IR <sup>1</sup>               | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total | Count <sup>6</sup>       | %    |
| 0                             | 4               | 4               | 4               | 0               | 12    | 1                        | 10.0 |
| 0                             | 0               | 8               | 0               | 0               | 8     | 2                        | 20.0 |
| 0                             | 0               | 4               | 4               | 0               | 8     | 3                        | 30.0 |

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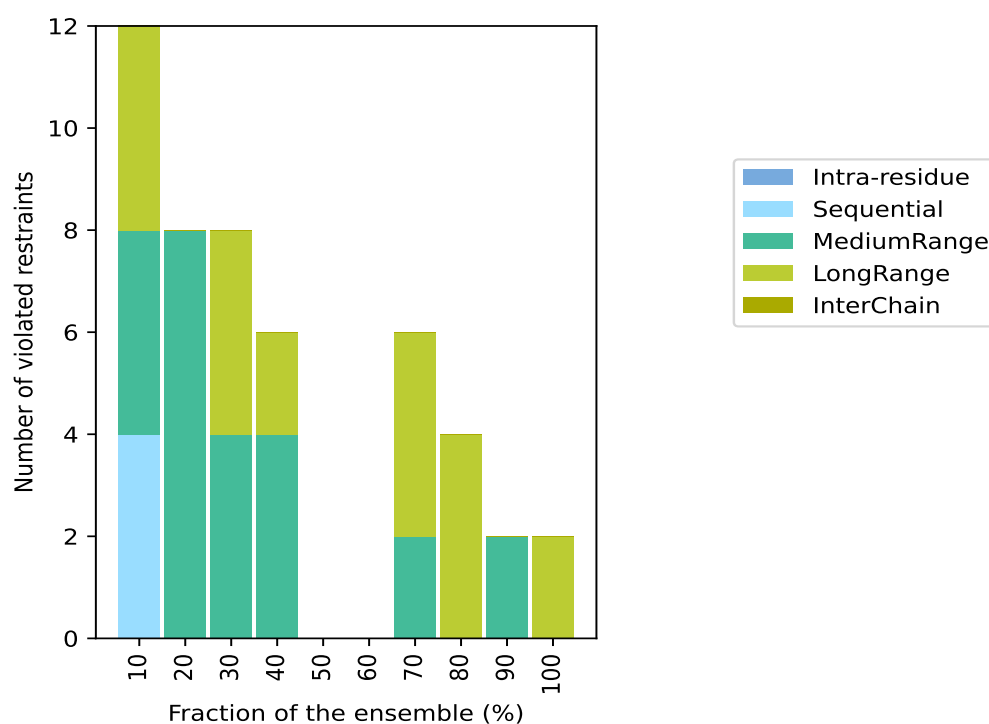
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| Number of violated restraints |                 |                 |                 |                 |       | Fraction of the ensemble |       |
|-------------------------------|-----------------|-----------------|-----------------|-----------------|-------|--------------------------|-------|
| IR <sup>1</sup>               | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total | Count <sup>6</sup>       | %     |
| 0                             | 0               | 4               | 2               | 0               | 6     | 4                        | 40.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 5                        | 50.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 6                        | 60.0  |
| 0                             | 0               | 2               | 4               | 0               | 6     | 7                        | 70.0  |
| 0                             | 0               | 0               | 4               | 0               | 4     | 8                        | 80.0  |
| 0                             | 0               | 2               | 0               | 0               | 2     | 9                        | 90.0  |
| 0                             | 0               | 0               | 2               | 0               | 2     | 10                       | 100.0 |

<sup>1</sup>Intra-residue restraints, <sup>2</sup>Sequential restraints, <sup>3</sup>Medium range restraints, <sup>4</sup>Long range restraints,

<sup>5</sup>Inter-chain restraints, <sup>6</sup> Number of models with violations

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

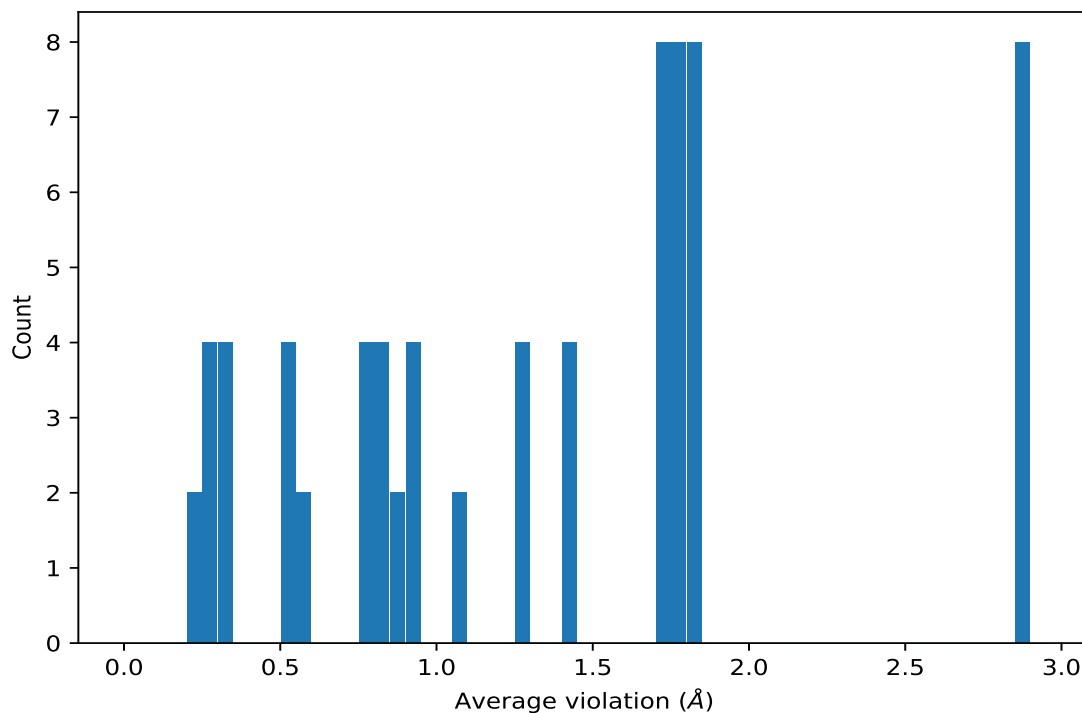


## 9.4 Most violated distance restraints in the ensemble [i](#)

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

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

in the ensemble



#### 9.4.2 Table: Most violated distance restraints [i](#)

The following table provides the mean and the standard deviation of the violation for each restraint sorted by number of violated models and the mean value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

| Key     | Atom-1        | Atom-2         | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|---------------|----------------|---------------------|----------|---------------------|------------|
| (1,33)  | 1:12:A:GLN:CG | 1:72:B:ILE:CD1 | 10                  | 1.72     | 0.69                | 1.72       |
| (1,33)  | 1:12:A:GLN:CG | 1:72:A:ILE:CD1 | 10                  | 1.72     | 0.69                | 1.72       |
| (1,33)  | 1:12:B:GLN:CG | 1:72:A:ILE:CD1 | 10                  | 1.72     | 0.69                | 1.72       |
| (1,33)  | 1:12:B:GLN:CG | 1:72:B:ILE:CD1 | 10                  | 1.72     | 0.69                | 1.72       |
| (1,69)  | 1:12:A:GLN:CG | 1:72:B:ILE:CD1 | 10                  | 1.72     | 0.69                | 1.72       |
| (1,69)  | 1:12:A:GLN:CG | 1:72:A:ILE:CD1 | 10                  | 1.72     | 0.69                | 1.72       |
| (1,69)  | 1:12:B:GLN:CG | 1:72:A:ILE:CD1 | 10                  | 1.72     | 0.69                | 1.72       |
| (1,69)  | 1:12:B:GLN:CG | 1:72:B:ILE:CD1 | 10                  | 1.72     | 0.69                | 1.72       |
| (1,306) | 1:28:A:SER:CA | 1:32:A:TRP:CE2 | 9                   | 0.75     | 0.38                | 0.75       |
| (1,306) | 1:28:B:SER:CA | 1:32:B:TRP:CE2 | 9                   | 0.75     | 0.38                | 0.75       |
| (1,370) | 1:28:A:SER:CA | 1:32:A:TRP:CE2 | 9                   | 0.75     | 0.38                | 0.75       |
| (1,370) | 1:28:B:SER:CA | 1:32:B:TRP:CE2 | 9                   | 0.75     | 0.38                | 0.75       |
| (1,315) | 1:51:A:ASN:CA | 1:56:A:VAL:CG2 | 8                   | 1.82     | 1.04                | 1.75       |
| (1,315) | 1:51:B:ASN:CA | 1:56:B:VAL:CG2 | 8                   | 1.82     | 1.04                | 1.75       |
| (1,379) | 1:51:A:ASN:CA | 1:56:A:VAL:CG2 | 8                   | 1.82     | 1.04                | 1.75       |

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| Key     | Atom-1         | Atom-2         | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|----------------|----------------|---------------------|----------|---------------------|------------|
| (1,379) | 1:51:B:ASN:CA  | 1:56:B:VAL:CG2 | 8                   | 1.82     | 1.04                | 1.75       |
| (1,25)  | 1:72:B:ILE:CD1 | 1:29:B:LEU:CD2 | 8                   | 1.81     | 1.09                | 1.89       |
| (1,25)  | 1:72:A:ILE:CD1 | 1:29:A:LEU:CD2 | 8                   | 1.81     | 1.09                | 1.89       |
| (1,61)  | 1:72:B:ILE:CD1 | 1:29:B:LEU:CD2 | 8                   | 1.81     | 1.09                | 1.89       |
| (1,61)  | 1:72:A:ILE:CD1 | 1:29:A:LEU:CD2 | 8                   | 1.81     | 1.09                | 1.89       |
| (2,63)  | 1:35:B:TYR:OH  | 1:12:B:GLN:NE2 | 7                   | 2.88     | 1.12                | 2.88       |
| (2,63)  | 1:35:B:TYR:OH  | 1:12:A:GLN:NE2 | 7                   | 2.88     | 1.12                | 2.88       |
| (2,63)  | 1:35:A:TYR:OH  | 1:12:A:GLN:NE2 | 7                   | 2.88     | 1.12                | 2.88       |
| (2,63)  | 1:35:A:TYR:OH  | 1:12:B:GLN:NE2 | 7                   | 2.88     | 1.12                | 2.88       |
| (2,64)  | 1:35:B:TYR:OH  | 1:12:B:GLN:NE2 | 7                   | 2.88     | 1.12                | 2.88       |
| (2,64)  | 1:35:B:TYR:OH  | 1:12:A:GLN:NE2 | 7                   | 2.88     | 1.12                | 2.88       |
| (2,64)  | 1:35:A:TYR:OH  | 1:12:A:GLN:NE2 | 7                   | 2.88     | 1.12                | 2.88       |
| (2,64)  | 1:35:A:TYR:OH  | 1:12:B:GLN:NE2 | 7                   | 2.88     | 1.12                | 2.88       |
| (2,62)  | 1:29:A:LEU:N   | 1:79:A:THR:O   | 7                   | 0.84     | 0.39                | 0.88       |
| (2,62)  | 1:29:B:LEU:N   | 1:79:B:THR:O   | 7                   | 0.84     | 0.39                | 0.88       |
| (2,126) | 1:29:A:LEU:N   | 1:79:A:THR:O   | 7                   | 0.84     | 0.39                | 0.88       |
| (2,126) | 1:29:B:LEU:N   | 1:79:B:THR:O   | 7                   | 0.84     | 0.39                | 0.88       |
| (1,308) | 1:21:B:SER:CB  | 1:18:B:VAL:CB  | 7                   | 0.5      | 0.39                | 0.25       |
| (1,308) | 1:21:A:SER:CB  | 1:18:A:VAL:CB  | 7                   | 0.5      | 0.39                | 0.25       |
| (1,372) | 1:21:B:SER:CB  | 1:18:B:VAL:CB  | 7                   | 0.5      | 0.39                | 0.25       |
| (1,372) | 1:21:A:SER:CB  | 1:18:A:VAL:CB  | 7                   | 0.5      | 0.39                | 0.25       |
| (1,314) | 1:51:A:ASN:CA  | 1:54:A:ILE:CG2 | 4                   | 1.76     | 0.45                | 1.9        |
| (1,314) | 1:51:B:ASN:CA  | 1:54:B:ILE:CG2 | 4                   | 1.76     | 0.45                | 1.9        |
| (1,378) | 1:51:A:ASN:CA  | 1:54:A:ILE:CG2 | 4                   | 1.76     | 0.45                | 1.9        |
| (1,378) | 1:51:B:ASN:CA  | 1:54:B:ILE:CG2 | 4                   | 1.76     | 0.45                | 1.9        |
| (1,26)  | 1:46:B:GLY:CA  | 1:55:B:TRP:CE2 | 4                   | 1.42     | 0.1                 | 1.44       |
| (1,26)  | 1:46:A:GLY:CA  | 1:55:A:TRP:CE2 | 4                   | 1.42     | 0.1                 | 1.44       |
| (1,62)  | 1:46:B:GLY:CA  | 1:55:B:TRP:CE2 | 4                   | 1.42     | 0.1                 | 1.44       |
| (1,62)  | 1:46:A:GLY:CA  | 1:55:A:TRP:CE2 | 4                   | 1.42     | 0.1                 | 1.44       |
| (2,39)  | 1:49:A:HIS:O   | 1:51:A:ASN:ND2 | 4                   | 1.08     | 0.5                 | 1.05       |
| (2,103) | 1:49:A:HIS:O   | 1:51:A:ASN:ND2 | 4                   | 1.08     | 0.5                 | 1.05       |
| (2,35)  | 1:43:A:THR:OG1 | 1:58:A:ASN:ND2 | 3                   | 1.27     | 1.09                | 0.82       |
| (2,35)  | 1:43:B:THR:OG1 | 1:58:B:ASN:ND2 | 3                   | 1.27     | 1.09                | 0.82       |
| (2,99)  | 1:43:A:THR:OG1 | 1:58:A:ASN:ND2 | 3                   | 1.27     | 1.09                | 0.82       |
| (2,99)  | 1:43:B:THR:OG1 | 1:58:B:ASN:ND2 | 3                   | 1.27     | 1.09                | 0.82       |
| (2,59)  | 1:21:A:SER:O   | 1:75:A:HIS:ND1 | 3                   | 0.95     | 0.33                | 1.07       |
| (2,59)  | 1:21:B:SER:O   | 1:75:B:HIS:ND1 | 3                   | 0.95     | 0.33                | 1.07       |
| (2,123) | 1:21:A:SER:O   | 1:75:A:HIS:ND1 | 3                   | 0.95     | 0.33                | 1.07       |
| (2,123) | 1:21:B:SER:O   | 1:75:B:HIS:ND1 | 3                   | 0.95     | 0.33                | 1.07       |
| (2,61)  | 1:28:B:SER:OG  | 1:31:B:THR:N   | 3                   | 0.86     | 0.16                | 0.83       |
| (2,125) | 1:28:B:SER:OG  | 1:31:B:THR:N   | 3                   | 0.86     | 0.16                | 0.83       |
| (1,305) | 1:52:B:PRO:CD  | 1:55:B:TRP:CE2 | 3                   | 0.28     | 0.1                 | 0.23       |

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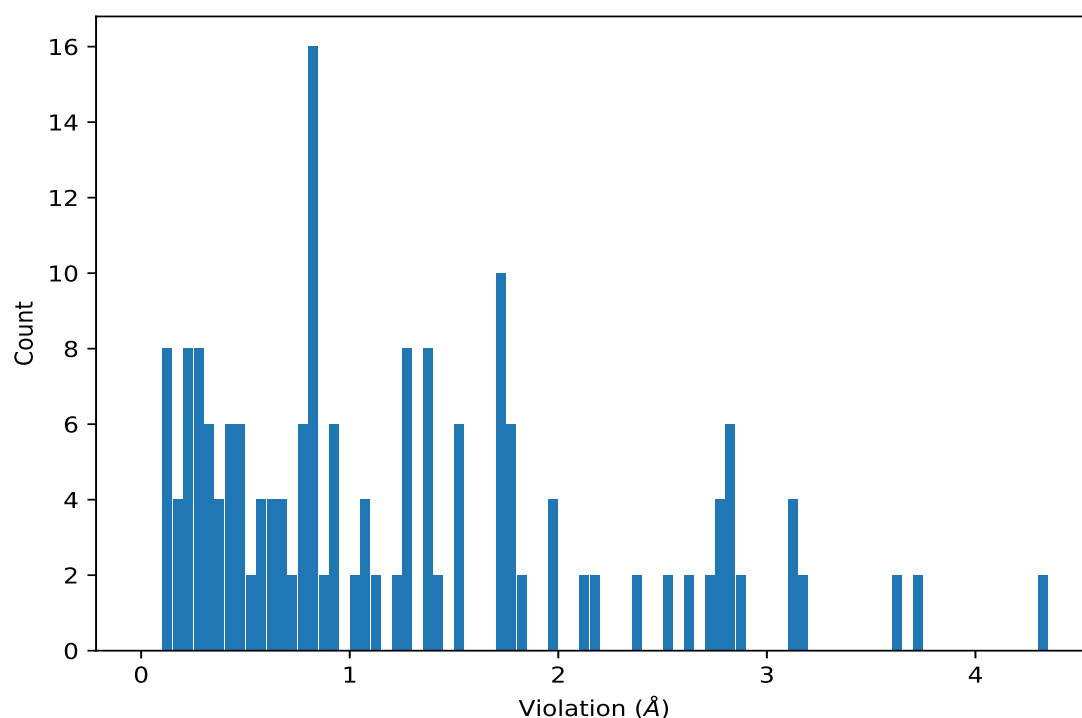
| Key     | Atom-1        | Atom-2         | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|---------------|----------------|---------------------|----------|---------------------|------------|
| (1,305) | 1:52:A:PRO:CD | 1:55:A:TRP:CE2 | 3                   | 0.28     | 0.1                 | 0.23       |
| (1,369) | 1:52:B:PRO:CD | 1:55:B:TRP:CE2 | 3                   | 0.28     | 0.1                 | 0.23       |
| (1,369) | 1:52:A:PRO:CD | 1:55:A:TRP:CE2 | 3                   | 0.28     | 0.1                 | 0.23       |
| (1,312) | 1:51:B:ASN:CA | 1:54:B:ILE:CD1 | 2                   | 1.76     | 0.02                | 1.76       |
| (1,312) | 1:51:A:ASN:CA | 1:54:A:ILE:CD1 | 2                   | 1.76     | 0.02                | 1.76       |
| (1,376) | 1:51:B:ASN:CA | 1:54:B:ILE:CD1 | 2                   | 1.76     | 0.02                | 1.76       |
| (1,376) | 1:51:A:ASN:CA | 1:54:A:ILE:CD1 | 2                   | 1.76     | 0.02                | 1.76       |
| (2,16)  | 1:28:B:SER:OG | 1:31:B:THR:OG1 | 2                   | 0.6      | 0.2                 | 0.6        |
| (2,80)  | 1:28:B:SER:OG | 1:31:B:THR:OG1 | 2                   | 0.6      | 0.2                 | 0.6        |
| (1,307) | 1:34:B:LEU:CA | 1:32:B:TRP:CE2 | 2                   | 0.34     | 0.02                | 0.34       |
| (1,307) | 1:34:A:LEU:CA | 1:32:A:TRP:CE2 | 2                   | 0.34     | 0.02                | 0.34       |
| (1,371) | 1:34:B:LEU:CA | 1:32:B:TRP:CE2 | 2                   | 0.34     | 0.02                | 0.34       |
| (1,371) | 1:34:A:LEU:CA | 1:32:A:TRP:CE2 | 2                   | 0.34     | 0.02                | 0.34       |
| (1,321) | 1:24:A:ALA:CB | 1:27:A:LEU:CA  | 2                   | 0.2      | 0.1                 | 0.2        |
| (1,385) | 1:24:A:ALA:CB | 1:27:A:LEU:CA  | 2                   | 0.2      | 0.1                 | 0.2        |

<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) |
|---------|----------------|----------------|----------|---------------|
| (2,64)  | 1:35:A:TYR:OH  | 1:12:A:GLN:NE2 | 8        | 4.32          |
| (2,63)  | 1:35:A:TYR:OH  | 1:12:A:GLN:NE2 | 8        | 4.32          |
| (2,64)  | 1:35:B:TYR:OH  | 1:12:B:GLN:NE2 | 1        | 3.73          |
| (2,63)  | 1:35:B:TYR:OH  | 1:12:B:GLN:NE2 | 1        | 3.73          |
| (1,61)  | 1:72:B:ILE:CD1 | 1:29:B:LEU:CD2 | 1        | 3.61          |
| (1,25)  | 1:72:B:ILE:CD1 | 1:29:B:LEU:CD2 | 1        | 3.61          |
| (2,64)  | 1:35:B:TYR:OH  | 1:12:A:GLN:NE2 | 6        | 3.19          |
| (2,63)  | 1:35:B:TYR:OH  | 1:12:A:GLN:NE2 | 6        | 3.19          |
| (1,379) | 1:51:A:ASN:CA  | 1:56:A:VAL:CG2 | 8        | 3.13          |
| (1,315) | 1:51:A:ASN:CA  | 1:56:A:VAL:CG2 | 8        | 3.13          |
| (1,379) | 1:51:A:ASN:CA  | 1:56:A:VAL:CG2 | 3        | 3.12          |
| (1,315) | 1:51:A:ASN:CA  | 1:56:A:VAL:CG2 | 3        | 3.12          |
| (2,64)  | 1:35:B:TYR:OH  | 1:12:A:GLN:NE2 | 9        | 2.88          |
| (2,63)  | 1:35:B:TYR:OH  | 1:12:A:GLN:NE2 | 9        | 2.88          |
| (2,64)  | 1:35:B:TYR:OH  | 1:12:B:GLN:NE2 | 5        | 2.84          |
| (2,63)  | 1:35:B:TYR:OH  | 1:12:B:GLN:NE2 | 5        | 2.84          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,69)  | 1:12:B:GLN:CG  | 1:72:A:ILE:CD1 | 8        | 2.84          |
| (1,33)  | 1:12:B:GLN:CG  | 1:72:A:ILE:CD1 | 8        | 2.84          |
| (1,379) | 1:51:B:ASN:CA  | 1:56:B:VAL:CG2 | 9        | 2.83          |
| (1,315) | 1:51:B:ASN:CA  | 1:56:B:VAL:CG2 | 9        | 2.83          |
| (2,99)  | 1:43:A:THR:OG1 | 1:58:A:ASN:ND2 | 8        | 2.77          |
| (2,35)  | 1:43:A:THR:OG1 | 1:58:A:ASN:ND2 | 8        | 2.77          |
| (2,64)  | 1:35:B:TYR:OH  | 1:12:B:GLN:NE2 | 4        | 2.75          |
| (2,63)  | 1:35:B:TYR:OH  | 1:12:B:GLN:NE2 | 4        | 2.75          |
| (1,61)  | 1:72:A:ILE:CD1 | 1:29:A:LEU:CD2 | 6        | 2.72          |
| (1,25)  | 1:72:A:ILE:CD1 | 1:29:A:LEU:CD2 | 6        | 2.72          |
| (1,61)  | 1:72:B:ILE:CD1 | 1:29:B:LEU:CD2 | 9        | 2.63          |
| (1,25)  | 1:72:B:ILE:CD1 | 1:29:B:LEU:CD2 | 9        | 2.63          |
| (1,69)  | 1:12:B:GLN:CG  | 1:72:B:ILE:CD1 | 10       | 2.5           |
| (1,33)  | 1:12:B:GLN:CG  | 1:72:B:ILE:CD1 | 10       | 2.5           |
| (1,69)  | 1:12:A:GLN:CG  | 1:72:A:ILE:CD1 | 4        | 2.37          |
| (1,33)  | 1:12:A:GLN:CG  | 1:72:A:ILE:CD1 | 4        | 2.37          |
| (1,378) | 1:51:A:ASN:CA  | 1:54:A:ILE:CG2 | 1        | 2.18          |
| (1,314) | 1:51:A:ASN:CA  | 1:54:A:ILE:CG2 | 1        | 2.18          |
| (1,378) | 1:51:B:ASN:CA  | 1:54:B:ILE:CG2 | 10       | 2.1           |
| (1,314) | 1:51:B:ASN:CA  | 1:54:B:ILE:CG2 | 10       | 2.1           |
| (1,61)  | 1:72:B:ILE:CD1 | 1:29:B:LEU:CD2 | 3        | 1.98          |
| (1,25)  | 1:72:B:ILE:CD1 | 1:29:B:LEU:CD2 | 3        | 1.98          |
| (1,69)  | 1:12:A:GLN:CG  | 1:72:B:ILE:CD1 | 3        | 1.95          |
| (1,33)  | 1:12:A:GLN:CG  | 1:72:B:ILE:CD1 | 3        | 1.95          |
| (1,61)  | 1:72:A:ILE:CD1 | 1:29:A:LEU:CD2 | 5        | 1.8           |
| (1,25)  | 1:72:A:ILE:CD1 | 1:29:A:LEU:CD2 | 5        | 1.8           |
| (1,376) | 1:51:A:ASN:CA  | 1:54:A:ILE:CD1 | 10       | 1.78          |
| (1,312) | 1:51:A:ASN:CA  | 1:54:A:ILE:CD1 | 10       | 1.78          |
| (1,379) | 1:51:A:ASN:CA  | 1:56:A:VAL:CG2 | 2        | 1.75          |
| (1,379) | 1:51:B:ASN:CA  | 1:56:B:VAL:CG2 | 10       | 1.75          |
| (1,315) | 1:51:A:ASN:CA  | 1:56:A:VAL:CG2 | 2        | 1.75          |
| (1,315) | 1:51:B:ASN:CA  | 1:56:B:VAL:CG2 | 10       | 1.75          |
| (1,376) | 1:51:B:ASN:CA  | 1:54:B:ILE:CD1 | 2        | 1.74          |
| (1,312) | 1:51:B:ASN:CA  | 1:54:B:ILE:CD1 | 2        | 1.74          |
| (1,69)  | 1:12:A:GLN:CG  | 1:72:B:ILE:CD1 | 2        | 1.74          |
| (1,33)  | 1:12:A:GLN:CG  | 1:72:B:ILE:CD1 | 2        | 1.74          |
| (2,103) | 1:49:A:HIS:O   | 1:51:A:ASN:ND2 | 8        | 1.73          |
| (2,39)  | 1:49:A:HIS:O   | 1:51:A:ASN:ND2 | 8        | 1.73          |
| (1,378) | 1:51:B:ASN:CA  | 1:54:B:ILE:CG2 | 2        | 1.71          |
| (1,314) | 1:51:B:ASN:CA  | 1:54:B:ILE:CG2 | 2        | 1.71          |
| (1,69)  | 1:12:B:GLN:CG  | 1:72:A:ILE:CD1 | 9        | 1.7           |
| (1,33)  | 1:12:B:GLN:CG  | 1:72:A:ILE:CD1 | 9        | 1.7           |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,370) | 1:28:A:SER:CA  | 1:32:A:TRP:CE2 | 8        | 1.53          |
| (1,306) | 1:28:A:SER:CA  | 1:32:A:TRP:CE2 | 8        | 1.53          |
| (1,62)  | 1:46:B:GLY:CA  | 1:55:B:TRP:CE2 | 1        | 1.53          |
| (1,26)  | 1:46:B:GLY:CA  | 1:55:B:TRP:CE2 | 1        | 1.53          |
| (1,62)  | 1:46:B:GLY:CA  | 1:55:B:TRP:CE2 | 10       | 1.5           |
| (1,26)  | 1:46:B:GLY:CA  | 1:55:B:TRP:CE2 | 10       | 1.5           |
| (1,69)  | 1:12:A:GLN:CG  | 1:72:B:ILE:CD1 | 5        | 1.41          |
| (1,33)  | 1:12:A:GLN:CG  | 1:72:B:ILE:CD1 | 5        | 1.41          |
| (2,103) | 1:49:A:HIS:O   | 1:51:A:ASN:ND2 | 10       | 1.39          |
| (2,39)  | 1:49:A:HIS:O   | 1:51:A:ASN:ND2 | 10       | 1.39          |
| (1,62)  | 1:46:A:GLY:CA  | 1:55:A:TRP:CE2 | 7        | 1.38          |
| (1,26)  | 1:46:A:GLY:CA  | 1:55:A:TRP:CE2 | 7        | 1.38          |
| (2,126) | 1:29:A:LEU:N   | 1:79:A:THR:O   | 3        | 1.37          |
| (2,62)  | 1:29:A:LEU:N   | 1:79:A:THR:O   | 3        | 1.37          |
| (2,126) | 1:29:A:LEU:N   | 1:79:A:THR:O   | 4        | 1.36          |
| (2,62)  | 1:29:A:LEU:N   | 1:79:A:THR:O   | 4        | 1.36          |
| (2,123) | 1:21:A:SER:O   | 1:75:A:HIS:ND1 | 7        | 1.29          |
| (2,59)  | 1:21:A:SER:O   | 1:75:A:HIS:ND1 | 7        | 1.29          |
| (1,62)  | 1:46:A:GLY:CA  | 1:55:A:TRP:CE2 | 2        | 1.29          |
| (1,26)  | 1:46:A:GLY:CA  | 1:55:A:TRP:CE2 | 2        | 1.29          |
| (1,69)  | 1:12:B:GLN:CG  | 1:72:A:ILE:CD1 | 6        | 1.26          |
| (1,33)  | 1:12:B:GLN:CG  | 1:72:A:ILE:CD1 | 6        | 1.26          |
| (1,368) | 1:72:A:ILE:CD1 | 1:76:A:THR:CG2 | 2        | 1.25          |
| (1,304) | 1:72:A:ILE:CD1 | 1:76:A:THR:CG2 | 2        | 1.25          |
| (1,372) | 1:21:B:SER:CB  | 1:18:B:VAL:CB  | 10       | 1.24          |
| (1,308) | 1:21:B:SER:CB  | 1:18:B:VAL:CB  | 10       | 1.24          |
| (1,370) | 1:28:B:SER:CA  | 1:32:B:TRP:CE2 | 7        | 1.12          |
| (1,306) | 1:28:B:SER:CA  | 1:32:B:TRP:CE2 | 7        | 1.12          |
| (2,125) | 1:28:B:SER:OG  | 1:31:B:THR:N   | 3        | 1.08          |
| (2,61)  | 1:28:B:SER:OG  | 1:31:B:THR:N   | 3        | 1.08          |
| (2,123) | 1:21:B:SER:O   | 1:75:B:HIS:ND1 | 4        | 1.07          |
| (2,59)  | 1:21:B:SER:O   | 1:75:B:HIS:ND1 | 4        | 1.07          |
| (1,378) | 1:51:B:ASN:CA  | 1:54:B:ILE:CG2 | 7        | 1.03          |
| (1,314) | 1:51:B:ASN:CA  | 1:54:B:ILE:CG2 | 7        | 1.03          |
| (1,370) | 1:28:A:SER:CA  | 1:32:A:TRP:CE2 | 4        | 0.92          |
| (1,306) | 1:28:A:SER:CA  | 1:32:A:TRP:CE2 | 4        | 0.92          |
| (2,126) | 1:29:B:LEU:N   | 1:79:B:THR:O   | 10       | 0.91          |
| (2,62)  | 1:29:B:LEU:N   | 1:79:B:THR:O   | 10       | 0.91          |
| (1,372) | 1:21:A:SER:CB  | 1:18:A:VAL:CB  | 4        | 0.91          |
| (1,308) | 1:21:A:SER:CB  | 1:18:A:VAL:CB  | 4        | 0.91          |
| (2,126) | 1:29:B:LEU:N   | 1:79:B:THR:O   | 8        | 0.88          |
| (2,62)  | 1:29:B:LEU:N   | 1:79:B:THR:O   | 8        | 0.88          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,379) | 1:51:B:ASN:CA  | 1:56:B:VAL:CG2 | 4        | 0.84          |
| (1,315) | 1:51:B:ASN:CA  | 1:56:B:VAL:CG2 | 4        | 0.84          |
| (2,125) | 1:28:B:SER:OG  | 1:31:B:THR:N   | 5        | 0.83          |
| (2,61)  | 1:28:B:SER:OG  | 1:31:B:THR:N   | 5        | 0.83          |
| (2,122) | 1:16:B:LEU:O   | 1:19:B:SER:OG  | 7        | 0.82          |
| (2,99)  | 1:43:A:THR:OG1 | 1:58:A:ASN:ND2 | 3        | 0.82          |
| (2,58)  | 1:16:B:LEU:O   | 1:19:B:SER:OG  | 7        | 0.82          |
| (2,35)  | 1:43:A:THR:OG1 | 1:58:A:ASN:ND2 | 3        | 0.82          |
| (1,69)  | 1:12:A:GLN:CG  | 1:72:B:ILE:CD1 | 1        | 0.82          |
| (1,61)  | 1:72:A:ILE:CD1 | 1:29:A:LEU:CD2 | 8        | 0.82          |
| (1,33)  | 1:12:A:GLN:CG  | 1:72:B:ILE:CD1 | 1        | 0.82          |
| (1,25)  | 1:72:A:ILE:CD1 | 1:29:A:LEU:CD2 | 8        | 0.82          |
| (2,80)  | 1:28:B:SER:OG  | 1:31:B:THR:OG1 | 8        | 0.81          |
| (2,16)  | 1:28:B:SER:OG  | 1:31:B:THR:OG1 | 8        | 0.81          |
| (1,370) | 1:28:A:SER:CA  | 1:32:A:TRP:CE2 | 5        | 0.8           |
| (1,306) | 1:28:A:SER:CA  | 1:32:A:TRP:CE2 | 5        | 0.8           |
| (1,63)  | 1:47:B:ILE:CD1 | 1:55:B:TRP:CE2 | 5        | 0.76          |
| (1,27)  | 1:47:B:ILE:CD1 | 1:55:B:TRP:CE2 | 5        | 0.76          |
| (1,379) | 1:51:B:ASN:CA  | 1:56:B:VAL:CG2 | 6        | 0.75          |
| (1,370) | 1:28:B:SER:CA  | 1:32:B:TRP:CE2 | 2        | 0.75          |
| (1,315) | 1:51:B:ASN:CA  | 1:56:B:VAL:CG2 | 6        | 0.75          |
| (1,306) | 1:28:B:SER:CA  | 1:32:B:TRP:CE2 | 2        | 0.75          |
| (2,103) | 1:49:A:HIS:O   | 1:51:A:ASN:ND2 | 5        | 0.71          |
| (2,39)  | 1:49:A:HIS:O   | 1:51:A:ASN:ND2 | 5        | 0.71          |
| (2,125) | 1:28:B:SER:OG  | 1:31:B:THR:N   | 6        | 0.68          |
| (2,61)  | 1:28:B:SER:OG  | 1:31:B:THR:N   | 6        | 0.68          |
| (2,126) | 1:29:B:LEU:N   | 1:79:B:THR:O   | 5        | 0.67          |
| (2,62)  | 1:29:B:LEU:N   | 1:79:B:THR:O   | 5        | 0.67          |
| (1,61)  | 1:72:B:ILE:CD1 | 1:29:B:LEU:CD2 | 2        | 0.64          |
| (1,25)  | 1:72:B:ILE:CD1 | 1:29:B:LEU:CD2 | 2        | 0.64          |
| (1,69)  | 1:12:B:GLN:CG  | 1:72:B:ILE:CD1 | 7        | 0.6           |
| (1,33)  | 1:12:B:GLN:CG  | 1:72:B:ILE:CD1 | 7        | 0.6           |
| (1,370) | 1:28:B:SER:CA  | 1:32:B:TRP:CE2 | 9        | 0.57          |
| (1,306) | 1:28:B:SER:CA  | 1:32:B:TRP:CE2 | 9        | 0.57          |
| (1,372) | 1:21:B:SER:CB  | 1:18:B:VAL:CB  | 5        | 0.55          |
| (1,308) | 1:21:B:SER:CB  | 1:18:B:VAL:CB  | 5        | 0.55          |
| (2,123) | 1:21:A:SER:O   | 1:75:A:HIS:ND1 | 10       | 0.5           |
| (2,59)  | 1:21:A:SER:O   | 1:75:A:HIS:ND1 | 10       | 0.5           |
| (2,103) | 1:49:A:HIS:O   | 1:51:A:ASN:ND2 | 4        | 0.48          |
| (2,39)  | 1:49:A:HIS:O   | 1:51:A:ASN:ND2 | 4        | 0.48          |
| (2,126) | 1:29:A:LEU:N   | 1:79:A:THR:O   | 7        | 0.47          |
| (2,64)  | 1:35:A:TYR:OH  | 1:12:B:GLN:NE2 | 10       | 0.47          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (2,63)  | 1:35:A:TYR:OH  | 1:12:B:GLN:NE2 | 10       | 0.47          |
| (2,62)  | 1:29:A:LEU:N   | 1:79:A:THR:O   | 7        | 0.47          |
| (1,369) | 1:52:A:PRO:CD  | 1:55:A:TRP:CE2 | 9        | 0.42          |
| (1,305) | 1:52:A:PRO:CD  | 1:55:A:TRP:CE2 | 9        | 0.42          |
| (2,80)  | 1:28:B:SER:OG  | 1:31:B:THR:OG1 | 3        | 0.4           |
| (2,16)  | 1:28:B:SER:OG  | 1:31:B:THR:OG1 | 3        | 0.4           |
| (1,370) | 1:28:A:SER:CA  | 1:32:A:TRP:CE2 | 10       | 0.4           |
| (1,306) | 1:28:A:SER:CA  | 1:32:A:TRP:CE2 | 10       | 0.4           |
| (1,379) | 1:51:B:ASN:CA  | 1:56:B:VAL:CG2 | 7        | 0.36          |
| (1,371) | 1:34:A:LEU:CA  | 1:32:A:TRP:CE2 | 3        | 0.36          |
| (1,315) | 1:51:B:ASN:CA  | 1:56:B:VAL:CG2 | 7        | 0.36          |
| (1,307) | 1:34:A:LEU:CA  | 1:32:A:TRP:CE2 | 3        | 0.36          |
| (1,370) | 1:28:A:SER:CA  | 1:32:A:TRP:CE2 | 1        | 0.34          |
| (1,306) | 1:28:A:SER:CA  | 1:32:A:TRP:CE2 | 1        | 0.34          |
| (1,371) | 1:34:B:LEU:CA  | 1:32:B:TRP:CE2 | 10       | 0.32          |
| (1,307) | 1:34:B:LEU:CA  | 1:32:B:TRP:CE2 | 10       | 0.32          |
| (1,385) | 1:24:A:ALA:CB  | 1:27:A:LEU:CA  | 4        | 0.31          |
| (1,321) | 1:24:A:ALA:CB  | 1:27:A:LEU:CA  | 4        | 0.31          |
| (1,370) | 1:28:A:SER:CA  | 1:32:A:TRP:CE2 | 6        | 0.29          |
| (1,306) | 1:28:A:SER:CA  | 1:32:A:TRP:CE2 | 6        | 0.29          |
| (1,61)  | 1:72:B:ILE:CD1 | 1:29:B:LEU:CD2 | 10       | 0.28          |
| (1,25)  | 1:72:B:ILE:CD1 | 1:29:B:LEU:CD2 | 10       | 0.28          |
| (2,126) | 1:29:A:LEU:N   | 1:79:A:THR:O   | 6        | 0.25          |
| (2,62)  | 1:29:A:LEU:N   | 1:79:A:THR:O   | 6        | 0.25          |
| (1,372) | 1:21:A:SER:CB  | 1:18:A:VAL:CB  | 9        | 0.25          |
| (1,308) | 1:21:A:SER:CB  | 1:18:A:VAL:CB  | 9        | 0.25          |
| (1,372) | 1:21:B:SER:CB  | 1:18:B:VAL:CB  | 7        | 0.23          |
| (1,369) | 1:52:B:PRO:CD  | 1:55:B:TRP:CE2 | 8        | 0.23          |
| (1,308) | 1:21:B:SER:CB  | 1:18:B:VAL:CB  | 7        | 0.23          |
| (1,305) | 1:52:B:PRO:CD  | 1:55:B:TRP:CE2 | 8        | 0.23          |
| (2,99)  | 1:43:B:THR:OG1 | 1:58:B:ASN:ND2 | 9        | 0.22          |
| (2,35)  | 1:43:B:THR:OG1 | 1:58:B:ASN:ND2 | 9        | 0.22          |
| (1,369) | 1:52:B:PRO:CD  | 1:55:B:TRP:CE2 | 3        | 0.2           |
| (1,305) | 1:52:B:PRO:CD  | 1:55:B:TRP:CE2 | 3        | 0.2           |
| (1,372) | 1:21:B:SER:CB  | 1:18:B:VAL:CB  | 1        | 0.16          |
| (1,372) | 1:21:A:SER:CB  | 1:18:A:VAL:CB  | 2        | 0.16          |
| (1,308) | 1:21:B:SER:CB  | 1:18:B:VAL:CB  | 1        | 0.16          |
| (1,308) | 1:21:A:SER:CB  | 1:18:A:VAL:CB  | 2        | 0.16          |
| (2,124) | 1:27:B:LEU:O   | 1:79:B:THR:OG1 | 9        | 0.13          |
| (2,60)  | 1:27:B:LEU:O   | 1:79:B:THR:OG1 | 9        | 0.13          |
| (1,252) | 1:56:B:VAL:CB  | 1:55:B:TRP:CE2 | 5        | 0.13          |
| (1,171) | 1:56:B:VAL:CB  | 1:55:B:TRP:CE2 | 5        | 0.13          |

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| Key     | Atom-1        | Atom-2         | Model ID | Violation (Å) |
|---------|---------------|----------------|----------|---------------|
| (1,255) | 1:31:B:THR:CB | 1:32:B:TRP:CE2 | 1        | 0.12          |
| (1,174) | 1:31:B:THR:CB | 1:32:B:TRP:CE2 | 1        | 0.12          |
| (1,385) | 1:24:A:ALA:CB | 1:27:A:LEU:CA  | 5        | 0.1           |
| (1,321) | 1:24:A:ALA:CB | 1:27:A:LEU:CA  | 5        | 0.1           |

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

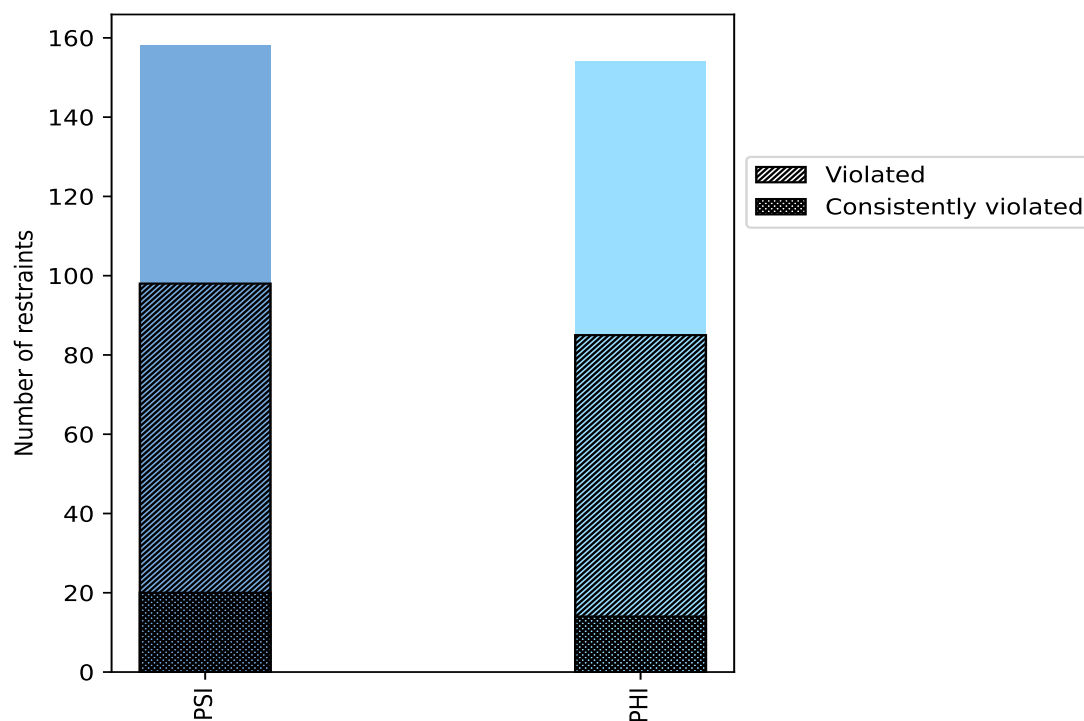
### 10.1 Summary of dihedral-angle violations [i](#)

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

| Angle type | Count | % <sup>1</sup> | Violated <sup>3</sup> |                |                | Consistently Violated <sup>4</sup> |                |                |
|------------|-------|----------------|-----------------------|----------------|----------------|------------------------------------|----------------|----------------|
|            |       |                | Count                 | % <sup>2</sup> | % <sup>1</sup> | Count                              | % <sup>2</sup> | % <sup>1</sup> |
| PSI        | 158   | 50.6           | 98                    | 62.0           | 31.4           | 20                                 | 12.7           | 6.4            |
| PHI        | 154   | 49.4           | 85                    | 55.2           | 27.2           | 14                                 | 9.1            | 4.5            |
| Total      | 312   | 100.0          | 183                   | 58.7           | 58.7           | 34                                 | 10.9           | 10.9           |

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

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



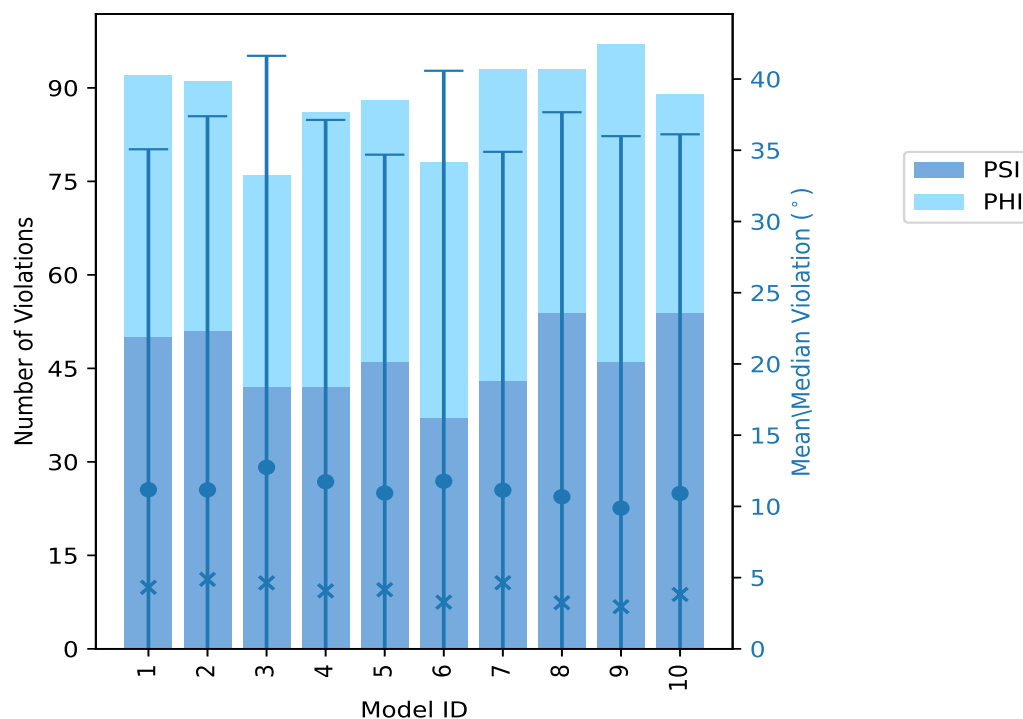
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

## 10.2 Dihedral-angle violation statistics for each model [i](#)

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

| Model ID | Number of violations |     |       | Mean (°) | Max (°) | SD (°) | Median (°) |
|----------|----------------------|-----|-------|----------|---------|--------|------------|
|          | PSI                  | PHI | Total |          |         |        |            |
| 1        | 50                   | 42  | 92    | 11.17    | 117.36  | 23.9   | 4.32       |
| 2        | 51                   | 40  | 91    | 11.16    | 153.76  | 26.23  | 4.88       |
| 3        | 42                   | 34  | 76    | 12.74    | 159.89  | 28.89  | 4.63       |
| 4        | 42                   | 44  | 86    | 11.73    | 118.91  | 25.4   | 4.07       |
| 5        | 46                   | 42  | 88    | 10.94    | 106.01  | 23.75  | 4.15       |
| 6        | 37                   | 41  | 78    | 11.77    | 159.39  | 28.81  | 3.28       |
| 7        | 43                   | 50  | 93    | 11.14    | 123.5   | 23.75  | 4.64       |
| 8        | 54                   | 39  | 93    | 10.68    | 159.26  | 26.99  | 3.24       |
| 9        | 46                   | 51  | 97    | 9.88     | 156.91  | 26.11  | 2.96       |
| 10       | 54                   | 35  | 89    | 10.91    | 128.36  | 25.21  | 3.82       |

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



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

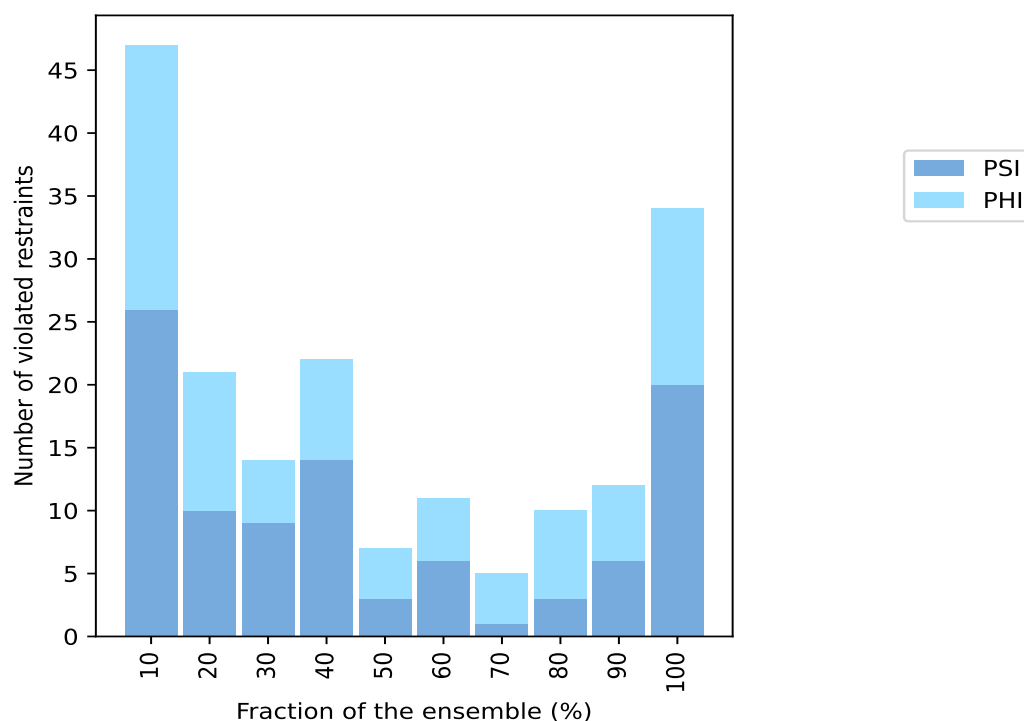
### 10.3 Dihedral-angle violation statistics for the ensemble [i](#)

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

| Number of violated restraints |     |       | Fraction of the ensemble |       |
|-------------------------------|-----|-------|--------------------------|-------|
| PSI                           | PHI | Total | Count <sup>1</sup>       | %     |
| 26                            | 21  | 47    | 1                        | 10.0  |
| 10                            | 11  | 21    | 2                        | 20.0  |
| 9                             | 5   | 14    | 3                        | 30.0  |
| 14                            | 8   | 22    | 4                        | 40.0  |
| 3                             | 4   | 7     | 5                        | 50.0  |
| 6                             | 5   | 11    | 6                        | 60.0  |
| 1                             | 4   | 5     | 7                        | 70.0  |
| 3                             | 7   | 10    | 8                        | 80.0  |
| 6                             | 6   | 12    | 9                        | 90.0  |
| 20                            | 14  | 34    | 10                       | 100.0 |

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

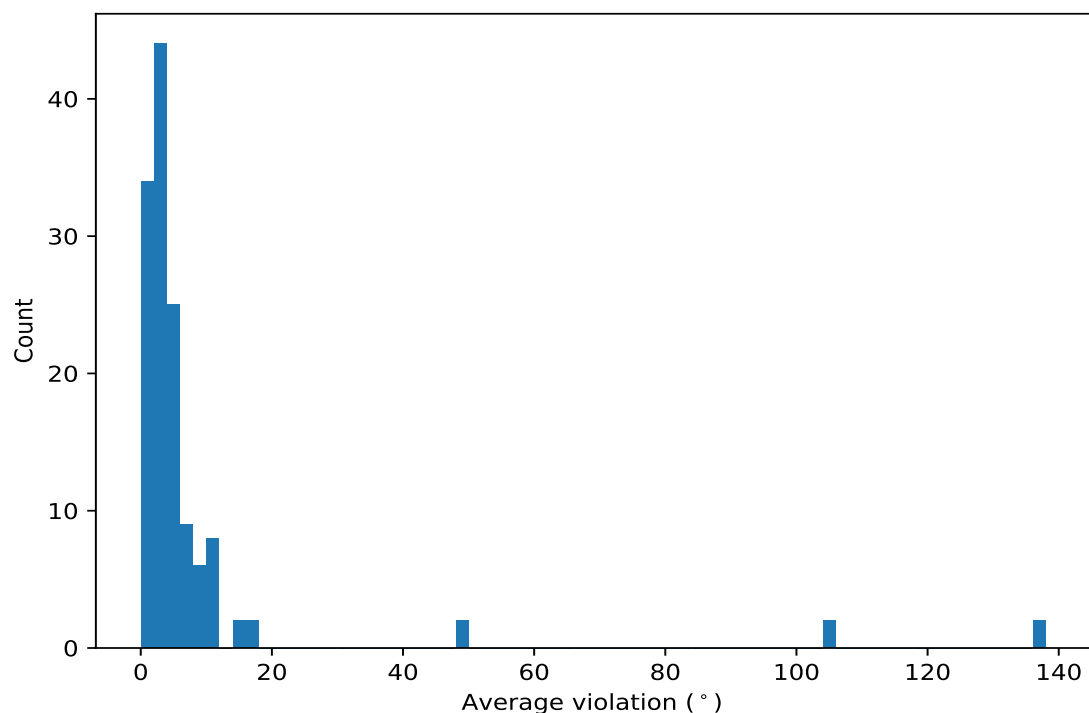
#### 10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



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

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

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



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

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

| Key     | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Models <sup>1</sup> | Mean   | SD <sup>2</sup> | Median |
|---------|--------------|---------------|---------------|--------------|---------------------|--------|-----------------|--------|
| (1,76)  | 1:20:B:HIS:N | 1:20:B:HIS:CA | 1:20:B:HIS:C  | 1:21:B:SER:N | 10                  | 137.57 | 21.4            | 141.0  |
| (1,75)  | 1:20:A:HIS:N | 1:20:A:HIS:CA | 1:20:A:HIS:C  | 1:21:A:SER:N | 10                  | 137.55 | 21.4            | 141.06 |
| (1,74)  | 1:19:B:SER:C | 1:20:B:HIS:N  | 1:20:B:HIS:CA | 1:20:B:HIS:C | 10                  | 105.56 | 7.35            | 104.03 |
| (1,73)  | 1:19:A:SER:C | 1:20:A:HIS:N  | 1:20:A:HIS:CA | 1:20:A:HIS:C | 10                  | 105.55 | 7.37            | 103.96 |
| (1,77)  | 1:20:A:HIS:C | 1:21:A:SER:N  | 1:21:A:SER:CA | 1:21:A:SER:C | 10                  | 49.59  | 22.02           | 36.27  |
| (1,78)  | 1:20:B:HIS:C | 1:21:B:SER:N  | 1:21:B:SER:CA | 1:21:B:SER:C | 10                  | 49.56  | 22.02           | 36.28  |
| (1,201) | 1:51:A:ASN:C | 1:52:A:PRO:N  | 1:52:A:PRO:CA | 1:52:A:PRO:C | 10                  | 10.9   | 3.51            | 10.4   |
| (1,202) | 1:51:B:ASN:C | 1:52:B:PRO:N  | 1:52:B:PRO:CA | 1:52:B:PRO:C | 10                  | 10.83  | 3.58            | 10.48  |
| (1,18)  | 1:5:B:SER:N  | 1:5:B:SER:CA  | 1:5:B:SER:C   | 1:6:B:PRO:N  | 10                  | 10.76  | 4.35            | 9.58   |
| (1,17)  | 1:5:A:SER:N  | 1:5:A:SER:CA  | 1:5:A:SER:C   | 1:6:A:PRO:N  | 10                  | 10.73  | 4.33            | 9.68   |
| (1,16)  | 1:4:B:ILE:C  | 1:5:B:SER:N   | 1:5:B:SER:CA  | 1:5:B:SER:C  | 10                  | 10.37  | 1.48            | 10.89  |
| (1,15)  | 1:4:A:ILE:C  | 1:5:A:SER:N   | 1:5:A:SER:CA  | 1:5:A:SER:C  | 10                  | 10.36  | 1.54            | 10.87  |
| (1,200) | 1:51:B:ASN:N | 1:51:B:ASN:CA | 1:51:B:ASN:C  | 1:52:B:PRO:N | 10                  | 9.17   | 1.96            | 8.57   |

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| Key     | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Models <sup>1</sup> | Mean  | SD <sup>2</sup> | Median |
|---------|--------------|---------------|---------------|--------------|---------------------|-------|-----------------|--------|
| (1,199) | 1:51:A:ASN:N | 1:51:A:ASN:CA | 1:51:A:ASN:C  | 1:52:A:PRO:N | 10                  | 9.13  | 1.84            | 8.52   |
| (1,13)  | 1:4:A:ILE:N  | 1:4:A:ILE:CA  | 1:4:A:ILE:C   | 1:5:A:SER:N  | 10                  | 7.81  | 1.15            | 7.42   |
| (1,14)  | 1:4:B:ILE:N  | 1:4:B:ILE:CA  | 1:4:B:ILE:C   | 1:5:B:SER:N  | 10                  | 7.75  | 1.16            | 7.37   |
| (1,83)  | 1:22:A:GLU:N | 1:22:A:GLU:CA | 1:22:A:GLU:C  | 1:23:A:HIS:N | 10                  | 6.83  | 2.19            | 7.12   |
| (1,84)  | 1:22:B:GLU:N | 1:22:B:GLU:CA | 1:22:B:GLU:C  | 1:23:B:HIS:N | 10                  | 6.82  | 2.16            | 7.09   |
| (1,92)  | 1:24:B:ALA:N | 1:24:B:ALA:CA | 1:24:B:ALA:C  | 1:25:B:LEU:N | 10                  | 6.68  | 2.28            | 7.3    |
| (1,91)  | 1:24:A:ALA:N | 1:24:A:ALA:CA | 1:24:A:ALA:C  | 1:25:A:LEU:N | 10                  | 6.64  | 2.25            | 7.28   |
| (1,93)  | 1:24:A:ALA:C | 1:25:A:LEU:N  | 1:25:A:LEU:CA | 1:25:A:LEU:C | 10                  | 5.69  | 1.99            | 6.29   |
| (1,94)  | 1:24:B:ALA:C | 1:25:B:LEU:N  | 1:25:B:LEU:CA | 1:25:B:LEU:C | 10                  | 5.68  | 1.99            | 6.34   |
| (1,95)  | 1:25:A:LEU:N | 1:25:A:LEU:CA | 1:25:A:LEU:C  | 1:26:A:GLY:N | 10                  | 5.3   | 1.45            | 5.32   |
| (1,96)  | 1:25:B:LEU:N | 1:25:B:LEU:CA | 1:25:B:LEU:C  | 1:26:B:GLY:N | 10                  | 5.28  | 1.48            | 5.25   |
| (1,85)  | 1:22:A:GLU:C | 1:23:A:HIS:N  | 1:23:A:HIS:CA | 1:23:A:HIS:C | 10                  | 4.99  | 1.85            | 4.89   |
| (1,86)  | 1:22:B:GLU:C | 1:23:B:HIS:N  | 1:23:B:HIS:CA | 1:23:B:HIS:C | 10                  | 4.97  | 1.84            | 4.84   |
| (1,306) | 1:77:B:GLY:C | 1:78:B:GLY:N  | 1:78:B:GLY:CA | 1:78:B:GLY:C | 10                  | 4.65  | 1.22            | 4.44   |
| (1,305) | 1:77:A:GLY:C | 1:78:A:GLY:N  | 1:78:A:GLY:CA | 1:78:A:GLY:C | 10                  | 4.63  | 1.19            | 4.35   |
| (1,80)  | 1:21:B:SER:N | 1:21:B:SER:CA | 1:21:B:SER:C  | 1:22:B:GLU:N | 10                  | 3.89  | 0.68            | 3.99   |
| (1,79)  | 1:21:A:SER:N | 1:21:A:SER:CA | 1:21:A:SER:C  | 1:22:A:GLU:N | 10                  | 3.86  | 0.66            | 4.0    |
| (1,29)  | 1:8:A:ALA:N  | 1:8:A:ALA:CA  | 1:8:A:ALA:C   | 1:9:A:THR:N  | 10                  | 3.65  | 1.38            | 3.26   |
| (1,30)  | 1:8:B:ALA:N  | 1:8:B:ALA:CA  | 1:8:B:ALA:C   | 1:9:B:THR:N  | 10                  | 3.58  | 1.41            | 3.24   |
| (1,280) | 1:71:B:GLY:N | 1:71:B:GLY:CA | 1:71:B:GLY:C  | 1:72:B:ILE:N | 10                  | 2.45  | 0.75            | 2.36   |
| (1,279) | 1:71:A:GLY:N | 1:71:A:GLY:CA | 1:71:A:GLY:C  | 1:72:A:ILE:N | 10                  | 2.32  | 0.59            | 2.37   |
| (1,38)  | 1:10:B:MET:N | 1:10:B:MET:CA | 1:10:B:MET:C  | 1:11:B:PRO:N | 9                   | 6.51  | 3.36            | 8.21   |
| (1,37)  | 1:10:A:MET:N | 1:10:A:MET:CA | 1:10:A:MET:C  | 1:11:A:PRO:N | 9                   | 6.49  | 3.41            | 7.97   |
| (1,212) | 1:54:B:ILE:N | 1:54:B:ILE:CA | 1:54:B:ILE:C  | 1:55:B:TRP:N | 9                   | 5.3   | 1.32            | 5.23   |
| (1,211) | 1:54:A:ILE:N | 1:54:A:ILE:CA | 1:54:A:ILE:C  | 1:55:A:TRP:N | 9                   | 5.29  | 1.4             | 5.15   |
| (1,214) | 1:54:B:ILE:C | 1:55:B:TRP:N  | 1:55:B:TRP:CA | 1:55:B:TRP:C | 9                   | 4.96  | 1.12            | 4.42   |
| (1,213) | 1:54:A:ILE:C | 1:55:A:TRP:N  | 1:55:A:TRP:CA | 1:55:A:TRP:C | 9                   | 4.94  | 1.05            | 4.41   |
| (1,81)  | 1:21:A:SER:C | 1:22:A:GLU:N  | 1:22:A:GLU:CA | 1:22:A:GLU:C | 9                   | 3.63  | 1.21            | 4.2    |
| (1,82)  | 1:21:B:SER:C | 1:22:B:GLU:N  | 1:22:B:GLU:CA | 1:22:B:GLU:C | 9                   | 3.62  | 1.18            | 4.26   |
| (1,303) | 1:77:A:GLY:N | 1:77:A:GLY:CA | 1:77:A:GLY:C  | 1:78:A:GLY:N | 9                   | 3.35  | 1.41            | 3.09   |
| (1,304) | 1:77:B:GLY:N | 1:77:B:GLY:CA | 1:77:B:GLY:C  | 1:78:B:GLY:N | 9                   | 3.28  | 1.49            | 2.82   |
| (1,294) | 1:74:B:ALA:C | 1:75:B:HIS:N  | 1:75:B:HIS:CA | 1:75:B:HIS:C | 9                   | 2.37  | 0.62            | 2.19   |
| (1,293) | 1:74:A:ALA:C | 1:75:A:HIS:N  | 1:75:A:HIS:CA | 1:75:A:HIS:C | 9                   | 2.37  | 0.65            | 2.05   |
| (1,7)   | 1:2:A:GLY:C  | 1:3:A:LEU:N   | 1:3:A:LEU:CA  | 1:3:A:LEU:C  | 8                   | 5.81  | 2.57            | 6.69   |
| (1,198) | 1:50:B:LYS:C | 1:51:B:ASN:N  | 1:51:B:ASN:CA | 1:51:B:ASN:C | 8                   | 4.98  | 3.51            | 5.18   |
| (1,197) | 1:50:A:LYS:C | 1:51:A:ASN:N  | 1:51:A:ASN:CA | 1:51:A:ASN:C | 8                   | 4.95  | 3.51            | 5.04   |
| (1,182) | 1:46:B:GLY:C | 1:47:B:ILE:N  | 1:47:B:ILE:CA | 1:47:B:ILE:C | 8                   | 2.64  | 1.6             | 2.17   |
| (1,181) | 1:46:A:GLY:C | 1:47:A:ILE:N  | 1:47:A:ILE:CA | 1:47:A:ILE:C | 8                   | 2.54  | 1.65            | 1.93   |
| (1,43)  | 1:12:A:GLN:N | 1:12:A:GLN:CA | 1:12:A:GLN:C  | 1:13:A:LEU:N | 8                   | 2.44  | 1.02            | 2.16   |
| (1,281) | 1:71:A:GLY:C | 1:72:A:ILE:N  | 1:72:A:ILE:CA | 1:72:A:ILE:C | 8                   | 2.37  | 0.75            | 2.5    |
| (1,282) | 1:71:B:GLY:C | 1:72:B:ILE:N  | 1:72:B:ILE:CA | 1:72:B:ILE:C | 8                   | 2.32  | 0.65            | 2.36   |
| (1,63)  | 1:17:A:TYR:N | 1:17:A:TYR:CA | 1:17:A:TYR:C  | 1:18:A:VAL:N | 8                   | 1.9   | 0.41            | 1.86   |
| (1,64)  | 1:17:B:TYR:N | 1:17:B:TYR:CA | 1:17:B:TYR:C  | 1:18:B:VAL:N | 8                   | 1.87  | 0.39            | 1.86   |
| (1,8)   | 1:2:B:GLY:C  | 1:3:B:LEU:N   | 1:3:B:LEU:CA  | 1:3:B:LEU:C  | 7                   | 6.46  | 1.97            | 6.7    |
| (1,11)  | 1:3:A:LEU:C  | 1:4:A:ILE:N   | 1:4:A:ILE:CA  | 1:4:A:ILE:C  | 7                   | 4.25  | 1.78            | 3.58   |
| (1,12)  | 1:3:B:LEU:C  | 1:4:B:ILE:N   | 1:4:B:ILE:CA  | 1:4:B:ILE:C  | 7                   | 4.2   | 1.8             | 3.65   |
| (1,44)  | 1:12:B:GLN:N | 1:12:B:GLN:CA | 1:12:B:GLN:C  | 1:13:B:LEU:N | 7                   | 2.58  | 0.95            | 2.16   |
| (1,70)  | 1:18:B:VAL:C | 1:19:B:SER:N  | 1:19:B:SER:CA | 1:19:B:SER:C | 7                   | 1.64  | 0.51            | 1.59   |
| (1,208) | 1:53:B:THR:N | 1:53:B:THR:CA | 1:53:B:THR:C  | 1:54:B:ILE:N | 6                   | 17.85 | 1.16            | 17.51  |
| (1,207) | 1:53:A:THR:N | 1:53:A:THR:CA | 1:53:A:THR:C  | 1:54:A:ILE:N | 6                   | 17.84 | 1.09            | 17.54  |
| (1,209) | 1:53:A:THR:C | 1:54:A:ILE:N  | 1:54:A:ILE:CA | 1:54:A:ILE:C | 6                   | 15.28 | 0.44            | 15.13  |

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| Key     | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Models <sup>1</sup> | Mean  | SD <sup>2</sup> | Median |
|---------|--------------|---------------|---------------|--------------|---------------------|-------|-----------------|--------|
| (1,210) | 1:53:B:THR:C | 1:54:B:ILE:N  | 1:54:B:ILE:CA | 1:54:B:ILE:C | 6                   | 15.23 | 0.36            | 15.08  |
| (1,107) | 1:28:A:SER:N | 1:28:A:SER:CA | 1:28:A:SER:C  | 1:29:A:LEU:N | 6                   | 2.78  | 1.13            | 2.5    |
| (1,108) | 1:28:B:SER:N | 1:28:B:SER:CA | 1:28:B:SER:C  | 1:29:B:LEU:N | 6                   | 2.71  | 1.15            | 2.44   |
| (1,263) | 1:67:A:ALA:N | 1:67:A:ALA:CA | 1:67:A:ALA:C  | 1:68:A:MET:N | 6                   | 1.84  | 0.31            | 1.93   |
| (1,41)  | 1:11:A:PRO:C | 1:12:A:GLN:N  | 1:12:A:GLN:CA | 1:12:A:GLN:C | 6                   | 1.81  | 0.47            | 1.76   |
| (1,42)  | 1:11:B:PRO:C | 1:12:B:GLN:N  | 1:12:B:GLN:CA | 1:12:B:GLN:C | 6                   | 1.8   | 0.44            | 1.82   |
| (1,264) | 1:67:B:ALA:N | 1:67:B:ALA:CA | 1:67:B:ALA:C  | 1:68:B:MET:N | 6                   | 1.78  | 0.34            | 1.87   |
| (1,69)  | 1:18:A:VAL:C | 1:19:A:SER:N  | 1:19:A:SER:CA | 1:19:A:SER:C | 6                   | 1.75  | 0.49            | 1.83   |
| (1,195) | 1:50:A:LYS:N | 1:50:A:LYS:CA | 1:50:A:LYS:C  | 1:51:A:ASN:N | 5                   | 8.29  | 3.72            | 9.49   |
| (1,196) | 1:50:B:LYS:N | 1:50:B:LYS:CA | 1:50:B:LYS:C  | 1:51:B:ASN:N | 5                   | 8.23  | 3.71            | 9.38   |
| (1,222) | 1:56:B:VAL:C | 1:57:B:GLY:N  | 1:57:B:GLY:CA | 1:57:B:GLY:C | 5                   | 4.27  | 1.22            | 4.33   |
| (1,221) | 1:56:A:VAL:C | 1:57:A:GLY:N  | 1:57:A:GLY:CA | 1:57:A:GLY:C | 5                   | 4.22  | 1.15            | 4.21   |
| (1,179) | 1:46:A:GLY:N | 1:46:A:GLY:CA | 1:46:A:GLY:C  | 1:47:A:ILE:N | 5                   | 2.72  | 1.6             | 2.19   |
| (1,98)  | 1:25:B:LEU:C | 1:26:B:GLY:N  | 1:26:B:GLY:CA | 1:26:B:GLY:C | 5                   | 2.1   | 0.67            | 2.57   |
| (1,97)  | 1:25:A:LEU:C | 1:26:A:GLY:N  | 1:26:A:GLY:CA | 1:26:A:GLY:C | 5                   | 2.05  | 0.65            | 2.47   |
| (1,205) | 1:52:A:PRO:C | 1:53:A:THR:N  | 1:53:A:THR:CA | 1:53:A:THR:C | 4                   | 11.1  | 2.27            | 11.84  |
| (1,206) | 1:52:B:PRO:C | 1:53:B:THR:N  | 1:53:B:THR:CA | 1:53:B:THR:C | 4                   | 11.06 | 2.21            | 11.78  |
| (1,203) | 1:52:A:PRO:N | 1:52:A:PRO:CA | 1:52:A:PRO:C  | 1:53:A:THR:N | 4                   | 9.65  | 3.56            | 11.32  |
| (1,204) | 1:52:B:PRO:N | 1:52:B:PRO:CA | 1:52:B:PRO:C  | 1:53:B:THR:N | 4                   | 9.65  | 3.5             | 11.25  |
| (1,183) | 1:47:A:ILE:N | 1:47:A:ILE:CA | 1:47:A:ILE:C  | 1:48:A:TYR:N | 4                   | 4.98  | 1.74            | 4.76   |
| (1,184) | 1:47:B:ILE:N | 1:47:B:ILE:CA | 1:47:B:ILE:C  | 1:48:B:TYR:N | 4                   | 4.96  | 1.67            | 4.62   |
| (1,185) | 1:47:A:ILE:C | 1:48:A:TYR:N  | 1:48:A:TYR:CA | 1:48:A:TYR:C | 4                   | 3.75  | 1.5             | 3.0    |
| (1,186) | 1:47:B:ILE:C | 1:48:B:TYR:N  | 1:48:B:TYR:CA | 1:48:B:TYR:C | 4                   | 3.73  | 1.55            | 2.9    |
| (1,215) | 1:55:A:TRP:N | 1:55:A:TRP:CA | 1:55:A:TRP:C  | 1:56:A:VAL:N | 4                   | 3.51  | 0.85            | 3.28   |
| (1,216) | 1:55:B:TRP:N | 1:55:B:TRP:CA | 1:55:B:TRP:C  | 1:56:B:VAL:N | 4                   | 3.5   | 0.84            | 3.28   |
| (1,180) | 1:46:B:GLY:N | 1:46:B:GLY:CA | 1:46:B:GLY:C  | 1:47:B:ILE:N | 4                   | 3.03  | 1.7             | 2.44   |
| (1,189) | 1:48:A:TYR:C | 1:49:A:HIS:N  | 1:49:A:HIS:CA | 1:49:A:HIS:C | 4                   | 2.76  | 1.05            | 2.56   |
| (1,190) | 1:48:B:TYR:C | 1:49:B:HIS:N  | 1:49:B:HIS:CA | 1:49:B:HIS:C | 4                   | 2.76  | 1.01            | 2.55   |
| (1,220) | 1:56:B:VAL:N | 1:56:B:VAL:CA | 1:56:B:VAL:C  | 1:57:B:GLY:N | 4                   | 2.31  | 1.48            | 1.7    |
| (1,72)  | 1:19:B:SER:N | 1:19:B:SER:CA | 1:19:B:SER:C  | 1:20:B:HIS:N | 4                   | 1.9   | 0.23            | 1.96   |
| (1,71)  | 1:19:A:SER:N | 1:19:A:SER:CA | 1:19:A:SER:C  | 1:20:A:HIS:N | 4                   | 1.89  | 0.2             | 2.0    |
| (1,192) | 1:49:B:HIS:N | 1:49:B:HIS:CA | 1:49:B:HIS:C  | 1:50:B:LYS:N | 4                   | 1.67  | 0.53            | 1.52   |
| (1,191) | 1:49:A:HIS:N | 1:49:A:HIS:CA | 1:49:A:HIS:C  | 1:50:A:LYS:N | 4                   | 1.64  | 0.48            | 1.49   |
| (1,308) | 1:78:B:GLY:N | 1:78:B:GLY:CA | 1:78:B:GLY:C  | 1:79:B:THR:N | 4                   | 1.61  | 0.3             | 1.52   |
| (1,307) | 1:78:A:GLY:N | 1:78:A:GLY:CA | 1:78:A:GLY:C  | 1:79:A:THR:N | 4                   | 1.56  | 0.27            | 1.44   |
| (1,23)  | 1:6:A:PRO:C  | 1:7:A:LEU:N   | 1:7:A:LEU:CA  | 1:7:A:LEU:C  | 4                   | 1.37  | 0.26            | 1.28   |
| (1,24)  | 1:6:B:PRO:C  | 1:7:B:LEU:N   | 1:7:B:LEU:CA  | 1:7:B:LEU:C  | 4                   | 1.35  | 0.24            | 1.31   |
| (1,10)  | 1:3:B:LEU:N  | 1:3:B:LEU:CA  | 1:3:B:LEU:C   | 1:4:B:ILE:N  | 3                   | 4.83  | 0.62            | 4.42   |
| (1,9)   | 1:3:A:LEU:N  | 1:3:A:LEU:CA  | 1:3:A:LEU:C   | 1:4:A:ILE:N  | 3                   | 4.76  | 0.59            | 4.5    |
| (1,35)  | 1:9:A:THR:C  | 1:10:A:MET:N  | 1:10:A:MET:CA | 1:10:A:MET:C | 3                   | 3.99  | 1.3             | 4.48   |
| (1,36)  | 1:9:B:THR:C  | 1:10:B:MET:N  | 1:10:B:MET:CA | 1:10:B:MET:C | 3                   | 3.93  | 1.38            | 4.38   |
| (1,219) | 1:56:A:VAL:N | 1:56:A:VAL:CA | 1:56:A:VAL:C  | 1:57:A:GLY:N | 3                   | 2.75  | 1.4             | 1.89   |
| (1,262) | 1:66:B:VAL:C | 1:67:B:ALA:N  | 1:67:B:ALA:CA | 1:67:B:ALA:C | 3                   | 2.11  | 1.2             | 1.53   |
| (1,261) | 1:66:A:VAL:C | 1:67:A:ALA:N  | 1:67:A:ALA:CA | 1:67:A:ALA:C | 3                   | 2.09  | 1.16            | 1.56   |
| (1,143) | 1:37:A:PHE:N | 1:37:A:PHE:CA | 1:37:A:PHE:C  | 1:38:A:ILE:N | 3                   | 2.03  | 0.52            | 1.86   |
| (1,144) | 1:37:B:PHE:N | 1:37:B:PHE:CA | 1:37:B:PHE:C  | 1:38:B:ILE:N | 3                   | 1.9   | 0.54            | 1.61   |
| (1,59)  | 1:16:A:LEU:N | 1:16:A:LEU:CA | 1:16:A:LEU:C  | 1:17:A:TYR:N | 3                   | 1.78  | 0.76            | 1.3    |
| (1,60)  | 1:16:B:LEU:N | 1:16:B:LEU:CA | 1:16:B:LEU:C  | 1:17:B:TYR:N | 3                   | 1.78  | 0.74            | 1.37   |
| (1,87)  | 1:23:A:HIS:N | 1:23:A:HIS:CA | 1:23:A:HIS:C  | 1:24:A:ALA:N | 3                   | 1.73  | 0.17            | 1.63   |
| (1,88)  | 1:23:B:HIS:N | 1:23:B:HIS:CA | 1:23:B:HIS:C  | 1:24:B:ALA:N | 3                   | 1.71  | 0.17            | 1.6    |
| (1,229) | 1:58:A:ASN:C | 1:59:A:CYS:N  | 1:59:A:CYS:CA | 1:59:A:CYS:C | 3                   | 1.21  | 0.14            | 1.28   |

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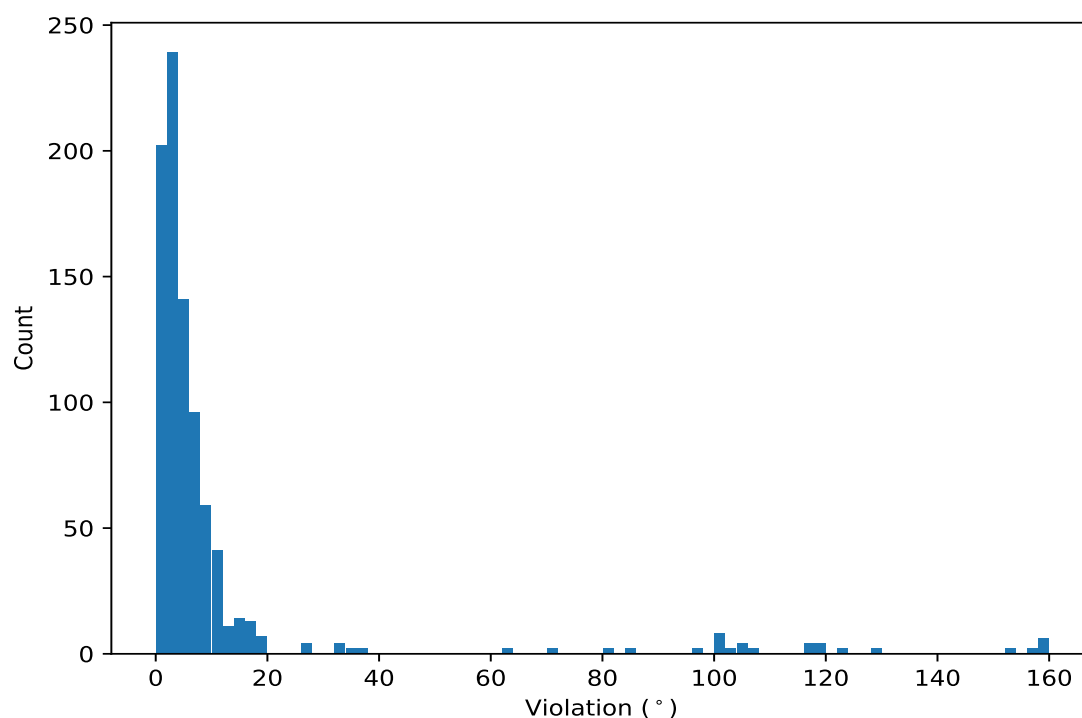
| Key     | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Models <sup>1</sup> | Mean | SD <sup>2</sup> | Median |
|---------|--------------|---------------|---------------|--------------|---------------------|------|-----------------|--------|
| (1,266) | 1:67:B:ALA:C | 1:68:B:MET:N  | 1:68:B:MET:CA | 1:68:B:MET:C | 2                   | 4.16 | 0.64            | 4.16   |
| (1,265) | 1:67:A:ALA:C | 1:68:A:MET:N  | 1:68:A:MET:CA | 1:68:A:MET:C | 2                   | 4.11 | 0.52            | 4.11   |
| (1,217) | 1:55:A:TRP:C | 1:56:A:VAL:N  | 1:56:A:VAL:CA | 1:56:A:VAL:C | 2                   | 3.62 | 2.01            | 3.62   |
| (1,218) | 1:55:B:TRP:C | 1:56:B:VAL:N  | 1:56:B:VAL:CA | 1:56:B:VAL:C | 2                   | 3.62 | 1.96            | 3.62   |
| (1,269) | 1:68:A:MET:C | 1:69:A:VAL:N  | 1:69:A:VAL:CA | 1:69:A:VAL:C | 2                   | 2.81 | 0.69            | 2.81   |
| (1,270) | 1:68:B:MET:C | 1:69:B:VAL:N  | 1:69:B:VAL:CA | 1:69:B:VAL:C | 2                   | 2.74 | 0.69            | 2.74   |
| (1,292) | 1:74:B:ALA:N | 1:74:B:ALA:CA | 1:74:B:ALA:C  | 1:75:B:HIS:N | 2                   | 2.1  | 0.09            | 2.1    |
| (1,167) | 1:43:A:THR:N | 1:43:A:THR:CA | 1:43:A:THR:C  | 1:44:A:ILE:N | 2                   | 2.02 | 0.68            | 2.02   |
| (1,291) | 1:74:A:ALA:N | 1:74:A:ALA:CA | 1:74:A:ALA:C  | 1:75:A:HIS:N | 2                   | 2.02 | 0.06            | 2.02   |
| (1,168) | 1:43:B:THR:N | 1:43:B:THR:CA | 1:43:B:THR:C  | 1:44:B:ILE:N | 2                   | 1.9  | 0.73            | 1.9    |
| (1,104) | 1:27:B:LEU:N | 1:27:B:LEU:CA | 1:27:B:LEU:C  | 1:28:B:SER:N | 2                   | 1.9  | 0.24            | 1.9    |
| (1,103) | 1:27:A:LEU:N | 1:27:A:LEU:CA | 1:27:A:LEU:C  | 1:28:A:SER:N | 2                   | 1.88 | 0.25            | 1.88   |
| (1,152) | 1:39:B:ALA:N | 1:39:B:ALA:CA | 1:39:B:ALA:C  | 1:40:B:LEU:N | 2                   | 1.86 | 0.05            | 1.86   |
| (1,151) | 1:39:A:ALA:N | 1:39:A:ALA:CA | 1:39:A:ALA:C  | 1:40:A:LEU:N | 2                   | 1.85 | 0.15            | 1.85   |
| (1,89)  | 1:23:A:HIS:C | 1:24:A:ALA:N  | 1:24:A:ALA:CA | 1:24:A:ALA:C | 2                   | 1.6  | 0.45            | 1.6    |
| (1,90)  | 1:23:B:HIS:C | 1:24:B:ALA:N  | 1:24:B:ALA:CA | 1:24:B:ALA:C | 2                   | 1.54 | 0.48            | 1.54   |
| (1,6)   | 1:2:B:GLY:N  | 1:2:B:GLY:CA  | 1:2:B:GLY:C   | 1:3:B:LEU:N  | 2                   | 1.43 | 0.21            | 1.43   |
| (1,5)   | 1:2:A:GLY:N  | 1:2:A:GLY:CA  | 1:2:A:GLY:C   | 1:3:A:LEU:N  | 2                   | 1.34 | 0.29            | 1.34   |
| (1,230) | 1:58:B:ASN:C | 1:59:B:CYS:N  | 1:59:B:CYS:CA | 1:59:B:CYS:C | 2                   | 1.26 | 0.12            | 1.26   |
| (1,49)  | 1:13:A:LEU:C | 1:14:A:TYR:N  | 1:14:A:TYR:CA | 1:14:A:TYR:C | 2                   | 1.25 | 0.14            | 1.25   |
| (1,50)  | 1:13:B:LEU:C | 1:14:B:TYR:N  | 1:14:B:TYR:CA | 1:14:B:TYR:C | 2                   | 1.21 | 0.15            | 1.21   |

<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 ⓘ

### 10.5.1 Histogram : Distribution of violations ⓘ

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 (°) |
|--------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,76) | 1:20:B:HIS:N | 1:20:B:HIS:CA | 1:20:B:HIS:C  | 1:21:B:SER:N | 3        | 159.89        |
| (1,75) | 1:20:A:HIS:N | 1:20:A:HIS:CA | 1:20:A:HIS:C  | 1:21:A:SER:N | 3        | 159.82        |
| (1,76) | 1:20:B:HIS:N | 1:20:B:HIS:CA | 1:20:B:HIS:C  | 1:21:B:SER:N | 6        | 159.39        |
| (1,75) | 1:20:A:HIS:N | 1:20:A:HIS:CA | 1:20:A:HIS:C  | 1:21:A:SER:N | 6        | 159.36        |
| (1,76) | 1:20:B:HIS:N | 1:20:B:HIS:CA | 1:20:B:HIS:C  | 1:21:B:SER:N | 8        | 159.26        |
| (1,75) | 1:20:A:HIS:N | 1:20:A:HIS:CA | 1:20:A:HIS:C  | 1:21:A:SER:N | 8        | 159.21        |
| (1,76) | 1:20:B:HIS:N | 1:20:B:HIS:CA | 1:20:B:HIS:C  | 1:21:B:SER:N | 9        | 156.91        |
| (1,75) | 1:20:A:HIS:N | 1:20:A:HIS:CA | 1:20:A:HIS:C  | 1:21:A:SER:N | 9        | 156.88        |
| (1,75) | 1:20:A:HIS:N | 1:20:A:HIS:CA | 1:20:A:HIS:C  | 1:21:A:SER:N | 2        | 153.76        |
| (1,76) | 1:20:B:HIS:N | 1:20:B:HIS:CA | 1:20:B:HIS:C  | 1:21:B:SER:N | 2        | 153.66        |
| (1,75) | 1:20:A:HIS:N | 1:20:A:HIS:CA | 1:20:A:HIS:C  | 1:21:A:SER:N | 10       | 128.36        |
| (1,76) | 1:20:B:HIS:N | 1:20:B:HIS:CA | 1:20:B:HIS:C  | 1:21:B:SER:N | 10       | 128.34        |
| (1,75) | 1:20:A:HIS:N | 1:20:A:HIS:CA | 1:20:A:HIS:C  | 1:21:A:SER:N | 7        | 123.5         |
| (1,76) | 1:20:B:HIS:N | 1:20:B:HIS:CA | 1:20:B:HIS:C  | 1:21:B:SER:N | 7        | 123.46        |
| (1,73) | 1:19:A:SER:C | 1:20:A:HIS:N  | 1:20:A:HIS:CA | 1:20:A:HIS:C | 10       | 119.67        |
| (1,74) | 1:19:B:SER:C | 1:20:B:HIS:N  | 1:20:B:HIS:CA | 1:20:B:HIS:C | 10       | 119.55        |
| (1,74) | 1:19:B:SER:C | 1:20:B:HIS:N  | 1:20:B:HIS:CA | 1:20:B:HIS:C | 4        | 118.91        |
| (1,73) | 1:19:A:SER:C | 1:20:A:HIS:N  | 1:20:A:HIS:CA | 1:20:A:HIS:C | 4        | 118.9         |
| (1,75) | 1:20:A:HIS:N | 1:20:A:HIS:CA | 1:20:A:HIS:C  | 1:21:A:SER:N | 1        | 117.36        |
| (1,76) | 1:20:B:HIS:N | 1:20:B:HIS:CA | 1:20:B:HIS:C  | 1:21:B:SER:N | 1        | 117.33        |
| (1,76) | 1:20:B:HIS:N | 1:20:B:HIS:CA | 1:20:B:HIS:C  | 1:21:B:SER:N | 4        | 117.2         |

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| Key     | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Model ID | Violation (°) |
|---------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,75)  | 1:20:A:HIS:N | 1:20:A:HIS:CA | 1:20:A:HIS:C  | 1:21:A:SER:N | 4        | 117.03        |
| (1,74)  | 1:19:B:SER:C | 1:20:B:HIS:N  | 1:20:B:HIS:CA | 1:20:B:HIS:C | 5        | 106.01        |
| (1,73)  | 1:19:A:SER:C | 1:20:A:HIS:N  | 1:20:A:HIS:CA | 1:20:A:HIS:C | 5        | 106.01        |
| (1,74)  | 1:19:B:SER:C | 1:20:B:HIS:N  | 1:20:B:HIS:CA | 1:20:B:HIS:C | 8        | 105.51        |
| (1,73)  | 1:19:A:SER:C | 1:20:A:HIS:N  | 1:20:A:HIS:CA | 1:20:A:HIS:C | 8        | 105.31        |
| (1,74)  | 1:19:B:SER:C | 1:20:B:HIS:N  | 1:20:B:HIS:CA | 1:20:B:HIS:C | 9        | 105.07        |
| (1,73)  | 1:19:A:SER:C | 1:20:A:HIS:N  | 1:20:A:HIS:CA | 1:20:A:HIS:C | 9        | 104.93        |
| (1,74)  | 1:19:B:SER:C | 1:20:B:HIS:N  | 1:20:B:HIS:CA | 1:20:B:HIS:C | 2        | 102.99        |
| (1,73)  | 1:19:A:SER:C | 1:20:A:HIS:N  | 1:20:A:HIS:CA | 1:20:A:HIS:C | 2        | 102.98        |
| (1,73)  | 1:19:A:SER:C | 1:20:A:HIS:N  | 1:20:A:HIS:CA | 1:20:A:HIS:C | 7        | 100.39        |
| (1,76)  | 1:20:B:HIS:N | 1:20:B:HIS:CA | 1:20:B:HIS:C  | 1:21:B:SER:N | 5        | 100.26        |
| (1,74)  | 1:19:B:SER:C | 1:20:B:HIS:N  | 1:20:B:HIS:CA | 1:20:B:HIS:C | 7        | 100.26        |
| (1,75)  | 1:20:A:HIS:N | 1:20:A:HIS:CA | 1:20:A:HIS:C  | 1:21:A:SER:N | 5        | 100.25        |
| (1,73)  | 1:19:A:SER:C | 1:20:A:HIS:N  | 1:20:A:HIS:CA | 1:20:A:HIS:C | 6        | 100.19        |
| (1,73)  | 1:19:A:SER:C | 1:20:A:HIS:N  | 1:20:A:HIS:CA | 1:20:A:HIS:C | 1        | 100.16        |
| (1,74)  | 1:19:B:SER:C | 1:20:B:HIS:N  | 1:20:B:HIS:CA | 1:20:B:HIS:C | 6        | 100.13        |
| (1,74)  | 1:19:B:SER:C | 1:20:B:HIS:N  | 1:20:B:HIS:CA | 1:20:B:HIS:C | 1        | 100.11        |
| (1,74)  | 1:19:B:SER:C | 1:20:B:HIS:N  | 1:20:B:HIS:CA | 1:20:B:HIS:C | 3        | 97.08         |
| (1,73)  | 1:19:A:SER:C | 1:20:A:HIS:N  | 1:20:A:HIS:CA | 1:20:A:HIS:C | 3        | 96.98         |
| (1,77)  | 1:20:A:HIS:C | 1:21:A:SER:N  | 1:21:A:SER:CA | 1:21:A:SER:C | 5        | 85.89         |
| (1,78)  | 1:20:B:HIS:C | 1:21:B:SER:N  | 1:21:B:SER:CA | 1:21:B:SER:C | 5        | 85.82         |
| (1,78)  | 1:20:B:HIS:C | 1:21:B:SER:N  | 1:21:B:SER:CA | 1:21:B:SER:C | 1        | 81.58         |
| (1,77)  | 1:20:A:HIS:C | 1:21:A:SER:N  | 1:21:A:SER:CA | 1:21:A:SER:C | 1        | 81.57         |
| (1,77)  | 1:20:A:HIS:C | 1:21:A:SER:N  | 1:21:A:SER:CA | 1:21:A:SER:C | 7        | 70.57         |
| (1,78)  | 1:20:B:HIS:C | 1:21:B:SER:N  | 1:21:B:SER:CA | 1:21:B:SER:C | 7        | 70.54         |
| (1,77)  | 1:20:A:HIS:C | 1:21:A:SER:N  | 1:21:A:SER:CA | 1:21:A:SER:C | 4        | 63.87         |
| (1,78)  | 1:20:B:HIS:C | 1:21:B:SER:N  | 1:21:B:SER:CA | 1:21:B:SER:C | 4        | 63.81         |
| (1,78)  | 1:20:B:HIS:C | 1:21:B:SER:N  | 1:21:B:SER:CA | 1:21:B:SER:C | 3        | 36.72         |
| (1,77)  | 1:20:A:HIS:C | 1:21:A:SER:N  | 1:21:A:SER:CA | 1:21:A:SER:C | 3        | 36.69         |
| (1,77)  | 1:20:A:HIS:C | 1:21:A:SER:N  | 1:21:A:SER:CA | 1:21:A:SER:C | 10       | 35.85         |
| (1,78)  | 1:20:B:HIS:C | 1:21:B:SER:N  | 1:21:B:SER:CA | 1:21:B:SER:C | 10       | 35.83         |
| (1,77)  | 1:20:A:HIS:C | 1:21:A:SER:N  | 1:21:A:SER:CA | 1:21:A:SER:C | 8        | 33.26         |
| (1,78)  | 1:20:B:HIS:C | 1:21:B:SER:N  | 1:21:B:SER:CA | 1:21:B:SER:C | 8        | 33.22         |
| (1,78)  | 1:20:B:HIS:C | 1:21:B:SER:N  | 1:21:B:SER:CA | 1:21:B:SER:C | 2        | 33.16         |
| (1,77)  | 1:20:A:HIS:C | 1:21:A:SER:N  | 1:21:A:SER:CA | 1:21:A:SER:C | 2        | 33.15         |
| (1,77)  | 1:20:A:HIS:C | 1:21:A:SER:N  | 1:21:A:SER:CA | 1:21:A:SER:C | 6        | 27.9          |
| (1,78)  | 1:20:B:HIS:C | 1:21:B:SER:N  | 1:21:B:SER:CA | 1:21:B:SER:C | 6        | 27.88         |
| (1,77)  | 1:20:A:HIS:C | 1:21:A:SER:N  | 1:21:A:SER:CA | 1:21:A:SER:C | 9        | 27.15         |
| (1,78)  | 1:20:B:HIS:C | 1:21:B:SER:N  | 1:21:B:SER:CA | 1:21:B:SER:C | 9        | 27.02         |
| (1,208) | 1:53:B:THR:N | 1:53:B:THR:CA | 1:53:B:THR:C  | 1:54:B:ILE:N | 5        | 19.48         |
| (1,207) | 1:53:A:THR:N | 1:53:A:THR:CA | 1:53:A:THR:C  | 1:54:A:ILE:N | 5        | 19.41         |
| (1,208) | 1:53:B:THR:N | 1:53:B:THR:CA | 1:53:B:THR:C  | 1:54:B:ILE:N | 8        | 19.26         |
| (1,207) | 1:53:A:THR:N | 1:53:A:THR:CA | 1:53:A:THR:C  | 1:54:A:ILE:N | 8        | 19.07         |
| (1,201) | 1:51:A:ASN:C | 1:52:A:PRO:N  | 1:52:A:PRO:CA | 1:52:A:PRO:C | 4        | 18.26         |
| (1,202) | 1:51:B:ASN:C | 1:52:B:PRO:N  | 1:52:B:PRO:CA | 1:52:B:PRO:C | 4        | 18.18         |
| (1,207) | 1:53:A:THR:N | 1:53:A:THR:CA | 1:53:A:THR:C  | 1:54:A:ILE:N | 3        | 18.04         |
| (1,208) | 1:53:B:THR:N | 1:53:B:THR:CA | 1:53:B:THR:C  | 1:54:B:ILE:N | 3        | 17.98         |
| (1,18)  | 1:5:B:SER:N  | 1:5:B:SER:CA  | 1:5:B:SER:C   | 1:6:B:PRO:N  | 6        | 17.5          |
| (1,17)  | 1:5:A:SER:N  | 1:5:A:SER:CA  | 1:5:A:SER:C   | 1:6:A:PRO:N  | 6        | 17.33         |
| (1,208) | 1:53:B:THR:N | 1:53:B:THR:CA | 1:53:B:THR:C  | 1:54:B:ILE:N | 4        | 17.04         |
| (1,207) | 1:53:A:THR:N | 1:53:A:THR:CA | 1:53:A:THR:C  | 1:54:A:ILE:N | 4        | 17.03         |

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| Key     | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Model ID | Violation (°) |
|---------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,207) | 1:53:A:THR:N | 1:53:A:THR:CA | 1:53:A:THR:C  | 1:54:A:ILE:N | 6        | 16.97         |
| (1,208) | 1:53:B:THR:N | 1:53:B:THR:CA | 1:53:B:THR:C  | 1:54:B:ILE:N | 6        | 16.87         |
| (1,207) | 1:53:A:THR:N | 1:53:A:THR:CA | 1:53:A:THR:C  | 1:54:A:ILE:N | 9        | 16.54         |
| (1,18)  | 1:5:B:SER:N  | 1:5:B:SER:CA  | 1:5:B:SER:C   | 1:6:B:PRO:N  | 10       | 16.52         |
| (1,208) | 1:53:B:THR:N | 1:53:B:THR:CA | 1:53:B:THR:C  | 1:54:B:ILE:N | 9        | 16.49         |
| (1,17)  | 1:5:A:SER:N  | 1:5:A:SER:CA  | 1:5:A:SER:C   | 1:6:A:PRO:N  | 10       | 16.48         |
| (1,18)  | 1:5:B:SER:N  | 1:5:B:SER:CA  | 1:5:B:SER:C   | 1:6:B:PRO:N  | 2        | 16.44         |
| (1,17)  | 1:5:A:SER:N  | 1:5:A:SER:CA  | 1:5:A:SER:C   | 1:6:A:PRO:N  | 2        | 16.38         |
| (1,209) | 1:53:A:THR:C | 1:54:A:ILE:N  | 1:54:A:ILE:CA | 1:54:A:ILE:C | 3        | 15.96         |
| (1,210) | 1:53:B:THR:C | 1:54:B:ILE:N  | 1:54:B:ILE:CA | 1:54:B:ILE:C | 3        | 15.89         |
| (1,209) | 1:53:A:THR:C | 1:54:A:ILE:N  | 1:54:A:ILE:CA | 1:54:A:ILE:C | 8        | 15.74         |
| (1,210) | 1:53:B:THR:C | 1:54:B:ILE:N  | 1:54:B:ILE:CA | 1:54:B:ILE:C | 8        | 15.53         |
| (1,209) | 1:53:A:THR:C | 1:54:A:ILE:N  | 1:54:A:ILE:CA | 1:54:A:ILE:C | 6        | 15.19         |
| (1,210) | 1:53:B:THR:C | 1:54:B:ILE:N  | 1:54:B:ILE:CA | 1:54:B:ILE:C | 9        | 15.08         |
| (1,210) | 1:53:B:THR:C | 1:54:B:ILE:N  | 1:54:B:ILE:CA | 1:54:B:ILE:C | 6        | 15.07         |
| (1,209) | 1:53:A:THR:C | 1:54:A:ILE:N  | 1:54:A:ILE:CA | 1:54:A:ILE:C | 9        | 15.07         |
| (1,209) | 1:53:A:THR:C | 1:54:A:ILE:N  | 1:54:A:ILE:CA | 1:54:A:ILE:C | 5        | 15.02         |
| (1,210) | 1:53:B:THR:C | 1:54:B:ILE:N  | 1:54:B:ILE:CA | 1:54:B:ILE:C | 5        | 14.96         |
| (1,210) | 1:53:B:THR:C | 1:54:B:ILE:N  | 1:54:B:ILE:CA | 1:54:B:ILE:C | 4        | 14.84         |
| (1,209) | 1:53:A:THR:C | 1:54:A:ILE:N  | 1:54:A:ILE:CA | 1:54:A:ILE:C | 4        | 14.67         |
| (1,202) | 1:51:B:ASN:C | 1:52:B:PRO:N  | 1:52:B:PRO:CA | 1:52:B:PRO:C | 6        | 14.25         |
| (1,201) | 1:51:A:ASN:C | 1:52:A:PRO:N  | 1:52:A:PRO:CA | 1:52:A:PRO:C | 6        | 14.24         |
| (1,200) | 1:51:B:ASN:N | 1:51:B:ASN:CA | 1:51:B:ASN:C  | 1:52:B:PRO:N | 2        | 13.5          |
| (1,205) | 1:52:A:PRO:C | 1:53:A:THR:N  | 1:53:A:THR:CA | 1:53:A:THR:C | 7        | 13.37         |
| (1,201) | 1:51:A:ASN:C | 1:52:A:PRO:N  | 1:52:A:PRO:CA | 1:52:A:PRO:C | 9        | 13.36         |
| (1,206) | 1:52:B:PRO:C | 1:53:B:THR:N  | 1:53:B:THR:CA | 1:53:B:THR:C | 7        | 13.29         |
| (1,202) | 1:51:B:ASN:C | 1:52:B:PRO:N  | 1:52:B:PRO:CA | 1:52:B:PRO:C | 9        | 13.18         |
| (1,199) | 1:51:A:ASN:N | 1:51:A:ASN:CA | 1:51:A:ASN:C  | 1:52:A:PRO:N | 2        | 12.93         |
| (1,204) | 1:52:B:PRO:N | 1:52:B:PRO:CA | 1:52:B:PRO:C  | 1:53:B:THR:N | 1        | 12.44         |
| (1,203) | 1:52:A:PRO:N | 1:52:A:PRO:CA | 1:52:A:PRO:C  | 1:53:A:THR:N | 1        | 12.44         |
| (1,205) | 1:52:A:PRO:C | 1:53:A:THR:N  | 1:53:A:THR:CA | 1:53:A:THR:C | 1        | 12.1          |
| (1,15)  | 1:4:A:ILE:C  | 1:5:A:SER:N   | 1:5:A:SER:CA  | 1:5:A:SER:C  | 9        | 12.03         |
| (1,206) | 1:52:B:PRO:C | 1:53:B:THR:N  | 1:53:B:THR:CA | 1:53:B:THR:C | 1        | 12.02         |
| (1,15)  | 1:4:A:ILE:C  | 1:5:A:SER:N   | 1:5:A:SER:CA  | 1:5:A:SER:C  | 3        | 11.9          |
| (1,16)  | 1:4:B:ILE:C  | 1:5:B:SER:N   | 1:5:B:SER:CA  | 1:5:B:SER:C  | 9        | 11.89         |
| (1,16)  | 1:4:B:ILE:C  | 1:5:B:SER:N   | 1:5:B:SER:CA  | 1:5:B:SER:C  | 3        | 11.88         |
| (1,195) | 1:50:A:LYS:N | 1:50:A:LYS:CA | 1:50:A:LYS:C  | 1:51:A:ASN:N | 2        | 11.79         |
| (1,196) | 1:50:B:LYS:N | 1:50:B:LYS:CA | 1:50:B:LYS:C  | 1:51:B:ASN:N | 2        | 11.66         |
| (1,201) | 1:51:A:ASN:C | 1:52:A:PRO:N  | 1:52:A:PRO:CA | 1:52:A:PRO:C | 3        | 11.61         |
| (1,18)  | 1:5:B:SER:N  | 1:5:B:SER:CA  | 1:5:B:SER:C   | 1:6:B:PRO:N  | 1        | 11.6          |
| (1,205) | 1:52:A:PRO:C | 1:53:A:THR:N  | 1:53:A:THR:CA | 1:53:A:THR:C | 10       | 11.58         |
| (1,203) | 1:52:A:PRO:N | 1:52:A:PRO:CA | 1:52:A:PRO:C  | 1:53:A:THR:N | 10       | 11.56         |
| (1,17)  | 1:5:A:SER:N  | 1:5:A:SER:CA  | 1:5:A:SER:C   | 1:6:A:PRO:N  | 1        | 11.55         |
| (1,206) | 1:52:B:PRO:C | 1:53:B:THR:N  | 1:53:B:THR:CA | 1:53:B:THR:C | 10       | 11.54         |
| (1,202) | 1:51:B:ASN:C | 1:52:B:PRO:N  | 1:52:B:PRO:CA | 1:52:B:PRO:C | 3        | 11.53         |
| (1,204) | 1:52:B:PRO:N | 1:52:B:PRO:CA | 1:52:B:PRO:C  | 1:53:B:THR:N | 10       | 11.48         |
| (1,83)  | 1:22:A:GLU:N | 1:22:A:GLU:CA | 1:22:A:GLU:C  | 1:23:A:HIS:N | 5        | 11.37         |
| (1,15)  | 1:4:A:ILE:C  | 1:5:A:SER:N   | 1:5:A:SER:CA  | 1:5:A:SER:C  | 8        | 11.35         |
| (1,16)  | 1:4:B:ILE:C  | 1:5:B:SER:N   | 1:5:B:SER:CA  | 1:5:B:SER:C  | 8        | 11.32         |
| (1,84)  | 1:22:B:GLU:N | 1:22:B:GLU:CA | 1:22:B:GLU:C  | 1:23:B:HIS:N | 5        | 11.26         |
| (1,17)  | 1:5:A:SER:N  | 1:5:A:SER:CA  | 1:5:A:SER:C   | 1:6:A:PRO:N  | 7        | 11.25         |

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| Key     | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Model ID | Violation (°) |
|---------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,16)  | 1:4:B:ILE:C  | 1:5:B:SER:N   | 1:5:B:SER:CA  | 1:5:B:SER:C  | 4        | 11.1          |
| (1,203) | 1:52:A:PRO:N | 1:52:A:PRO:CA | 1:52:A:PRO:C  | 1:53:A:THR:N | 7        | 11.07         |
| (1,15)  | 1:4:A:ILE:C  | 1:5:A:SER:N   | 1:5:A:SER:CA  | 1:5:A:SER:C  | 4        | 11.05         |
| (1,18)  | 1:5:B:SER:N  | 1:5:B:SER:CA  | 1:5:B:SER:C   | 1:6:B:PRO:N  | 7        | 11.04         |
| (1,16)  | 1:4:B:ILE:C  | 1:5:B:SER:N   | 1:5:B:SER:CA  | 1:5:B:SER:C  | 1        | 11.04         |
| (1,204) | 1:52:B:PRO:N | 1:52:B:PRO:CA | 1:52:B:PRO:C  | 1:53:B:THR:N | 7        | 11.02         |
| (1,202) | 1:51:B:ASN:C | 1:52:B:PRO:N  | 1:52:B:PRO:CA | 1:52:B:PRO:C | 7        | 11.0          |
| (1,15)  | 1:4:A:ILE:C  | 1:5:A:SER:N   | 1:5:A:SER:CA  | 1:5:A:SER:C  | 1        | 10.89         |
| (1,199) | 1:51:A:ASN:N | 1:51:A:ASN:CA | 1:51:A:ASN:C  | 1:52:A:PRO:N | 7        | 10.87         |
| (1,15)  | 1:4:A:ILE:C  | 1:5:A:SER:N   | 1:5:A:SER:CA  | 1:5:A:SER:C  | 7        | 10.85         |
| (1,200) | 1:51:B:ASN:N | 1:51:B:ASN:CA | 1:51:B:ASN:C  | 1:52:B:PRO:N | 10       | 10.83         |
| (1,201) | 1:51:A:ASN:C | 1:52:A:PRO:N  | 1:52:A:PRO:CA | 1:52:A:PRO:C | 7        | 10.81         |
| (1,15)  | 1:4:A:ILE:C  | 1:5:A:SER:N   | 1:5:A:SER:CA  | 1:5:A:SER:C  | 2        | 10.77         |
| (1,199) | 1:51:A:ASN:N | 1:51:A:ASN:CA | 1:51:A:ASN:C  | 1:52:A:PRO:N | 10       | 10.76         |
| (1,16)  | 1:4:B:ILE:C  | 1:5:B:SER:N   | 1:5:B:SER:CA  | 1:5:B:SER:C  | 2        | 10.74         |
| (1,16)  | 1:4:B:ILE:C  | 1:5:B:SER:N   | 1:5:B:SER:CA  | 1:5:B:SER:C  | 7        | 10.7          |
| (1,37)  | 1:10:A:MET:N | 1:10:A:MET:CA | 1:10:A:MET:C  | 1:11:A:PRO:N | 8        | 10.65         |
| (1,200) | 1:51:B:ASN:N | 1:51:B:ASN:CA | 1:51:B:ASN:C  | 1:52:B:PRO:N | 7        | 10.63         |
| (1,38)  | 1:10:B:MET:N | 1:10:B:MET:CA | 1:10:B:MET:C  | 1:11:B:PRO:N | 8        | 10.63         |
| (1,37)  | 1:10:A:MET:N | 1:10:A:MET:CA | 1:10:A:MET:C  | 1:11:A:PRO:N | 10       | 10.25         |
| (1,38)  | 1:10:B:MET:N | 1:10:B:MET:CA | 1:10:B:MET:C  | 1:11:B:PRO:N | 10       | 10.07         |
| (1,13)  | 1:4:A:ILE:N  | 1:4:A:ILE:CA  | 1:4:A:ILE:C   | 1:5:A:SER:N  | 2        | 10.05         |
| (1,195) | 1:50:A:LYS:N | 1:50:A:LYS:CA | 1:50:A:LYS:C  | 1:51:A:ASN:N | 10       | 10.0          |
| (1,201) | 1:51:A:ASN:C | 1:52:A:PRO:N  | 1:52:A:PRO:CA | 1:52:A:PRO:C | 1        | 9.98          |
| (1,200) | 1:51:B:ASN:N | 1:51:B:ASN:CA | 1:51:B:ASN:C  | 1:52:B:PRO:N | 1        | 9.98          |
| (1,199) | 1:51:A:ASN:N | 1:51:A:ASN:CA | 1:51:A:ASN:C  | 1:52:A:PRO:N | 1        | 9.98          |
| (1,202) | 1:51:B:ASN:C | 1:52:B:PRO:N  | 1:52:B:PRO:CA | 1:52:B:PRO:C | 1        | 9.96          |
| (1,14)  | 1:4:B:ILE:N  | 1:4:B:ILE:CA  | 1:4:B:ILE:C   | 1:5:B:SER:N  | 2        | 9.95          |
| (1,196) | 1:50:B:LYS:N | 1:50:B:LYS:CA | 1:50:B:LYS:C  | 1:51:B:ASN:N | 10       | 9.85          |
| (1,16)  | 1:4:B:ILE:C  | 1:5:B:SER:N   | 1:5:B:SER:CA  | 1:5:B:SER:C  | 6        | 9.76          |
| (1,92)  | 1:24:B:ALA:N | 1:24:B:ALA:CA | 1:24:B:ALA:C  | 1:25:B:LEU:N | 1        | 9.73          |
| (1,15)  | 1:4:A:ILE:C  | 1:5:A:SER:N   | 1:5:A:SER:CA  | 1:5:A:SER:C  | 6        | 9.68          |
| (1,201) | 1:51:A:ASN:C | 1:52:A:PRO:N  | 1:52:A:PRO:CA | 1:52:A:PRO:C | 10       | 9.62          |
| (1,91)  | 1:24:A:ALA:N | 1:24:A:ALA:CA | 1:24:A:ALA:C  | 1:25:A:LEU:N | 1        | 9.61          |
| (1,37)  | 1:10:A:MET:N | 1:10:A:MET:CA | 1:10:A:MET:C  | 1:11:A:PRO:N | 4        | 9.58          |
| (1,202) | 1:51:B:ASN:C | 1:52:B:PRO:N  | 1:52:B:PRO:CA | 1:52:B:PRO:C | 10       | 9.56          |
| (1,195) | 1:50:A:LYS:N | 1:50:A:LYS:CA | 1:50:A:LYS:C  | 1:51:A:ASN:N | 1        | 9.49          |
| (1,92)  | 1:24:B:ALA:N | 1:24:B:ALA:CA | 1:24:B:ALA:C  | 1:25:B:LEU:N | 8        | 9.46          |
| (1,38)  | 1:10:B:MET:N | 1:10:B:MET:CA | 1:10:B:MET:C  | 1:11:B:PRO:N | 4        | 9.44          |
| (1,14)  | 1:4:B:ILE:N  | 1:4:B:ILE:CA  | 1:4:B:ILE:C   | 1:5:B:SER:N  | 3        | 9.43          |
| (1,13)  | 1:4:A:ILE:N  | 1:4:A:ILE:CA  | 1:4:A:ILE:C   | 1:5:A:SER:N  | 3        | 9.43          |
| (1,91)  | 1:24:A:ALA:N | 1:24:A:ALA:CA | 1:24:A:ALA:C  | 1:25:A:LEU:N | 8        | 9.41          |
| (1,196) | 1:50:B:LYS:N | 1:50:B:LYS:CA | 1:50:B:LYS:C  | 1:51:B:ASN:N | 1        | 9.38          |
| (1,196) | 1:50:B:LYS:N | 1:50:B:LYS:CA | 1:50:B:LYS:C  | 1:51:B:ASN:N | 7        | 9.25          |
| (1,195) | 1:50:A:LYS:N | 1:50:A:LYS:CA | 1:50:A:LYS:C  | 1:51:A:ASN:N | 7        | 9.07          |
| (1,198) | 1:50:B:LYS:C | 1:51:B:ASN:N  | 1:51:B:ASN:CA | 1:51:B:ASN:C | 2        | 9.05          |
| (1,197) | 1:50:A:LYS:C | 1:51:A:ASN:N  | 1:51:A:ASN:CA | 1:51:A:ASN:C | 2        | 9.0           |
| (1,202) | 1:51:B:ASN:C | 1:52:B:PRO:N  | 1:52:B:PRO:CA | 1:52:B:PRO:C | 8        | 8.8           |
| (1,86)  | 1:22:B:GLU:C | 1:23:B:HIS:N  | 1:23:B:HIS:CA | 1:23:B:HIS:C | 5        | 8.73          |
| (1,38)  | 1:10:B:MET:N | 1:10:B:MET:CA | 1:10:B:MET:C  | 1:11:B:PRO:N | 3        | 8.73          |
| (1,85)  | 1:22:A:GLU:C | 1:23:A:HIS:N  | 1:23:A:HIS:CA | 1:23:A:HIS:C | 5        | 8.71          |

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Continued from previous page...

| Key     | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Model ID | Violation (°) |
|---------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,8)   | 1:2:B:GLY:C  | 1:3:B:LEU:N   | 1:3:B:LEU:CA  | 1:3:B:LEU:C  | 7        | 8.7           |
| (1,201) | 1:51:A:ASN:C | 1:52:A:PRO:N  | 1:52:A:PRO:CA | 1:52:A:PRO:C | 8        | 8.64          |
| (1,37)  | 1:10:A:MET:N | 1:10:A:MET:CA | 1:10:A:MET:C  | 1:11:A:PRO:N | 3        | 8.63          |
| (1,84)  | 1:22:B:GLU:N | 1:22:B:GLU:CA | 1:22:B:GLU:C  | 1:23:B:HIS:N | 4        | 8.62          |
| (1,7)   | 1:2:A:GLY:C  | 1:3:A:LEU:N   | 1:3:A:LEU:CA  | 1:3:A:LEU:C  | 7        | 8.62          |
| (1,14)  | 1:4:B:ILE:N  | 1:4:B:ILE:CA  | 1:4:B:ILE:C   | 1:5:B:SER:N  | 7        | 8.61          |
| (1,94)  | 1:24:B:ALA:C | 1:25:B:LEU:N  | 1:25:B:LEU:CA | 1:25:B:LEU:C | 8        | 8.6           |
| (1,13)  | 1:4:A:ILE:N  | 1:4:A:ILE:CA  | 1:4:A:ILE:C   | 1:5:A:SER:N  | 7        | 8.59          |
| (1,200) | 1:51:B:ASN:N | 1:51:B:ASN:CA | 1:51:B:ASN:C  | 1:52:B:PRO:N | 9        | 8.58          |
| (1,199) | 1:51:A:ASN:N | 1:51:A:ASN:CA | 1:51:A:ASN:C  | 1:52:A:PRO:N | 8        | 8.56          |
| (1,200) | 1:51:B:ASN:N | 1:51:B:ASN:CA | 1:51:B:ASN:C  | 1:52:B:PRO:N | 8        | 8.55          |
| (1,93)  | 1:24:A:ALA:C | 1:25:A:LEU:N  | 1:25:A:LEU:CA | 1:25:A:LEU:C | 8        | 8.54          |
| (1,83)  | 1:22:A:GLU:N | 1:22:A:GLU:CA | 1:22:A:GLU:C  | 1:23:A:HIS:N | 4        | 8.54          |
| (1,199) | 1:51:A:ASN:N | 1:51:A:ASN:CA | 1:51:A:ASN:C  | 1:52:A:PRO:N | 9        | 8.48          |
| (1,198) | 1:50:B:LYS:C | 1:51:B:ASN:N  | 1:51:B:ASN:CA | 1:51:B:ASN:C | 1        | 8.37          |
| (1,197) | 1:50:A:LYS:C | 1:51:A:ASN:N  | 1:51:A:ASN:CA | 1:51:A:ASN:C | 1        | 8.36          |
| (1,11)  | 1:3:A:LEU:C  | 1:4:A:ILE:N   | 1:4:A:ILE:CA  | 1:4:A:ILE:C  | 7        | 8.36          |
| (1,12)  | 1:3:B:LEU:C  | 1:4:B:ILE:N   | 1:4:B:ILE:CA  | 1:4:B:ILE:C  | 7        | 8.33          |
| (1,198) | 1:50:B:LYS:C | 1:51:B:ASN:N  | 1:51:B:ASN:CA | 1:51:B:ASN:C | 10       | 8.26          |
| (1,197) | 1:50:A:LYS:C | 1:51:A:ASN:N  | 1:51:A:ASN:CA | 1:51:A:ASN:C | 7        | 8.25          |
| (1,38)  | 1:10:B:MET:N | 1:10:B:MET:CA | 1:10:B:MET:C  | 1:11:B:PRO:N | 2        | 8.21          |
| (1,198) | 1:50:B:LYS:C | 1:51:B:ASN:N  | 1:51:B:ASN:CA | 1:51:B:ASN:C | 7        | 8.2           |
| (1,92)  | 1:24:B:ALA:N | 1:24:B:ALA:CA | 1:24:B:ALA:C  | 1:25:B:LEU:N | 9        | 8.2           |
| (1,91)  | 1:24:A:ALA:N | 1:24:A:ALA:CA | 1:24:A:ALA:C  | 1:25:A:LEU:N | 9        | 8.19          |
| (1,197) | 1:50:A:LYS:C | 1:51:A:ASN:N  | 1:51:A:ASN:CA | 1:51:A:ASN:C | 10       | 8.17          |
| (1,18)  | 1:5:B:SER:N  | 1:5:B:SER:CA  | 1:5:B:SER:C   | 1:6:B:PRO:N  | 4        | 8.12          |
| (1,17)  | 1:5:A:SER:N  | 1:5:A:SER:CA  | 1:5:A:SER:C   | 1:6:A:PRO:N  | 4        | 8.12          |
| (1,13)  | 1:4:A:ILE:N  | 1:4:A:ILE:CA  | 1:4:A:ILE:C   | 1:5:A:SER:N  | 8        | 8.05          |
| (1,7)   | 1:2:A:GLY:C  | 1:3:A:LEU:N   | 1:3:A:LEU:CA  | 1:3:A:LEU:C  | 4        | 8.03          |
| (1,8)   | 1:2:B:GLY:C  | 1:3:B:LEU:N   | 1:3:B:LEU:CA  | 1:3:B:LEU:C  | 1        | 8.02          |
| (1,7)   | 1:2:A:GLY:C  | 1:3:A:LEU:N   | 1:3:A:LEU:CA  | 1:3:A:LEU:C  | 1        | 8.01          |
| (1,83)  | 1:22:A:GLU:N | 1:22:A:GLU:CA | 1:22:A:GLU:C  | 1:23:A:HIS:N | 1        | 7.99          |
| (1,37)  | 1:10:A:MET:N | 1:10:A:MET:CA | 1:10:A:MET:C  | 1:11:A:PRO:N | 2        | 7.97          |
| (1,14)  | 1:4:B:ILE:N  | 1:4:B:ILE:CA  | 1:4:B:ILE:C   | 1:5:B:SER:N  | 8        | 7.95          |
| (1,84)  | 1:22:B:GLU:N | 1:22:B:GLU:CA | 1:22:B:GLU:C  | 1:23:B:HIS:N | 1        | 7.93          |
| (1,8)   | 1:2:B:GLY:C  | 1:3:B:LEU:N   | 1:3:B:LEU:CA  | 1:3:B:LEU:C  | 4        | 7.93          |
| (1,92)  | 1:24:B:ALA:N | 1:24:B:ALA:CA | 1:24:B:ALA:C  | 1:25:B:LEU:N | 6        | 7.92          |
| (1,16)  | 1:4:B:ILE:C  | 1:5:B:SER:N   | 1:5:B:SER:CA  | 1:5:B:SER:C  | 10       | 7.92          |
| (1,199) | 1:51:A:ASN:N | 1:51:A:ASN:CA | 1:51:A:ASN:C  | 1:52:A:PRO:N | 4        | 7.91          |
| (1,200) | 1:51:B:ASN:N | 1:51:B:ASN:CA | 1:51:B:ASN:C  | 1:52:B:PRO:N | 4        | 7.89          |
| (1,15)  | 1:4:A:ILE:C  | 1:5:A:SER:N   | 1:5:A:SER:CA  | 1:5:A:SER:C  | 10       | 7.88          |
| (1,211) | 1:54:A:ILE:N | 1:54:A:ILE:CA | 1:54:A:ILE:C  | 1:55:A:TRP:N | 7        | 7.83          |
| (1,212) | 1:54:B:ILE:N | 1:54:B:ILE:CA | 1:54:B:ILE:C  | 1:55:B:TRP:N | 7        | 7.79          |
| (1,91)  | 1:24:A:ALA:N | 1:24:A:ALA:CA | 1:24:A:ALA:C  | 1:25:A:LEU:N | 6        | 7.76          |
| (1,92)  | 1:24:B:ALA:N | 1:24:B:ALA:CA | 1:24:B:ALA:C  | 1:25:B:LEU:N | 7        | 7.68          |
| (1,83)  | 1:22:A:GLU:N | 1:22:A:GLU:CA | 1:22:A:GLU:C  | 1:23:A:HIS:N | 7        | 7.65          |
| (1,91)  | 1:24:A:ALA:N | 1:24:A:ALA:CA | 1:24:A:ALA:C  | 1:25:A:LEU:N | 7        | 7.64          |
| (1,200) | 1:51:B:ASN:N | 1:51:B:ASN:CA | 1:51:B:ASN:C  | 1:52:B:PRO:N | 3        | 7.63          |
| (1,199) | 1:51:A:ASN:N | 1:51:A:ASN:CA | 1:51:A:ASN:C  | 1:52:A:PRO:N | 3        | 7.63          |
| (1,183) | 1:47:A:ILE:N | 1:47:A:ILE:CA | 1:47:A:ILE:C  | 1:48:A:TYR:N | 2        | 7.63          |
| (1,184) | 1:47:B:ILE:N | 1:47:B:ILE:CA | 1:47:B:ILE:C  | 1:48:B:TYR:N | 2        | 7.59          |

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Continued from previous page...

| Key     | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Model ID | Violation (°) |
|---------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,93)  | 1:24:A:ALA:C | 1:25:A:LEU:N  | 1:25:A:LEU:CA | 1:25:A:LEU:C | 7        | 7.58          |
| (1,84)  | 1:22:B:GLU:N | 1:22:B:GLU:CA | 1:22:B:GLU:C  | 1:23:B:HIS:N | 7        | 7.56          |
| (1,13)  | 1:4:A:ILE:N  | 1:4:A:ILE:CA  | 1:4:A:ILE:C   | 1:5:A:SER:N  | 6        | 7.52          |
| (1,214) | 1:54:B:ILE:C | 1:55:B:TRP:N  | 1:55:B:TRP:CA | 1:55:B:TRP:C | 7        | 7.48          |
| (1,199) | 1:51:A:ASN:N | 1:51:A:ASN:CA | 1:51:A:ASN:C  | 1:52:A:PRO:N | 6        | 7.46          |
| (1,94)  | 1:24:B:ALA:C | 1:25:B:LEU:N  | 1:25:B:LEU:CA | 1:25:B:LEU:C | 7        | 7.45          |
| (1,96)  | 1:25:B:LEU:N | 1:25:B:LEU:CA | 1:25:B:LEU:C  | 1:26:B:GLY:N | 4        | 7.44          |
| (1,95)  | 1:25:A:LEU:N | 1:25:A:LEU:CA | 1:25:A:LEU:C  | 1:26:A:GLY:N | 4        | 7.43          |
| (1,200) | 1:51:B:ASN:N | 1:51:B:ASN:CA | 1:51:B:ASN:C  | 1:52:B:PRO:N | 6        | 7.4           |
| (1,206) | 1:52:B:PRO:C | 1:53:B:THR:N  | 1:53:B:THR:CA | 1:53:B:THR:C | 2        | 7.39          |
| (1,16)  | 1:4:B:ILE:C  | 1:5:B:SER:N   | 1:5:B:SER:CA  | 1:5:B:SER:C  | 5        | 7.39          |
| (1,14)  | 1:4:B:ILE:N  | 1:4:B:ILE:CA  | 1:4:B:ILE:C   | 1:5:B:SER:N  | 6        | 7.39          |
| (1,18)  | 1:5:B:SER:N  | 1:5:B:SER:CA  | 1:5:B:SER:C   | 1:6:B:PRO:N  | 8        | 7.37          |
| (1,213) | 1:54:A:ILE:C | 1:55:A:TRP:N  | 1:55:A:TRP:CA | 1:55:A:TRP:C | 7        | 7.35          |
| (1,14)  | 1:4:B:ILE:N  | 1:4:B:ILE:CA  | 1:4:B:ILE:C   | 1:5:B:SER:N  | 10       | 7.35          |
| (1,205) | 1:52:A:PRO:C | 1:53:A:THR:N  | 1:53:A:THR:CA | 1:53:A:THR:C | 2        | 7.33          |
| (1,13)  | 1:4:A:ILE:N  | 1:4:A:ILE:CA  | 1:4:A:ILE:C   | 1:5:A:SER:N  | 10       | 7.33          |
| (1,83)  | 1:22:A:GLU:N | 1:22:A:GLU:CA | 1:22:A:GLU:C  | 1:23:A:HIS:N | 3        | 7.27          |
| (1,29)  | 1:8:A:ALA:N  | 1:8:A:ALA:CA  | 1:8:A:ALA:C   | 1:9:A:THR:N  | 9        | 7.27          |
| (1,30)  | 1:8:B:ALA:N  | 1:8:B:ALA:CA  | 1:8:B:ALA:C   | 1:9:B:THR:N  | 9        | 7.26          |
| (1,84)  | 1:22:B:GLU:N | 1:22:B:GLU:CA | 1:22:B:GLU:C  | 1:23:B:HIS:N | 3        | 7.25          |
| (1,15)  | 1:4:A:ILE:C  | 1:5:A:SER:N   | 1:5:A:SER:CA  | 1:5:A:SER:C  | 5        | 7.24          |
| (1,17)  | 1:5:A:SER:N  | 1:5:A:SER:CA  | 1:5:A:SER:C   | 1:6:A:PRO:N  | 8        | 7.23          |
| (1,13)  | 1:4:A:ILE:N  | 1:4:A:ILE:CA  | 1:4:A:ILE:C   | 1:5:A:SER:N  | 4        | 7.18          |
| (1,96)  | 1:25:B:LEU:N | 1:25:B:LEU:CA | 1:25:B:LEU:C  | 1:26:B:GLY:N | 7        | 7.16          |
| (1,96)  | 1:25:B:LEU:N | 1:25:B:LEU:CA | 1:25:B:LEU:C  | 1:26:B:GLY:N | 8        | 7.12          |
| (1,93)  | 1:24:A:ALA:C | 1:25:A:LEU:N  | 1:25:A:LEU:CA | 1:25:A:LEU:C | 1        | 7.11          |
| (1,95)  | 1:25:A:LEU:N | 1:25:A:LEU:CA | 1:25:A:LEU:C  | 1:26:A:GLY:N | 8        | 7.1           |
| (1,94)  | 1:24:B:ALA:C | 1:25:B:LEU:N  | 1:25:B:LEU:CA | 1:25:B:LEU:C | 1        | 7.08          |
| (1,95)  | 1:25:A:LEU:N | 1:25:A:LEU:CA | 1:25:A:LEU:C  | 1:26:A:GLY:N | 7        | 7.07          |
| (1,93)  | 1:24:A:ALA:C | 1:25:A:LEU:N  | 1:25:A:LEU:CA | 1:25:A:LEU:C | 6        | 7.06          |
| (1,83)  | 1:22:A:GLU:N | 1:22:A:GLU:CA | 1:22:A:GLU:C  | 1:23:A:HIS:N | 2        | 6.98          |
| (1,94)  | 1:24:B:ALA:C | 1:25:B:LEU:N  | 1:25:B:LEU:CA | 1:25:B:LEU:C | 3        | 6.96          |
| (1,14)  | 1:4:B:ILE:N  | 1:4:B:ILE:CA  | 1:4:B:ILE:C   | 1:5:B:SER:N  | 4        | 6.95          |
| (1,92)  | 1:24:B:ALA:N | 1:24:B:ALA:CA | 1:24:B:ALA:C  | 1:25:B:LEU:N | 3        | 6.93          |
| (1,91)  | 1:24:A:ALA:N | 1:24:A:ALA:CA | 1:24:A:ALA:C  | 1:25:A:LEU:N | 3        | 6.93          |
| (1,84)  | 1:22:B:GLU:N | 1:22:B:GLU:CA | 1:22:B:GLU:C  | 1:23:B:HIS:N | 2        | 6.93          |
| (1,94)  | 1:24:B:ALA:C | 1:25:B:LEU:N  | 1:25:B:LEU:CA | 1:25:B:LEU:C | 6        | 6.9           |
| (1,93)  | 1:24:A:ALA:C | 1:25:A:LEU:N  | 1:25:A:LEU:CA | 1:25:A:LEU:C | 3        | 6.9           |
| (1,13)  | 1:4:A:ILE:N  | 1:4:A:ILE:CA  | 1:4:A:ILE:C   | 1:5:A:SER:N  | 5        | 6.9           |
| (1,14)  | 1:4:B:ILE:N  | 1:4:B:ILE:CA  | 1:4:B:ILE:C   | 1:5:B:SER:N  | 9        | 6.85          |
| (1,202) | 1:51:B:ASN:C | 1:52:B:PRO:N  | 1:52:B:PRO:CA | 1:52:B:PRO:C | 5        | 6.81          |
| (1,14)  | 1:4:B:ILE:N  | 1:4:B:ILE:CA  | 1:4:B:ILE:C   | 1:5:B:SER:N  | 5        | 6.81          |
| (1,13)  | 1:4:A:ILE:N  | 1:4:A:ILE:CA  | 1:4:A:ILE:C   | 1:5:A:SER:N  | 9        | 6.8           |
| (1,201) | 1:51:A:ASN:C | 1:52:A:PRO:N  | 1:52:A:PRO:CA | 1:52:A:PRO:C | 5        | 6.79          |
| (1,181) | 1:46:A:GLY:C | 1:47:A:ILE:N  | 1:47:A:ILE:CA | 1:47:A:ILE:C | 2        | 6.76          |
| (1,7)   | 1:2:A:GLY:C  | 1:3:A:LEU:N   | 1:3:A:LEU:CA  | 1:3:A:LEU:C  | 5        | 6.76          |
| (1,199) | 1:51:A:ASN:N | 1:51:A:ASN:CA | 1:51:A:ASN:C  | 1:52:A:PRO:N | 5        | 6.73          |
| (1,17)  | 1:5:A:SER:N  | 1:5:A:SER:CA  | 1:5:A:SER:C   | 1:6:A:PRO:N  | 3        | 6.73          |
| (1,182) | 1:46:B:GLY:C | 1:47:B:ILE:N  | 1:47:B:ILE:CA | 1:47:B:ILE:C | 2        | 6.71          |
| (1,85)  | 1:22:A:GLU:C | 1:23:A:HIS:N  | 1:23:A:HIS:CA | 1:23:A:HIS:C | 1        | 6.7           |

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| Key     | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Model ID | Violation (°) |
|---------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,8)   | 1:2:B:GLY:C  | 1:3:B:LEU:N   | 1:3:B:LEU:CA  | 1:3:B:LEU:C  | 5        | 6.7           |
| (1,211) | 1:54:A:ILE:N | 1:54:A:ILE:CA | 1:54:A:ILE:C  | 1:55:A:TRP:N | 10       | 6.69          |
| (1,86)  | 1:22:B:GLU:C | 1:23:B:HIS:N  | 1:23:B:HIS:CA | 1:23:B:HIS:C | 1        | 6.69          |
| (1,200) | 1:51:B:ASN:N | 1:51:B:ASN:CA | 1:51:B:ASN:C  | 1:52:B:PRO:N | 5        | 6.68          |
| (1,18)  | 1:5:B:SER:N  | 1:5:B:SER:CA  | 1:5:B:SER:C   | 1:6:B:PRO:N  | 3        | 6.67          |
| (1,7)   | 1:2:A:GLY:C  | 1:3:A:LEU:N   | 1:3:A:LEU:CA  | 1:3:A:LEU:C  | 9        | 6.62          |
| (1,8)   | 1:2:B:GLY:C  | 1:3:B:LEU:N   | 1:3:B:LEU:CA  | 1:3:B:LEU:C  | 9        | 6.6           |
| (1,305) | 1:77:A:GLY:C | 1:78:A:GLY:N  | 1:78:A:GLY:CA | 1:78:A:GLY:C | 2        | 6.57          |
| (1,306) | 1:77:B:GLY:C | 1:78:B:GLY:N  | 1:78:B:GLY:CA | 1:78:B:GLY:C | 2        | 6.53          |
| (1,212) | 1:54:B:ILE:N | 1:54:B:ILE:CA | 1:54:B:ILE:C  | 1:55:B:TRP:N | 10       | 6.53          |
| (1,18)  | 1:5:B:SER:N  | 1:5:B:SER:CA  | 1:5:B:SER:C   | 1:6:B:PRO:N  | 5        | 6.47          |
| (1,306) | 1:77:B:GLY:C | 1:78:B:GLY:N  | 1:78:B:GLY:CA | 1:78:B:GLY:C | 10       | 6.46          |
| (1,305) | 1:77:A:GLY:C | 1:78:A:GLY:N  | 1:78:A:GLY:CA | 1:78:A:GLY:C | 10       | 6.43          |
| (1,186) | 1:47:B:ILE:C | 1:48:B:TYR:N  | 1:48:B:TYR:CA | 1:48:B:TYR:C | 2        | 6.42          |
| (1,185) | 1:47:A:ILE:C | 1:48:A:TYR:N  | 1:48:A:TYR:CA | 1:48:A:TYR:C | 2        | 6.33          |
| (1,17)  | 1:5:A:SER:N  | 1:5:A:SER:CA  | 1:5:A:SER:C   | 1:6:A:PRO:N  | 5        | 6.32          |
| (1,211) | 1:54:A:ILE:N | 1:54:A:ILE:CA | 1:54:A:ILE:C  | 1:55:A:TRP:N | 2        | 6.3           |
| (1,85)  | 1:22:A:GLU:C | 1:23:A:HIS:N  | 1:23:A:HIS:CA | 1:23:A:HIS:C | 4        | 6.29          |
| (1,13)  | 1:4:A:ILE:N  | 1:4:A:ILE:CA  | 1:4:A:ILE:C   | 1:5:A:SER:N  | 1        | 6.24          |
| (1,86)  | 1:22:B:GLU:C | 1:23:B:HIS:N  | 1:23:B:HIS:CA | 1:23:B:HIS:C | 4        | 6.23          |
| (1,14)  | 1:4:B:ILE:N  | 1:4:B:ILE:CA  | 1:4:B:ILE:C   | 1:5:B:SER:N  | 1        | 6.2           |
| (1,222) | 1:56:B:VAL:C | 1:57:B:GLY:N  | 1:57:B:GLY:CA | 1:57:B:GLY:C | 7        | 6.19          |
| (1,212) | 1:54:B:ILE:N | 1:54:B:ILE:CA | 1:54:B:ILE:C  | 1:55:B:TRP:N | 2        | 6.08          |
| (1,304) | 1:77:B:GLY:N | 1:77:B:GLY:CA | 1:77:B:GLY:C  | 1:78:B:GLY:N | 2        | 6.05          |
| (1,221) | 1:56:A:VAL:C | 1:57:A:GLY:N  | 1:57:A:GLY:CA | 1:57:A:GLY:C | 7        | 6.04          |
| (1,214) | 1:54:B:ILE:C | 1:55:B:TRP:N  | 1:55:B:TRP:CA | 1:55:B:TRP:C | 10       | 5.97          |
| (1,303) | 1:77:A:GLY:N | 1:77:A:GLY:CA | 1:77:A:GLY:C  | 1:78:A:GLY:N | 2        | 5.92          |
| (1,17)  | 1:5:A:SER:N  | 1:5:A:SER:CA  | 1:5:A:SER:C   | 1:6:A:PRO:N  | 9        | 5.92          |
| (1,213) | 1:54:A:ILE:C | 1:55:A:TRP:N  | 1:55:A:TRP:CA | 1:55:A:TRP:C | 10       | 5.85          |
| (1,18)  | 1:5:B:SER:N  | 1:5:B:SER:CA  | 1:5:B:SER:C   | 1:6:B:PRO:N  | 9        | 5.85          |
| (1,91)  | 1:24:A:ALA:N | 1:24:A:ALA:CA | 1:24:A:ALA:C  | 1:25:A:LEU:N | 2        | 5.84          |
| (1,180) | 1:46:B:GLY:N | 1:46:B:GLY:CA | 1:46:B:GLY:C  | 1:47:B:ILE:N | 2        | 5.81          |
| (1,92)  | 1:24:B:ALA:N | 1:24:B:ALA:CA | 1:24:B:ALA:C  | 1:25:B:LEU:N | 2        | 5.79          |
| (1,94)  | 1:24:B:ALA:C | 1:25:B:LEU:N  | 1:25:B:LEU:CA | 1:25:B:LEU:C | 9        | 5.77          |
| (1,179) | 1:46:A:GLY:N | 1:46:A:GLY:CA | 1:46:A:GLY:C  | 1:47:A:ILE:N | 2        | 5.72          |
| (1,10)  | 1:3:B:LEU:N  | 1:3:B:LEU:CA  | 1:3:B:LEU:C   | 1:4:B:ILE:N  | 10       | 5.71          |
| (1,201) | 1:51:A:ASN:C | 1:52:A:PRO:N  | 1:52:A:PRO:CA | 1:52:A:PRO:C | 2        | 5.69          |
| (1,93)  | 1:24:A:ALA:C | 1:25:A:LEU:N  | 1:25:A:LEU:CA | 1:25:A:LEU:C | 9        | 5.68          |
| (1,84)  | 1:22:B:GLU:N | 1:22:B:GLU:CA | 1:22:B:GLU:C  | 1:23:B:HIS:N | 8        | 5.65          |
| (1,217) | 1:55:A:TRP:C | 1:56:A:VAL:N  | 1:56:A:VAL:CA | 1:56:A:VAL:C | 5        | 5.64          |
| (1,212) | 1:54:B:ILE:N | 1:54:B:ILE:CA | 1:54:B:ILE:C  | 1:55:B:TRP:N | 1        | 5.61          |
| (1,211) | 1:54:A:ILE:N | 1:54:A:ILE:CA | 1:54:A:ILE:C  | 1:55:A:TRP:N | 1        | 5.6           |
| (1,306) | 1:77:B:GLY:C | 1:78:B:GLY:N  | 1:78:B:GLY:CA | 1:78:B:GLY:C | 8        | 5.59          |
| (1,218) | 1:55:B:TRP:C | 1:56:B:VAL:N  | 1:56:B:VAL:CA | 1:56:B:VAL:C | 5        | 5.58          |
| (1,9)   | 1:3:A:LEU:N  | 1:3:A:LEU:CA  | 1:3:A:LEU:C   | 1:4:A:ILE:N  | 10       | 5.58          |
| (1,95)  | 1:25:A:LEU:N | 1:25:A:LEU:CA | 1:25:A:LEU:C  | 1:26:A:GLY:N | 3        | 5.56          |
| (1,95)  | 1:25:A:LEU:N | 1:25:A:LEU:CA | 1:25:A:LEU:C  | 1:26:A:GLY:N | 1        | 5.54          |
| (1,214) | 1:54:B:ILE:C | 1:55:B:TRP:N  | 1:55:B:TRP:CA | 1:55:B:TRP:C | 2        | 5.51          |
| (1,96)  | 1:25:B:LEU:N | 1:25:B:LEU:CA | 1:25:B:LEU:C  | 1:26:B:GLY:N | 1        | 5.5           |
| (1,83)  | 1:22:A:GLU:N | 1:22:A:GLU:CA | 1:22:A:GLU:C  | 1:23:A:HIS:N | 8        | 5.48          |
| (1,96)  | 1:25:B:LEU:N | 1:25:B:LEU:CA | 1:25:B:LEU:C  | 1:26:B:GLY:N | 3        | 5.44          |

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| Key     | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Model ID | Violation (°) |
|---------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,305) | 1:77:A:GLY:C | 1:78:A:GLY:N  | 1:78:A:GLY:CA | 1:78:A:GLY:C | 8        | 5.39          |
| (1,85)  | 1:22:A:GLU:C | 1:23:A:HIS:N  | 1:23:A:HIS:CA | 1:23:A:HIS:C | 7        | 5.37          |
| (1,36)  | 1:9:B:THR:C  | 1:10:B:MET:N  | 1:10:B:MET:CA | 1:10:B:MET:C | 1        | 5.36          |
| (1,86)  | 1:22:B:GLU:C | 1:23:B:HIS:N  | 1:23:B:HIS:CA | 1:23:B:HIS:C | 7        | 5.33          |
| (1,304) | 1:77:B:GLY:N | 1:77:B:GLY:CA | 1:77:B:GLY:C  | 1:78:B:GLY:N | 10       | 5.3           |
| (1,35)  | 1:9:A:THR:C  | 1:10:A:MET:N  | 1:10:A:MET:CA | 1:10:A:MET:C | 1        | 5.29          |
| (1,213) | 1:54:A:ILE:C | 1:55:A:TRP:N  | 1:55:A:TRP:CA | 1:55:A:TRP:C | 2        | 5.27          |
| (1,212) | 1:54:B:ILE:N | 1:54:B:ILE:CA | 1:54:B:ILE:C  | 1:55:B:TRP:N | 3        | 5.23          |
| (1,303) | 1:77:A:GLY:N | 1:77:A:GLY:CA | 1:77:A:GLY:C  | 1:78:A:GLY:N | 10       | 5.21          |
| (1,305) | 1:77:A:GLY:C | 1:78:A:GLY:N  | 1:78:A:GLY:CA | 1:78:A:GLY:C | 3        | 5.19          |
| (1,213) | 1:54:A:ILE:C | 1:55:A:TRP:N  | 1:55:A:TRP:CA | 1:55:A:TRP:C | 1        | 5.18          |
| (1,83)  | 1:22:A:GLU:N | 1:22:A:GLU:CA | 1:22:A:GLU:C  | 1:23:A:HIS:N | 9        | 5.16          |
| (1,211) | 1:54:A:ILE:N | 1:54:A:ILE:CA | 1:54:A:ILE:C  | 1:55:A:TRP:N | 3        | 5.15          |
| (1,306) | 1:77:B:GLY:C | 1:78:B:GLY:N  | 1:78:B:GLY:CA | 1:78:B:GLY:C | 3        | 5.14          |
| (1,84)  | 1:22:B:GLU:N | 1:22:B:GLU:CA | 1:22:B:GLU:C  | 1:23:B:HIS:N | 9        | 5.11          |
| (1,95)  | 1:25:A:LEU:N | 1:25:A:LEU:CA | 1:25:A:LEU:C  | 1:26:A:GLY:N | 5        | 5.1           |
| (1,96)  | 1:25:B:LEU:N | 1:25:B:LEU:CA | 1:25:B:LEU:C  | 1:26:B:GLY:N | 5        | 5.06          |
| (1,214) | 1:54:B:ILE:C | 1:55:B:TRP:N  | 1:55:B:TRP:CA | 1:55:B:TRP:C | 1        | 5.03          |
| (1,202) | 1:51:B:ASN:C | 1:52:B:PRO:N  | 1:52:B:PRO:CA | 1:52:B:PRO:C | 2        | 5.02          |
| (1,215) | 1:55:A:TRP:N | 1:55:A:TRP:CA | 1:55:A:TRP:C  | 1:56:A:VAL:N | 4        | 4.91          |
| (1,85)  | 1:22:A:GLU:C | 1:23:A:HIS:N  | 1:23:A:HIS:CA | 1:23:A:HIS:C | 3        | 4.91          |
| (1,80)  | 1:21:B:SER:N | 1:21:B:SER:CA | 1:21:B:SER:C  | 1:22:B:GLU:N | 5        | 4.9           |
| (1,216) | 1:55:B:TRP:N | 1:55:B:TRP:CA | 1:55:B:TRP:C  | 1:56:B:VAL:N | 4        | 4.88          |
| (1,183) | 1:47:A:ILE:N | 1:47:A:ILE:CA | 1:47:A:ILE:C  | 1:48:A:TYR:N | 10       | 4.88          |
| (1,86)  | 1:22:B:GLU:C | 1:23:B:HIS:N  | 1:23:B:HIS:CA | 1:23:B:HIS:C | 2        | 4.88          |
| (1,85)  | 1:22:A:GLU:C | 1:23:A:HIS:N  | 1:23:A:HIS:CA | 1:23:A:HIS:C | 2        | 4.88          |
| (1,222) | 1:56:B:VAL:C | 1:57:B:GLY:N  | 1:57:B:GLY:CA | 1:57:B:GLY:C | 10       | 4.87          |
| (1,184) | 1:47:B:ILE:N | 1:47:B:ILE:CA | 1:47:B:ILE:C  | 1:48:B:TYR:N | 10       | 4.84          |
| (1,220) | 1:56:B:VAL:N | 1:56:B:VAL:CA | 1:56:B:VAL:C  | 1:57:B:GLY:N | 5        | 4.83          |
| (1,212) | 1:54:B:ILE:N | 1:54:B:ILE:CA | 1:54:B:ILE:C  | 1:55:B:TRP:N | 8        | 4.82          |
| (1,266) | 1:67:B:ALA:C | 1:68:B:MET:N  | 1:68:B:MET:CA | 1:68:B:MET:C | 8        | 4.81          |
| (1,82)  | 1:21:B:SER:C | 1:22:B:GLU:N  | 1:22:B:GLU:CA | 1:22:B:GLU:C | 7        | 4.81          |
| (1,86)  | 1:22:B:GLU:C | 1:23:B:HIS:N  | 1:23:B:HIS:CA | 1:23:B:HIS:C | 3        | 4.8           |
| (1,221) | 1:56:A:VAL:C | 1:57:A:GLY:N  | 1:57:A:GLY:CA | 1:57:A:GLY:C | 10       | 4.79          |
| (1,81)  | 1:21:A:SER:C | 1:22:A:GLU:N  | 1:22:A:GLU:CA | 1:22:A:GLU:C | 5        | 4.77          |
| (1,81)  | 1:21:A:SER:C | 1:22:A:GLU:N  | 1:22:A:GLU:CA | 1:22:A:GLU:C | 7        | 4.74          |
| (1,219) | 1:56:A:VAL:N | 1:56:A:VAL:CA | 1:56:A:VAL:C  | 1:57:A:GLY:N | 5        | 4.72          |
| (1,81)  | 1:21:A:SER:C | 1:22:A:GLU:N  | 1:22:A:GLU:CA | 1:22:A:GLU:C | 4        | 4.71          |
| (1,211) | 1:54:A:ILE:N | 1:54:A:ILE:CA | 1:54:A:ILE:C  | 1:55:A:TRP:N | 8        | 4.67          |
| (1,80)  | 1:21:B:SER:N | 1:21:B:SER:CA | 1:21:B:SER:C  | 1:22:B:GLU:N | 3        | 4.67          |
| (1,79)  | 1:21:A:SER:N | 1:21:A:SER:CA | 1:21:A:SER:C  | 1:22:A:GLU:N | 3        | 4.67          |
| (1,83)  | 1:22:A:GLU:N | 1:22:A:GLU:CA | 1:22:A:GLU:C  | 1:23:A:HIS:N | 6        | 4.66          |
| (1,306) | 1:77:B:GLY:C | 1:78:B:GLY:N  | 1:78:B:GLY:CA | 1:78:B:GLY:C | 6        | 4.64          |
| (1,183) | 1:47:A:ILE:N | 1:47:A:ILE:CA | 1:47:A:ILE:C  | 1:48:A:TYR:N | 7        | 4.64          |
| (1,79)  | 1:21:A:SER:N | 1:21:A:SER:CA | 1:21:A:SER:C  | 1:22:A:GLU:N | 5        | 4.64          |
| (1,265) | 1:67:A:ALA:C | 1:68:A:MET:N  | 1:68:A:MET:CA | 1:68:A:MET:C | 8        | 4.63          |
| (1,84)  | 1:22:B:GLU:N | 1:22:B:GLU:CA | 1:22:B:GLU:C  | 1:23:B:HIS:N | 6        | 4.63          |
| (1,82)  | 1:21:B:SER:C | 1:22:B:GLU:N  | 1:22:B:GLU:CA | 1:22:B:GLU:C | 4        | 4.63          |
| (1,82)  | 1:21:B:SER:C | 1:22:B:GLU:N  | 1:22:B:GLU:CA | 1:22:B:GLU:C | 5        | 4.63          |
| (1,305) | 1:77:A:GLY:C | 1:78:A:GLY:N  | 1:78:A:GLY:CA | 1:78:A:GLY:C | 6        | 4.62          |
| (1,29)  | 1:8:A:ALA:N  | 1:8:A:ALA:CA  | 1:8:A:ALA:C   | 1:9:A:THR:N  | 5        | 4.61          |

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| Key     | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Model ID | Violation (°) |
|---------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,212) | 1:54:B:ILE:N | 1:54:B:ILE:CA | 1:54:B:ILE:C  | 1:55:B:TRP:N | 6        | 4.59          |
| (1,79)  | 1:21:A:SER:N | 1:21:A:SER:CA | 1:21:A:SER:C  | 1:22:A:GLU:N | 1        | 4.59          |
| (1,7)   | 1:2:A:GLY:C  | 1:3:A:LEU:N   | 1:3:A:LEU:CA  | 1:3:A:LEU:C  | 3        | 4.59          |
| (1,95)  | 1:25:A:LEU:N | 1:25:A:LEU:CA | 1:25:A:LEU:C  | 1:26:A:GLY:N | 10       | 4.58          |
| (1,80)  | 1:21:B:SER:N | 1:21:B:SER:CA | 1:21:B:SER:C  | 1:22:B:GLU:N | 1        | 4.58          |
| (1,96)  | 1:25:B:LEU:N | 1:25:B:LEU:CA | 1:25:B:LEU:C  | 1:26:B:GLY:N | 10       | 4.54          |
| (1,92)  | 1:24:B:ALA:N | 1:24:B:ALA:CA | 1:24:B:ALA:C  | 1:25:B:LEU:N | 5        | 4.53          |
| (1,30)  | 1:8:B:ALA:N  | 1:8:B:ALA:CA  | 1:8:B:ALA:C   | 1:9:B:THR:N  | 5        | 4.53          |
| (1,91)  | 1:24:A:ALA:N | 1:24:A:ALA:CA | 1:24:A:ALA:C  | 1:25:A:LEU:N | 5        | 4.52          |
| (1,9)   | 1:3:A:LEU:N  | 1:3:A:LEU:CA  | 1:3:A:LEU:C   | 1:4:A:ILE:N  | 6        | 4.5           |
| (1,35)  | 1:9:A:THR:C  | 1:10:A:MET:N  | 1:10:A:MET:CA | 1:10:A:MET:C | 5        | 4.48          |
| (1,8)   | 1:2:B:GLY:C  | 1:3:B:LEU:N   | 1:3:B:LEU:CA  | 1:3:B:LEU:C  | 3        | 4.48          |
| (1,94)  | 1:24:B:ALA:C | 1:25:B:LEU:N  | 1:25:B:LEU:CA | 1:25:B:LEU:C | 2        | 4.46          |
| (1,93)  | 1:24:A:ALA:C | 1:25:A:LEU:N  | 1:25:A:LEU:CA | 1:25:A:LEU:C | 2        | 4.46          |
| (1,214) | 1:54:B:ILE:C | 1:55:B:TRP:N  | 1:55:B:TRP:CA | 1:55:B:TRP:C | 9        | 4.42          |
| (1,10)  | 1:3:B:LEU:N  | 1:3:B:LEU:CA  | 1:3:B:LEU:C   | 1:4:B:ILE:N  | 6        | 4.42          |
| (1,213) | 1:54:A:ILE:C | 1:55:A:TRP:N  | 1:55:A:TRP:CA | 1:55:A:TRP:C | 9        | 4.41          |
| (1,184) | 1:47:B:ILE:N | 1:47:B:ILE:CA | 1:47:B:ILE:C  | 1:48:B:TYR:N | 7        | 4.41          |
| (1,211) | 1:54:A:ILE:N | 1:54:A:ILE:CA | 1:54:A:ILE:C  | 1:55:A:TRP:N | 6        | 4.38          |
| (1,107) | 1:28:A:SER:N | 1:28:A:SER:CA | 1:28:A:SER:C  | 1:29:A:LEU:N | 4        | 4.38          |
| (1,36)  | 1:9:B:THR:C  | 1:10:B:MET:N  | 1:10:B:MET:CA | 1:10:B:MET:C | 5        | 4.38          |
| (1,11)  | 1:3:A:LEU:C  | 1:4:A:ILE:N   | 1:4:A:ILE:CA  | 1:4:A:ILE:C  | 4        | 4.37          |
| (1,10)  | 1:3:B:LEU:N  | 1:3:B:LEU:CA  | 1:3:B:LEU:C   | 1:4:B:ILE:N  | 2        | 4.37          |
| (1,189) | 1:48:A:TYR:C | 1:49:A:HIS:N  | 1:49:A:HIS:CA | 1:49:A:HIS:C | 4        | 4.35          |
| (1,108) | 1:28:B:SER:N | 1:28:B:SER:CA | 1:28:B:SER:C  | 1:29:B:LEU:N | 4        | 4.35          |
| (1,11)  | 1:3:A:LEU:C  | 1:4:A:ILE:N   | 1:4:A:ILE:CA  | 1:4:A:ILE:C  | 1        | 4.34          |
| (1,222) | 1:56:B:VAL:C | 1:57:B:GLY:N  | 1:57:B:GLY:CA | 1:57:B:GLY:C | 1        | 4.33          |
| (1,81)  | 1:21:A:SER:C | 1:22:A:GLU:N  | 1:22:A:GLU:CA | 1:22:A:GLU:C | 3        | 4.33          |
| (1,82)  | 1:21:B:SER:C | 1:22:B:GLU:N  | 1:22:B:GLU:CA | 1:22:B:GLU:C | 3        | 4.32          |
| (1,12)  | 1:3:B:LEU:C  | 1:4:B:ILE:N   | 1:4:B:ILE:CA  | 1:4:B:ILE:C  | 1        | 4.32          |
| (1,12)  | 1:3:B:LEU:C  | 1:4:B:ILE:N   | 1:4:B:ILE:CA  | 1:4:B:ILE:C  | 4        | 4.32          |
| (1,190) | 1:48:B:TYR:C | 1:49:B:HIS:N  | 1:49:B:HIS:CA | 1:49:B:HIS:C | 4        | 4.29          |
| (1,94)  | 1:24:B:ALA:C | 1:25:B:LEU:N  | 1:25:B:LEU:CA | 1:25:B:LEU:C | 5        | 4.29          |
| (1,93)  | 1:24:A:ALA:C | 1:25:A:LEU:N  | 1:25:A:LEU:CA | 1:25:A:LEU:C | 5        | 4.29          |
| (1,82)  | 1:21:B:SER:C | 1:22:B:GLU:N  | 1:22:B:GLU:CA | 1:22:B:GLU:C | 2        | 4.26          |
| (1,306) | 1:77:B:GLY:C | 1:78:B:GLY:N  | 1:78:B:GLY:CA | 1:78:B:GLY:C | 1        | 4.25          |
| (1,44)  | 1:12:B:GLN:N | 1:12:B:GLN:CA | 1:12:B:GLN:C  | 1:13:B:LEU:N | 2        | 4.23          |
| (1,221) | 1:56:A:VAL:C | 1:57:A:GLY:N  | 1:57:A:GLY:CA | 1:57:A:GLY:C | 1        | 4.21          |
| (1,213) | 1:54:A:ILE:C | 1:55:A:TRP:N  | 1:55:A:TRP:CA | 1:55:A:TRP:C | 3        | 4.21          |
| (1,92)  | 1:24:B:ALA:N | 1:24:B:ALA:CA | 1:24:B:ALA:C  | 1:25:B:LEU:N | 4        | 4.21          |
| (1,81)  | 1:21:A:SER:C | 1:22:A:GLU:N  | 1:22:A:GLU:CA | 1:22:A:GLU:C | 2        | 4.2           |
| (1,9)   | 1:3:A:LEU:N  | 1:3:A:LEU:CA  | 1:3:A:LEU:C   | 1:4:A:ILE:N  | 2        | 4.2           |
| (1,214) | 1:54:B:ILE:C | 1:55:B:TRP:N  | 1:55:B:TRP:CA | 1:55:B:TRP:C | 3        | 4.17          |
| (1,80)  | 1:21:B:SER:N | 1:21:B:SER:CA | 1:21:B:SER:C  | 1:22:B:GLU:N | 2        | 4.17          |
| (1,43)  | 1:12:A:GLN:N | 1:12:A:GLN:CA | 1:12:A:GLN:C  | 1:13:A:LEU:N | 2        | 4.17          |
| (1,213) | 1:54:A:ILE:C | 1:55:A:TRP:N  | 1:55:A:TRP:CA | 1:55:A:TRP:C | 6        | 4.15          |
| (1,86)  | 1:22:B:GLU:C | 1:23:B:HIS:N  | 1:23:B:HIS:CA | 1:23:B:HIS:C | 9        | 4.15          |
| (1,214) | 1:54:B:ILE:C | 1:55:B:TRP:N  | 1:55:B:TRP:CA | 1:55:B:TRP:C | 6        | 4.14          |
| (1,107) | 1:28:A:SER:N | 1:28:A:SER:CA | 1:28:A:SER:C  | 1:29:A:LEU:N | 7        | 4.14          |
| (1,79)  | 1:21:A:SER:N | 1:21:A:SER:CA | 1:21:A:SER:C  | 1:22:A:GLU:N | 10       | 4.14          |
| (1,79)  | 1:21:A:SER:N | 1:21:A:SER:CA | 1:21:A:SER:C  | 1:22:A:GLU:N | 2        | 4.13          |

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| Key     | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Model ID | Violation (°) |
|---------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,33)  | 1:9:A:THR:N  | 1:9:A:THR:CA  | 1:9:A:THR:C   | 1:10:A:MET:N | 1        | 4.13          |
| (1,303) | 1:77:A:GLY:N | 1:77:A:GLY:CA | 1:77:A:GLY:C  | 1:78:A:GLY:N | 3        | 4.11          |
| (1,213) | 1:54:A:ILE:C | 1:55:A:TRP:N  | 1:55:A:TRP:CA | 1:55:A:TRP:C | 4        | 4.1           |
| (1,108) | 1:28:B:SER:N | 1:28:B:SER:CA | 1:28:B:SER:C  | 1:29:B:LEU:N | 7        | 4.09          |
| (1,85)  | 1:22:A:GLU:C | 1:23:A:HIS:N  | 1:23:A:HIS:CA | 1:23:A:HIS:C | 9        | 4.09          |
| (1,305) | 1:77:A:GLY:C | 1:78:A:GLY:N  | 1:78:A:GLY:CA | 1:78:A:GLY:C | 1        | 4.08          |
| (1,304) | 1:77:B:GLY:N | 1:77:B:GLY:CA | 1:77:B:GLY:C  | 1:78:B:GLY:N | 3        | 4.08          |
| (1,214) | 1:54:B:ILE:C | 1:55:B:TRP:N  | 1:55:B:TRP:CA | 1:55:B:TRP:C | 4        | 4.08          |
| (1,91)  | 1:24:A:ALA:N | 1:24:A:ALA:CA | 1:24:A:ALA:C  | 1:25:A:LEU:N | 4        | 4.06          |
| (1,34)  | 1:9:B:THR:N  | 1:9:B:THR:CA  | 1:9:B:THR:C   | 1:10:B:MET:N | 1        | 4.05          |
| (1,80)  | 1:21:B:SER:N | 1:21:B:SER:CA | 1:21:B:SER:C  | 1:22:B:GLU:N | 10       | 4.04          |
| (1,30)  | 1:8:B:ALA:N  | 1:8:B:ALA:CA  | 1:8:B:ALA:C   | 1:9:B:THR:N  | 7        | 4.04          |
| (1,306) | 1:77:B:GLY:C | 1:78:B:GLY:N  | 1:78:B:GLY:CA | 1:78:B:GLY:C | 5        | 4.01          |
| (1,29)  | 1:8:A:ALA:N  | 1:8:A:ALA:CA  | 1:8:A:ALA:C   | 1:9:A:THR:N  | 7        | 3.99          |
| (1,211) | 1:54:A:ILE:N | 1:54:A:ILE:CA | 1:54:A:ILE:C  | 1:55:A:TRP:N | 4        | 3.98          |
| (1,43)  | 1:12:A:GLN:N | 1:12:A:GLN:CA | 1:12:A:GLN:C  | 1:13:A:LEU:N | 5        | 3.98          |
| (1,212) | 1:54:B:ILE:N | 1:54:B:ILE:CA | 1:54:B:ILE:C  | 1:55:B:TRP:N | 4        | 3.97          |
| (1,305) | 1:77:A:GLY:C | 1:78:A:GLY:N  | 1:78:A:GLY:CA | 1:78:A:GLY:C | 5        | 3.96          |
| (1,213) | 1:54:A:ILE:C | 1:55:A:TRP:N  | 1:55:A:TRP:CA | 1:55:A:TRP:C | 8        | 3.95          |
| (1,80)  | 1:21:B:SER:N | 1:21:B:SER:CA | 1:21:B:SER:C  | 1:22:B:GLU:N | 7        | 3.94          |
| (1,85)  | 1:22:A:GLU:C | 1:23:A:HIS:N  | 1:23:A:HIS:CA | 1:23:A:HIS:C | 6        | 3.93          |
| (1,86)  | 1:22:B:GLU:C | 1:23:B:HIS:N  | 1:23:B:HIS:CA | 1:23:B:HIS:C | 6        | 3.9           |
| (1,214) | 1:54:B:ILE:C | 1:55:B:TRP:N  | 1:55:B:TRP:CA | 1:55:B:TRP:C | 8        | 3.87          |
| (1,79)  | 1:21:A:SER:N | 1:21:A:SER:CA | 1:21:A:SER:C  | 1:22:A:GLU:N | 7        | 3.87          |
| (1,306) | 1:77:B:GLY:C | 1:78:B:GLY:N  | 1:78:B:GLY:CA | 1:78:B:GLY:C | 9        | 3.82          |
| (1,99)  | 1:26:A:GLY:N | 1:26:A:GLY:CA | 1:26:A:GLY:C  | 1:27:A:LEU:N | 10       | 3.82          |
| (1,96)  | 1:25:B:LEU:N | 1:25:B:LEU:CA | 1:25:B:LEU:C  | 1:26:B:GLY:N | 2        | 3.81          |
| (1,95)  | 1:25:A:LEU:N | 1:25:A:LEU:CA | 1:25:A:LEU:C  | 1:26:A:GLY:N | 2        | 3.81          |
| (1,262) | 1:66:B:VAL:C | 1:67:B:ALA:N  | 1:67:B:ALA:CA | 1:67:B:ALA:C | 9        | 3.79          |
| (1,100) | 1:26:B:GLY:N | 1:26:B:GLY:CA | 1:26:B:GLY:C  | 1:27:B:LEU:N | 10       | 3.79          |
| (1,44)  | 1:12:B:GLN:N | 1:12:B:GLN:CA | 1:12:B:GLN:C  | 1:13:B:LEU:N | 5        | 3.79          |
| (1,38)  | 1:10:B:MET:N | 1:10:B:MET:CA | 1:10:B:MET:C  | 1:11:B:PRO:N | 5        | 3.78          |
| (1,37)  | 1:10:A:MET:N | 1:10:A:MET:CA | 1:10:A:MET:C  | 1:11:A:PRO:N | 5        | 3.78          |
| (1,293) | 1:74:A:ALA:C | 1:75:A:HIS:N  | 1:75:A:HIS:CA | 1:75:A:HIS:C | 8        | 3.77          |
| (1,39)  | 1:11:A:PRO:N | 1:11:A:PRO:CA | 1:11:A:PRO:C  | 1:12:A:GLN:N | 1        | 3.77          |
| (1,280) | 1:71:B:GLY:N | 1:71:B:GLY:CA | 1:71:B:GLY:C  | 1:72:B:ILE:N | 8        | 3.76          |
| (1,305) | 1:77:A:GLY:C | 1:78:A:GLY:N  | 1:78:A:GLY:CA | 1:78:A:GLY:C | 9        | 3.75          |
| (1,261) | 1:66:A:VAL:C | 1:67:A:ALA:N  | 1:67:A:ALA:CA | 1:67:A:ALA:C | 9        | 3.71          |
| (1,305) | 1:77:A:GLY:C | 1:78:A:GLY:N  | 1:78:A:GLY:CA | 1:78:A:GLY:C | 4        | 3.69          |
| (1,40)  | 1:11:B:PRO:N | 1:11:B:PRO:CA | 1:11:B:PRO:C  | 1:12:B:GLN:N | 1        | 3.67          |
| (1,294) | 1:74:B:ALA:C | 1:75:B:HIS:N  | 1:75:B:HIS:CA | 1:75:B:HIS:C | 8        | 3.66          |
| (1,204) | 1:52:B:PRO:N | 1:52:B:PRO:CA | 1:52:B:PRO:C  | 1:53:B:THR:N | 2        | 3.66          |
| (1,12)  | 1:3:B:LEU:C  | 1:4:B:ILE:N   | 1:4:B:ILE:CA  | 1:4:B:ILE:C  | 9        | 3.65          |
| (1,38)  | 1:10:B:MET:N | 1:10:B:MET:CA | 1:10:B:MET:C  | 1:11:B:PRO:N | 9        | 3.62          |
| (1,95)  | 1:25:A:LEU:N | 1:25:A:LEU:CA | 1:25:A:LEU:C  | 1:26:A:GLY:N | 9        | 3.61          |
| (1,265) | 1:67:A:ALA:C | 1:68:A:MET:N  | 1:68:A:MET:CA | 1:68:A:MET:C | 2        | 3.59          |
| (1,37)  | 1:10:A:MET:N | 1:10:A:MET:CA | 1:10:A:MET:C  | 1:11:A:PRO:N | 9        | 3.59          |
| (1,11)  | 1:3:A:LEU:C  | 1:4:A:ILE:N   | 1:4:A:ILE:CA  | 1:4:A:ILE:C  | 9        | 3.58          |
| (1,203) | 1:52:A:PRO:N | 1:52:A:PRO:CA | 1:52:A:PRO:C  | 1:53:A:THR:N | 2        | 3.54          |
| (1,266) | 1:67:B:ALA:C | 1:68:B:MET:N  | 1:68:B:MET:CA | 1:68:B:MET:C | 2        | 3.52          |
| (1,79)  | 1:21:A:SER:N | 1:21:A:SER:CA | 1:21:A:SER:C  | 1:22:A:GLU:N | 4        | 3.51          |

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| Key     | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Model ID | Violation (°) |
|---------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,269) | 1:68:A:MET:C | 1:69:A:VAL:N  | 1:69:A:VAL:CA | 1:69:A:VAL:C | 3        | 3.5           |
| (1,29)  | 1:8:A:ALA:N  | 1:8:A:ALA:CA  | 1:8:A:ALA:C   | 1:9:A:THR:N  | 3        | 3.49          |
| (1,11)  | 1:3:A:LEU:C  | 1:4:A:ILE:N   | 1:4:A:ILE:CA  | 1:4:A:ILE:C  | 5        | 3.49          |
| (1,306) | 1:77:B:GLY:C | 1:78:B:GLY:N  | 1:78:B:GLY:CA | 1:78:B:GLY:C | 4        | 3.47          |
| (1,274) | 1:69:B:VAL:C | 1:70:B:VAL:N  | 1:70:B:VAL:CA | 1:70:B:VAL:C | 4        | 3.47          |
| (1,80)  | 1:21:B:SER:N | 1:21:B:SER:CA | 1:21:B:SER:C  | 1:22:B:GLU:N | 4        | 3.46          |
| (1,270) | 1:68:B:MET:C | 1:69:B:VAL:N  | 1:69:B:VAL:CA | 1:69:B:VAL:C | 3        | 3.43          |
| (1,96)  | 1:25:B:LEU:N | 1:25:B:LEU:CA | 1:25:B:LEU:C  | 1:26:B:GLY:N | 9        | 3.43          |
| (1,30)  | 1:8:B:ALA:N  | 1:8:B:ALA:CA  | 1:8:B:ALA:C   | 1:9:B:THR:N  | 3        | 3.39          |
| (1,12)  | 1:3:B:LEU:C  | 1:4:B:ILE:N   | 1:4:B:ILE:CA  | 1:4:B:ILE:C  | 5        | 3.39          |
| (1,280) | 1:71:B:GLY:N | 1:71:B:GLY:CA | 1:71:B:GLY:C  | 1:72:B:ILE:N | 6        | 3.38          |
| (1,273) | 1:69:A:VAL:C | 1:70:A:VAL:N  | 1:70:A:VAL:CA | 1:70:A:VAL:C | 4        | 3.37          |
| (1,215) | 1:55:A:TRP:N | 1:55:A:TRP:CA | 1:55:A:TRP:C  | 1:56:A:VAL:N | 5        | 3.35          |
| (1,93)  | 1:24:A:ALA:C | 1:25:A:LEU:N  | 1:25:A:LEU:CA | 1:25:A:LEU:C | 4        | 3.35          |
| (1,294) | 1:74:B:ALA:C | 1:75:B:HIS:N  | 1:75:B:HIS:CA | 1:75:B:HIS:C | 7        | 3.34          |
| (1,281) | 1:71:A:GLY:C | 1:72:A:ILE:N  | 1:72:A:ILE:CA | 1:72:A:ILE:C | 6        | 3.33          |
| (1,30)  | 1:8:B:ALA:N  | 1:8:B:ALA:CA  | 1:8:B:ALA:C   | 1:9:B:THR:N  | 4        | 3.33          |
| (1,303) | 1:77:A:GLY:N | 1:77:A:GLY:CA | 1:77:A:GLY:C  | 1:78:A:GLY:N | 8        | 3.31          |
| (1,282) | 1:71:B:GLY:C | 1:72:B:ILE:N  | 1:72:B:ILE:CA | 1:72:B:ILE:C | 6        | 3.3           |
| (1,216) | 1:55:B:TRP:N | 1:55:B:TRP:CA | 1:55:B:TRP:C  | 1:56:B:VAL:N | 8        | 3.3           |
| (1,293) | 1:74:A:ALA:C | 1:75:A:HIS:N  | 1:75:A:HIS:CA | 1:75:A:HIS:C | 7        | 3.29          |
| (1,221) | 1:56:A:VAL:C | 1:57:A:GLY:N  | 1:57:A:GLY:CA | 1:57:A:GLY:C | 5        | 3.29          |
| (1,86)  | 1:22:B:GLU:C | 1:23:B:HIS:N  | 1:23:B:HIS:CA | 1:23:B:HIS:C | 8        | 3.29          |
| (1,85)  | 1:22:A:GLU:C | 1:23:A:HIS:N  | 1:23:A:HIS:CA | 1:23:A:HIS:C | 8        | 3.29          |
| (1,29)  | 1:8:A:ALA:N  | 1:8:A:ALA:CA  | 1:8:A:ALA:C   | 1:9:A:THR:N  | 4        | 3.29          |
| (1,222) | 1:56:B:VAL:C | 1:57:B:GLY:N  | 1:57:B:GLY:CA | 1:57:B:GLY:C | 5        | 3.28          |
| (1,84)  | 1:22:B:GLU:N | 1:22:B:GLU:CA | 1:22:B:GLU:C  | 1:23:B:HIS:N | 10       | 3.28          |
| (1,81)  | 1:21:A:SER:C | 1:22:A:GLU:N  | 1:22:A:GLU:CA | 1:22:A:GLU:C | 8        | 3.27          |
| (1,96)  | 1:25:B:LEU:N | 1:25:B:LEU:CA | 1:25:B:LEU:C  | 1:26:B:GLY:N | 6        | 3.26          |
| (1,216) | 1:55:B:TRP:N | 1:55:B:TRP:CA | 1:55:B:TRP:C  | 1:56:B:VAL:N | 5        | 3.25          |
| (1,94)  | 1:24:B:ALA:C | 1:25:B:LEU:N  | 1:25:B:LEU:CA | 1:25:B:LEU:C | 4        | 3.24          |
| (1,79)  | 1:21:A:SER:N | 1:21:A:SER:CA | 1:21:A:SER:C  | 1:22:A:GLU:N | 8        | 3.24          |
| (1,279) | 1:71:A:GLY:N | 1:71:A:GLY:CA | 1:71:A:GLY:C  | 1:72:A:ILE:N | 6        | 3.23          |
| (1,82)  | 1:21:B:SER:C | 1:22:B:GLU:N  | 1:22:B:GLU:CA | 1:22:B:GLU:C | 10       | 3.23          |
| (1,81)  | 1:21:A:SER:C | 1:22:A:GLU:N  | 1:22:A:GLU:CA | 1:22:A:GLU:C | 10       | 3.23          |
| (1,29)  | 1:8:A:ALA:N  | 1:8:A:ALA:CA  | 1:8:A:ALA:C   | 1:9:A:THR:N  | 6        | 3.23          |
| (1,95)  | 1:25:A:LEU:N | 1:25:A:LEU:CA | 1:25:A:LEU:C  | 1:26:A:GLY:N | 6        | 3.22          |
| (1,83)  | 1:22:A:GLU:N | 1:22:A:GLU:CA | 1:22:A:GLU:C  | 1:23:A:HIS:N | 10       | 3.22          |
| (1,80)  | 1:21:B:SER:N | 1:21:B:SER:CA | 1:21:B:SER:C  | 1:22:B:GLU:N | 8        | 3.22          |
| (1,215) | 1:55:A:TRP:N | 1:55:A:TRP:CA | 1:55:A:TRP:C  | 1:56:A:VAL:N | 8        | 3.2           |
| (1,30)  | 1:8:B:ALA:N  | 1:8:B:ALA:CA  | 1:8:B:ALA:C   | 1:9:B:THR:N  | 6        | 3.16          |
| (1,185) | 1:47:A:ILE:C | 1:48:A:TYR:N  | 1:48:A:TYR:CA | 1:48:A:TYR:C | 1        | 3.14          |
| (1,82)  | 1:21:B:SER:C | 1:22:B:GLU:N  | 1:22:B:GLU:CA | 1:22:B:GLU:C | 8        | 3.14          |
| (1,281) | 1:71:A:GLY:C | 1:72:A:ILE:N  | 1:72:A:ILE:CA | 1:72:A:ILE:C | 4        | 3.12          |
| (1,212) | 1:54:B:ILE:N | 1:54:B:ILE:CA | 1:54:B:ILE:C  | 1:55:B:TRP:N | 9        | 3.12          |
| (1,303) | 1:77:A:GLY:N | 1:77:A:GLY:CA | 1:77:A:GLY:C  | 1:78:A:GLY:N | 6        | 3.09          |
| (1,304) | 1:77:B:GLY:N | 1:77:B:GLY:CA | 1:77:B:GLY:C  | 1:78:B:GLY:N | 6        | 3.07          |
| (1,211) | 1:54:A:ILE:N | 1:54:A:ILE:CA | 1:54:A:ILE:C  | 1:55:A:TRP:N | 9        | 3.04          |
| (1,29)  | 1:8:A:ALA:N  | 1:8:A:ALA:CA  | 1:8:A:ALA:C   | 1:9:A:THR:N  | 2        | 3.04          |
| (1,189) | 1:48:A:TYR:C | 1:49:A:HIS:N  | 1:49:A:HIS:CA | 1:49:A:HIS:C | 9        | 3.03          |
| (1,29)  | 1:8:A:ALA:N  | 1:8:A:ALA:CA  | 1:8:A:ALA:C   | 1:9:A:THR:N  | 10       | 3.03          |

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| Key     | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Model ID | Violation (°) |
|---------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,280) | 1:71:B:GLY:N | 1:71:B:GLY:CA | 1:71:B:GLY:C  | 1:72:B:ILE:N | 4        | 3.02          |
| (1,282) | 1:71:B:GLY:C | 1:72:B:ILE:N  | 1:72:B:ILE:CA | 1:72:B:ILE:C | 4        | 3.01          |
| (1,180) | 1:46:B:GLY:N | 1:46:B:GLY:CA | 1:46:B:GLY:C  | 1:47:B:ILE:N | 5        | 3.01          |
| (1,281) | 1:71:A:GLY:C | 1:72:A:ILE:N  | 1:72:A:ILE:CA | 1:72:A:ILE:C | 8        | 3.0           |
| (1,170) | 1:43:B:THR:C | 1:44:B:ILE:N  | 1:44:B:ILE:CA | 1:44:B:ILE:C | 9        | 2.99          |
| (1,279) | 1:71:A:GLY:N | 1:71:A:GLY:CA | 1:71:A:GLY:C  | 1:72:A:ILE:N | 4        | 2.98          |
| (1,184) | 1:47:B:ILE:N | 1:47:B:ILE:CA | 1:47:B:ILE:C  | 1:48:B:TYR:N | 1        | 2.98          |
| (1,190) | 1:48:B:TYR:C | 1:49:B:HIS:N  | 1:49:B:HIS:CA | 1:49:B:HIS:C | 9        | 2.96          |
| (1,80)  | 1:21:B:SER:N | 1:21:B:SER:CA | 1:21:B:SER:C  | 1:22:B:GLU:N | 9        | 2.96          |
| (1,11)  | 1:3:A:LEU:C  | 1:4:A:ILE:N   | 1:4:A:ILE:CA  | 1:4:A:ILE:C  | 3        | 2.96          |
| (1,12)  | 1:3:B:LEU:C  | 1:4:B:ILE:N   | 1:4:B:ILE:CA  | 1:4:B:ILE:C  | 3        | 2.94          |
| (1,80)  | 1:21:B:SER:N | 1:21:B:SER:CA | 1:21:B:SER:C  | 1:22:B:GLU:N | 6        | 2.93          |
| (1,186) | 1:47:B:ILE:C | 1:48:B:TYR:N  | 1:48:B:TYR:CA | 1:48:B:TYR:C | 10       | 2.91          |
| (1,79)  | 1:21:A:SER:N | 1:21:A:SER:CA | 1:21:A:SER:C  | 1:22:A:GLU:N | 6        | 2.91          |
| (1,30)  | 1:8:B:ALA:N  | 1:8:B:ALA:CA  | 1:8:B:ALA:C   | 1:9:B:THR:N  | 2        | 2.91          |
| (1,30)  | 1:8:B:ALA:N  | 1:8:B:ALA:CA  | 1:8:B:ALA:C   | 1:9:B:THR:N  | 10       | 2.9           |
| (1,179) | 1:46:A:GLY:N | 1:46:A:GLY:CA | 1:46:A:GLY:C  | 1:47:A:ILE:N | 5        | 2.89          |
| (1,281) | 1:71:A:GLY:C | 1:72:A:ILE:N  | 1:72:A:ILE:CA | 1:72:A:ILE:C | 3        | 2.88          |
| (1,186) | 1:47:B:ILE:C | 1:48:B:TYR:N  | 1:48:B:TYR:CA | 1:48:B:TYR:C | 1        | 2.88          |
| (1,182) | 1:46:B:GLY:C | 1:47:B:ILE:N  | 1:47:B:ILE:CA | 1:47:B:ILE:C | 9        | 2.88          |
| (1,79)  | 1:21:A:SER:N | 1:21:A:SER:CA | 1:21:A:SER:C  | 1:22:A:GLU:N | 9        | 2.87          |
| (1,185) | 1:47:A:ILE:C | 1:48:A:TYR:N  | 1:48:A:TYR:CA | 1:48:A:TYR:C | 10       | 2.86          |
| (1,59)  | 1:16:A:LEU:N | 1:16:A:LEU:CA | 1:16:A:LEU:C  | 1:17:A:TYR:N | 3        | 2.85          |
| (1,7)   | 1:2:A:GLY:C  | 1:3:A:LEU:N   | 1:3:A:LEU:CA  | 1:3:A:LEU:C  | 8        | 2.84          |
| (1,304) | 1:77:B:GLY:N | 1:77:B:GLY:CA | 1:77:B:GLY:C  | 1:78:B:GLY:N | 8        | 2.82          |
| (1,280) | 1:71:B:GLY:N | 1:71:B:GLY:CA | 1:71:B:GLY:C  | 1:72:B:ILE:N | 3        | 2.82          |
| (1,60)  | 1:16:B:LEU:N | 1:16:B:LEU:CA | 1:16:B:LEU:C  | 1:17:B:TYR:N | 3        | 2.82          |
| (1,279) | 1:71:A:GLY:N | 1:71:A:GLY:CA | 1:71:A:GLY:C  | 1:72:A:ILE:N | 8        | 2.79          |
| (1,282) | 1:71:B:GLY:C | 1:72:B:ILE:N  | 1:72:B:ILE:CA | 1:72:B:ILE:C | 3        | 2.77          |
| (1,8)   | 1:2:B:GLY:C  | 1:3:B:LEU:N   | 1:3:B:LEU:CA  | 1:3:B:LEU:C  | 8        | 2.77          |
| (1,279) | 1:71:A:GLY:N | 1:71:A:GLY:CA | 1:71:A:GLY:C  | 1:72:A:ILE:N | 3        | 2.76          |
| (1,183) | 1:47:A:ILE:N | 1:47:A:ILE:CA | 1:47:A:ILE:C  | 1:48:A:TYR:N | 1        | 2.76          |
| (1,181) | 1:46:A:GLY:C | 1:47:A:ILE:N  | 1:47:A:ILE:CA | 1:47:A:ILE:C | 9        | 2.76          |
| (1,169) | 1:43:A:THR:C | 1:44:A:ILE:N  | 1:44:A:ILE:CA | 1:44:A:ILE:C | 9        | 2.76          |
| (1,221) | 1:56:A:VAL:C | 1:57:A:GLY:N  | 1:57:A:GLY:CA | 1:57:A:GLY:C | 2        | 2.75          |
| (1,143) | 1:37:A:PHE:N | 1:37:A:PHE:CA | 1:37:A:PHE:C  | 1:38:A:ILE:N | 10       | 2.74          |
| (1,98)  | 1:25:B:LEU:C | 1:26:B:GLY:N  | 1:26:B:GLY:CA | 1:26:B:GLY:C | 5        | 2.73          |
| (1,186) | 1:47:B:ILE:C | 1:48:B:TYR:N  | 1:48:B:TYR:CA | 1:48:B:TYR:C | 7        | 2.71          |
| (1,222) | 1:56:B:VAL:C | 1:57:B:GLY:N  | 1:57:B:GLY:CA | 1:57:B:GLY:C | 2        | 2.7           |
| (1,167) | 1:43:A:THR:N | 1:43:A:THR:CA | 1:43:A:THR:C  | 1:44:A:ILE:N | 9        | 2.7           |
| (1,280) | 1:71:B:GLY:N | 1:71:B:GLY:CA | 1:71:B:GLY:C  | 1:72:B:ILE:N | 2        | 2.67          |
| (1,185) | 1:47:A:ILE:C | 1:48:A:TYR:N  | 1:48:A:TYR:CA | 1:48:A:TYR:C | 7        | 2.67          |
| (1,305) | 1:77:A:GLY:C | 1:78:A:GLY:N  | 1:78:A:GLY:CA | 1:78:A:GLY:C | 7        | 2.66          |
| (1,144) | 1:37:B:PHE:N | 1:37:B:PHE:CA | 1:37:B:PHE:C  | 1:38:B:ILE:N | 10       | 2.66          |
| (1,98)  | 1:25:B:LEU:C | 1:26:B:GLY:N  | 1:26:B:GLY:CA | 1:26:B:GLY:C | 10       | 2.64          |
| (1,97)  | 1:25:A:LEU:C | 1:26:A:GLY:N  | 1:26:A:GLY:CA | 1:26:A:GLY:C | 10       | 2.64          |
| (1,168) | 1:43:B:THR:N | 1:43:B:THR:CA | 1:43:B:THR:C  | 1:44:B:ILE:N | 9        | 2.63          |
| (1,11)  | 1:3:A:LEU:C  | 1:4:A:ILE:N   | 1:4:A:ILE:CA  | 1:4:A:ILE:C  | 8        | 2.63          |
| (1,279) | 1:71:A:GLY:N | 1:71:A:GLY:CA | 1:71:A:GLY:C  | 1:72:A:ILE:N | 2        | 2.61          |
| (1,107) | 1:28:A:SER:N | 1:28:A:SER:CA | 1:28:A:SER:C  | 1:29:A:LEU:N | 1        | 2.61          |
| (1,97)  | 1:25:A:LEU:C | 1:26:A:GLY:N  | 1:26:A:GLY:CA | 1:26:A:GLY:C | 5        | 2.61          |

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| Key     | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Model ID | Violation (°) |
|---------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,215) | 1:55:A:TRP:N | 1:55:A:TRP:CA | 1:55:A:TRP:C  | 1:56:A:VAL:N | 3        | 2.6           |
| (1,216) | 1:55:B:TRP:N | 1:55:B:TRP:CA | 1:55:B:TRP:C  | 1:56:B:VAL:N | 3        | 2.59          |
| (1,306) | 1:77:B:GLY:C | 1:78:B:GLY:N  | 1:78:B:GLY:CA | 1:78:B:GLY:C | 7        | 2.57          |
| (1,98)  | 1:25:B:LEU:C | 1:26:B:GLY:N  | 1:26:B:GLY:CA | 1:26:B:GLY:C | 4        | 2.57          |
| (1,192) | 1:49:B:HIS:N | 1:49:B:HIS:CA | 1:49:B:HIS:C  | 1:50:B:LYS:N | 4        | 2.54          |
| (1,282) | 1:71:B:GLY:C | 1:72:B:ILE:N  | 1:72:B:ILE:CA | 1:72:B:ILE:C | 8        | 2.53          |
| (1,82)  | 1:21:B:SER:C | 1:22:B:GLU:N  | 1:22:B:GLU:CA | 1:22:B:GLU:C | 6        | 2.53          |
| (1,303) | 1:77:A:GLY:N | 1:77:A:GLY:CA | 1:77:A:GLY:C  | 1:78:A:GLY:N | 1        | 2.52          |
| (1,304) | 1:77:B:GLY:N | 1:77:B:GLY:CA | 1:77:B:GLY:C  | 1:78:B:GLY:N | 9        | 2.5           |
| (1,108) | 1:28:B:SER:N | 1:28:B:SER:CA | 1:28:B:SER:C  | 1:29:B:LEU:N | 1        | 2.5           |
| (1,97)  | 1:25:A:LEU:C | 1:26:A:GLY:N  | 1:26:A:GLY:CA | 1:26:A:GLY:C | 4        | 2.47          |
| (1,63)  | 1:17:A:TYR:N | 1:17:A:TYR:CA | 1:17:A:TYR:C  | 1:18:A:VAL:N | 10       | 2.47          |
| (1,303) | 1:77:A:GLY:N | 1:77:A:GLY:CA | 1:77:A:GLY:C  | 1:78:A:GLY:N | 9        | 2.46          |
| (1,91)  | 1:24:A:ALA:N | 1:24:A:ALA:CA | 1:24:A:ALA:C  | 1:25:A:LEU:N | 10       | 2.46          |
| (1,12)  | 1:3:B:LEU:C  | 1:4:B:ILE:N   | 1:4:B:ILE:CA  | 1:4:B:ILE:C  | 8        | 2.46          |
| (1,81)  | 1:21:A:SER:C | 1:22:A:GLU:N  | 1:22:A:GLU:CA | 1:22:A:GLU:C | 6        | 2.44          |
| (1,191) | 1:49:A:HIS:N | 1:49:A:HIS:CA | 1:49:A:HIS:C  | 1:50:A:LYS:N | 4        | 2.42          |
| (1,107) | 1:28:A:SER:N | 1:28:A:SER:CA | 1:28:A:SER:C  | 1:29:A:LEU:N | 3        | 2.4           |
| (1,38)  | 1:10:B:MET:N | 1:10:B:MET:CA | 1:10:B:MET:C  | 1:11:B:PRO:N | 7        | 2.4           |
| (1,43)  | 1:12:A:GLN:N | 1:12:A:GLN:CA | 1:12:A:GLN:C  | 1:13:A:LEU:N | 9        | 2.39          |
| (1,64)  | 1:17:B:TYR:N | 1:17:B:TYR:CA | 1:17:B:TYR:C  | 1:18:B:VAL:N | 10       | 2.38          |
| (1,41)  | 1:11:A:PRO:C | 1:12:A:GLN:N  | 1:12:A:GLN:CA | 1:12:A:GLN:C | 1        | 2.38          |
| (1,304) | 1:77:B:GLY:N | 1:77:B:GLY:CA | 1:77:B:GLY:C  | 1:78:B:GLY:N | 1        | 2.37          |
| (1,108) | 1:28:B:SER:N | 1:28:B:SER:CA | 1:28:B:SER:C  | 1:29:B:LEU:N | 3        | 2.37          |
| (1,92)  | 1:24:B:ALA:N | 1:24:B:ALA:CA | 1:24:B:ALA:C  | 1:25:B:LEU:N | 10       | 2.37          |
| (1,44)  | 1:12:B:GLN:N | 1:12:B:GLN:CA | 1:12:B:GLN:C  | 1:13:B:LEU:N | 9        | 2.36          |
| (1,42)  | 1:11:B:PRO:C | 1:12:B:GLN:N  | 1:12:B:GLN:CA | 1:12:B:GLN:C | 1        | 2.36          |
| (1,303) | 1:77:A:GLY:N | 1:77:A:GLY:CA | 1:77:A:GLY:C  | 1:78:A:GLY:N | 5        | 2.35          |
| (1,41)  | 1:11:A:PRO:C | 1:12:A:GLN:N  | 1:12:A:GLN:CA | 1:12:A:GLN:C | 10       | 2.35          |
| (1,70)  | 1:18:B:VAL:C | 1:19:B:SER:N  | 1:19:B:SER:CA | 1:19:B:SER:C | 5        | 2.34          |
| (1,63)  | 1:17:A:TYR:N | 1:17:A:TYR:CA | 1:17:A:TYR:C  | 1:18:A:VAL:N | 1        | 2.34          |
| (1,294) | 1:74:B:ALA:C | 1:75:B:HIS:N  | 1:75:B:HIS:CA | 1:75:B:HIS:C | 4        | 2.33          |
| (1,293) | 1:74:A:ALA:C | 1:75:A:HIS:N  | 1:75:A:HIS:CA | 1:75:A:HIS:C | 4        | 2.32          |
| (1,69)  | 1:18:A:VAL:C | 1:19:A:SER:N  | 1:19:A:SER:CA | 1:19:A:SER:C | 5        | 2.32          |
| (1,182) | 1:46:B:GLY:C | 1:47:B:ILE:N  | 1:47:B:ILE:CA | 1:47:B:ILE:C | 7        | 2.3           |
| (1,264) | 1:67:B:ALA:N | 1:67:B:ALA:CA | 1:67:B:ALA:C  | 1:68:B:MET:N | 3        | 2.28          |
| (1,293) | 1:74:A:ALA:C | 1:75:A:HIS:N  | 1:75:A:HIS:CA | 1:75:A:HIS:C | 10       | 2.26          |
| (1,29)  | 1:8:A:ALA:N  | 1:8:A:ALA:CA  | 1:8:A:ALA:C   | 1:9:A:THR:N  | 8        | 2.26          |
| (1,64)  | 1:17:B:TYR:N | 1:17:B:TYR:CA | 1:17:B:TYR:C  | 1:18:B:VAL:N | 2        | 2.25          |
| (1,42)  | 1:11:B:PRO:C | 1:12:B:GLN:N  | 1:12:B:GLN:CA | 1:12:B:GLN:C | 10       | 2.25          |
| (1,37)  | 1:10:A:MET:N | 1:10:A:MET:CA | 1:10:A:MET:C  | 1:11:A:PRO:N | 7        | 2.24          |
| (1,29)  | 1:8:A:ALA:N  | 1:8:A:ALA:CA  | 1:8:A:ALA:C   | 1:9:A:THR:N  | 1        | 2.24          |
| (1,304) | 1:77:B:GLY:N | 1:77:B:GLY:CA | 1:77:B:GLY:C  | 1:78:B:GLY:N | 5        | 2.23          |
| (1,43)  | 1:12:A:GLN:N | 1:12:A:GLN:CA | 1:12:A:GLN:C  | 1:13:A:LEU:N | 8        | 2.22          |
| (1,63)  | 1:17:A:TYR:N | 1:17:A:TYR:CA | 1:17:A:TYR:C  | 1:18:A:VAL:N | 2        | 2.21          |
| (1,35)  | 1:9:A:THR:C  | 1:10:A:MET:N  | 1:10:A:MET:CA | 1:10:A:MET:C | 9        | 2.21          |
| (1,294) | 1:74:B:ALA:C | 1:75:B:HIS:N  | 1:75:B:HIS:CA | 1:75:B:HIS:C | 10       | 2.2           |
| (1,294) | 1:74:B:ALA:C | 1:75:B:HIS:N  | 1:75:B:HIS:CA | 1:75:B:HIS:C | 5        | 2.19          |
| (1,292) | 1:74:B:ALA:N | 1:74:B:ALA:CA | 1:74:B:ALA:C  | 1:75:B:HIS:N | 8        | 2.19          |
| (1,282) | 1:71:B:GLY:C | 1:72:B:ILE:N  | 1:72:B:ILE:CA | 1:72:B:ILE:C | 9        | 2.19          |
| (1,263) | 1:67:A:ALA:N | 1:67:A:ALA:CA | 1:67:A:ALA:C  | 1:68:A:MET:N | 3        | 2.19          |

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Continued from previous page...

| Key     | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Model ID | Violation (°) |
|---------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,179) | 1:46:A:GLY:N | 1:46:A:GLY:CA | 1:46:A:GLY:C  | 1:47:A:ILE:N | 9        | 2.19          |
| (1,182) | 1:46:B:GLY:C | 1:47:B:ILE:N  | 1:47:B:ILE:CA | 1:47:B:ILE:C | 4        | 2.18          |
| (1,69)  | 1:18:A:VAL:C | 1:19:A:SER:N  | 1:19:A:SER:CA | 1:19:A:SER:C | 7        | 2.17          |
| (1,30)  | 1:8:B:ALA:N  | 1:8:B:ALA:CA  | 1:8:B:ALA:C   | 1:9:B:THR:N  | 8        | 2.17          |
| (1,182) | 1:46:B:GLY:C | 1:47:B:ILE:N  | 1:47:B:ILE:CA | 1:47:B:ILE:C | 1        | 2.16          |
| (1,72)  | 1:19:B:SER:N | 1:19:B:SER:CA | 1:19:B:SER:C  | 1:20:B:HIS:N | 10       | 2.16          |
| (1,69)  | 1:18:A:VAL:C | 1:19:A:SER:N  | 1:19:A:SER:CA | 1:19:A:SER:C | 2        | 2.16          |
| (1,44)  | 1:12:B:GLN:N | 1:12:B:GLN:CA | 1:12:B:GLN:C  | 1:13:B:LEU:N | 8        | 2.16          |
| (1,30)  | 1:8:B:ALA:N  | 1:8:B:ALA:CA  | 1:8:B:ALA:C   | 1:9:B:THR:N  | 1        | 2.16          |
| (1,198) | 1:50:B:LYS:C | 1:51:B:ASN:N  | 1:51:B:ASN:CA | 1:51:B:ASN:C | 4        | 2.15          |
| (1,190) | 1:48:B:TYR:C | 1:49:B:HIS:N  | 1:49:B:HIS:CA | 1:49:B:HIS:C | 6        | 2.15          |
| (1,64)  | 1:17:B:TYR:N | 1:17:B:TYR:CA | 1:17:B:TYR:C  | 1:18:B:VAL:N | 1        | 2.15          |
| (1,70)  | 1:18:B:VAL:C | 1:19:B:SER:N  | 1:19:B:SER:CA | 1:19:B:SER:C | 7        | 2.14          |
| (1,281) | 1:71:A:GLY:C | 1:72:A:ILE:N  | 1:72:A:ILE:CA | 1:72:A:ILE:C | 9        | 2.13          |
| (1,279) | 1:71:A:GLY:N | 1:71:A:GLY:CA | 1:71:A:GLY:C  | 1:72:A:ILE:N | 5        | 2.13          |
| (1,268) | 1:68:B:MET:N | 1:68:B:MET:CA | 1:68:B:MET:C  | 1:69:B:VAL:N | 3        | 2.13          |
| (1,104) | 1:27:B:LEU:N | 1:27:B:LEU:CA | 1:27:B:LEU:C  | 1:28:B:SER:N | 9        | 2.13          |
| (1,103) | 1:27:A:LEU:N | 1:27:A:LEU:CA | 1:27:A:LEU:C  | 1:28:A:SER:N | 9        | 2.13          |
| (1,269) | 1:68:A:MET:C | 1:69:A:VAL:N  | 1:69:A:VAL:CA | 1:69:A:VAL:C | 6        | 2.12          |
| (1,267) | 1:68:A:MET:N | 1:68:A:MET:CA | 1:68:A:MET:C  | 1:69:A:VAL:N | 3        | 2.11          |
| (1,44)  | 1:12:B:GLN:N | 1:12:B:GLN:CA | 1:12:B:GLN:C  | 1:13:B:LEU:N | 4        | 2.11          |
| (1,308) | 1:78:B:GLY:N | 1:78:B:GLY:CA | 1:78:B:GLY:C  | 1:79:B:THR:N | 10       | 2.1           |
| (1,189) | 1:48:A:TYR:C | 1:49:A:HIS:N  | 1:49:A:HIS:CA | 1:49:A:HIS:C | 6        | 2.1           |
| (1,181) | 1:46:A:GLY:C | 1:47:A:ILE:N  | 1:47:A:ILE:CA | 1:47:A:ILE:C | 1        | 2.1           |
| (1,43)  | 1:12:A:GLN:N | 1:12:A:GLN:CA | 1:12:A:GLN:C  | 1:13:A:LEU:N | 3        | 2.09          |
| (1,43)  | 1:12:A:GLN:N | 1:12:A:GLN:CA | 1:12:A:GLN:C  | 1:13:A:LEU:N | 4        | 2.09          |
| (1,291) | 1:74:A:ALA:N | 1:74:A:ALA:CA | 1:74:A:ALA:C  | 1:75:A:HIS:N | 10       | 2.08          |
| (1,263) | 1:67:A:ALA:N | 1:67:A:ALA:CA | 1:67:A:ALA:C  | 1:68:A:MET:N | 2        | 2.08          |
| (1,70)  | 1:18:B:VAL:C | 1:19:B:SER:N  | 1:19:B:SER:CA | 1:19:B:SER:C | 2        | 2.08          |
| (1,250) | 1:63:B:LEU:C | 1:64:B:MET:N  | 1:64:B:MET:CA | 1:64:B:MET:C | 7        | 2.07          |
| (1,41)  | 1:11:A:PRO:C | 1:12:A:GLN:N  | 1:12:A:GLN:CA | 1:12:A:GLN:C | 7        | 2.07          |
| (1,36)  | 1:9:B:THR:C  | 1:10:B:MET:N  | 1:10:B:MET:CA | 1:10:B:MET:C | 9        | 2.06          |
| (1,293) | 1:74:A:ALA:C | 1:75:A:HIS:N  | 1:75:A:HIS:CA | 1:75:A:HIS:C | 9        | 2.05          |
| (1,280) | 1:71:B:GLY:N | 1:71:B:GLY:CA | 1:71:B:GLY:C  | 1:72:B:ILE:N | 5        | 2.05          |
| (1,270) | 1:68:B:MET:C | 1:69:B:VAL:N  | 1:69:B:VAL:CA | 1:69:B:VAL:C | 6        | 2.05          |
| (1,89)  | 1:23:A:HIS:C | 1:24:A:ALA:N  | 1:24:A:ALA:CA | 1:24:A:ALA:C | 3        | 2.05          |
| (1,72)  | 1:19:B:SER:N | 1:19:B:SER:CA | 1:19:B:SER:C  | 1:20:B:HIS:N | 8        | 2.04          |
| (1,71)  | 1:19:A:SER:N | 1:19:A:SER:CA | 1:19:A:SER:C  | 1:20:A:HIS:N | 8        | 2.04          |
| (1,293) | 1:74:A:ALA:C | 1:75:A:HIS:N  | 1:75:A:HIS:CA | 1:75:A:HIS:C | 1        | 2.03          |
| (1,42)  | 1:11:B:PRO:C | 1:12:B:GLN:N  | 1:12:B:GLN:CA | 1:12:B:GLN:C | 7        | 2.03          |
| (1,307) | 1:78:A:GLY:N | 1:78:A:GLY:CA | 1:78:A:GLY:C  | 1:79:A:THR:N | 10       | 2.02          |
| (1,90)  | 1:23:B:HIS:C | 1:24:B:ALA:N  | 1:24:B:ALA:CA | 1:24:B:ALA:C | 3        | 2.02          |
| (1,292) | 1:74:B:ALA:N | 1:74:B:ALA:CA | 1:74:B:ALA:C  | 1:75:B:HIS:N | 10       | 2.01          |
| (1,182) | 1:46:B:GLY:C | 1:47:B:ILE:N  | 1:47:B:ILE:CA | 1:47:B:ILE:C | 10       | 2.01          |
| (1,94)  | 1:24:B:ALA:C | 1:25:B:LEU:N  | 1:25:B:LEU:CA | 1:25:B:LEU:C | 10       | 2.01          |
| (1,71)  | 1:19:A:SER:N | 1:19:A:SER:CA | 1:19:A:SER:C  | 1:20:A:HIS:N | 10       | 2.01          |
| (1,64)  | 1:17:B:TYR:N | 1:17:B:TYR:CA | 1:17:B:TYR:C  | 1:18:B:VAL:N | 6        | 2.01          |
| (1,151) | 1:39:A:ALA:N | 1:39:A:ALA:CA | 1:39:A:ALA:C  | 1:40:A:LEU:N | 8        | 2.0           |
| (1,181) | 1:46:A:GLY:C | 1:47:A:ILE:N  | 1:47:A:ILE:CA | 1:47:A:ILE:C | 10       | 1.99          |
| (1,44)  | 1:12:B:GLN:N | 1:12:B:GLN:CA | 1:12:B:GLN:C  | 1:13:B:LEU:N | 3        | 1.99          |
| (1,264) | 1:67:B:ALA:N | 1:67:B:ALA:CA | 1:67:B:ALA:C  | 1:68:B:MET:N | 2        | 1.98          |

Continued on next page...

Continued from previous page...

| Key     | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Model ID | Violation (°) |
|---------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,263) | 1:67:A:ALA:N | 1:67:A:ALA:CA | 1:67:A:ALA:C  | 1:68:A:MET:N | 9        | 1.98          |
| (1,155) | 1:40:A:LEU:N | 1:40:A:LEU:CA | 1:40:A:LEU:C  | 1:41:A:LEU:N | 1        | 1.98          |
| (1,93)  | 1:24:A:ALA:C | 1:25:A:LEU:N  | 1:25:A:LEU:CA | 1:25:A:LEU:C | 10       | 1.98          |
| (1,71)  | 1:19:A:SER:N | 1:19:A:SER:CA | 1:19:A:SER:C  | 1:20:A:HIS:N | 5        | 1.98          |
| (1,63)  | 1:17:A:TYR:N | 1:17:A:TYR:CA | 1:17:A:TYR:C  | 1:18:A:VAL:N | 6        | 1.98          |
| (1,291) | 1:74:A:ALA:N | 1:74:A:ALA:CA | 1:74:A:ALA:C  | 1:75:A:HIS:N | 8        | 1.96          |
| (1,280) | 1:71:B:GLY:N | 1:71:B:GLY:CA | 1:71:B:GLY:C  | 1:72:B:ILE:N | 10       | 1.96          |
| (1,88)  | 1:23:B:HIS:N | 1:23:B:HIS:CA | 1:23:B:HIS:C  | 1:24:B:ALA:N | 3        | 1.96          |
| (1,87)  | 1:23:A:HIS:N | 1:23:A:HIS:CA | 1:23:A:HIS:C  | 1:24:A:ALA:N | 3        | 1.96          |
| (1,294) | 1:74:B:ALA:C | 1:75:B:HIS:N  | 1:75:B:HIS:CA | 1:75:B:HIS:C | 9        | 1.95          |
| (1,293) | 1:74:A:ALA:C | 1:75:A:HIS:N  | 1:75:A:HIS:CA | 1:75:A:HIS:C | 6        | 1.95          |
| (1,294) | 1:74:B:ALA:C | 1:75:B:HIS:N  | 1:75:B:HIS:CA | 1:75:B:HIS:C | 1        | 1.94          |
| (1,156) | 1:40:B:LEU:N | 1:40:B:LEU:CA | 1:40:B:LEU:C  | 1:41:B:LEU:N | 1        | 1.93          |
| (1,264) | 1:67:B:ALA:N | 1:67:B:ALA:CA | 1:67:B:ALA:C  | 1:68:B:MET:N | 9        | 1.92          |
| (1,152) | 1:39:B:ALA:N | 1:39:B:ALA:CA | 1:39:B:ALA:C  | 1:40:B:LEU:N | 1        | 1.92          |
| (1,293) | 1:74:A:ALA:C | 1:75:A:HIS:N  | 1:75:A:HIS:CA | 1:75:A:HIS:C | 5        | 1.91          |
| (1,249) | 1:63:A:LEU:C | 1:64:A:MET:N  | 1:64:A:MET:CA | 1:64:A:MET:C | 7        | 1.91          |
| (1,197) | 1:50:A:LYS:C | 1:51:A:ASN:N  | 1:51:A:ASN:CA | 1:51:A:ASN:C | 4        | 1.9           |
| (1,294) | 1:74:B:ALA:C | 1:75:B:HIS:N  | 1:75:B:HIS:CA | 1:75:B:HIS:C | 6        | 1.89          |
| (1,219) | 1:56:A:VAL:N | 1:56:A:VAL:CA | 1:56:A:VAL:C  | 1:57:A:GLY:N | 1        | 1.89          |
| (1,2)   | 1:1:B:MET:N  | 1:1:B:MET:CA  | 1:1:B:MET:C   | 1:2:B:GLY:N  | 5        | 1.89          |
| (1,263) | 1:67:A:ALA:N | 1:67:A:ALA:CA | 1:67:A:ALA:C  | 1:68:A:MET:N | 8        | 1.88          |
| (1,294) | 1:74:B:ALA:C | 1:75:B:HIS:N  | 1:75:B:HIS:CA | 1:75:B:HIS:C | 3        | 1.87          |
| (1,181) | 1:46:A:GLY:C | 1:47:A:ILE:N  | 1:47:A:ILE:CA | 1:47:A:ILE:C | 7        | 1.87          |
| (1,180) | 1:46:B:GLY:N | 1:46:B:GLY:CA | 1:46:B:GLY:C  | 1:47:B:ILE:N | 9        | 1.87          |
| (1,72)  | 1:19:B:SER:N | 1:19:B:SER:CA | 1:19:B:SER:C  | 1:20:B:HIS:N | 5        | 1.87          |
| (1,279) | 1:71:A:GLY:N | 1:71:A:GLY:CA | 1:71:A:GLY:C  | 1:72:A:ILE:N | 10       | 1.86          |
| (1,143) | 1:37:A:PHE:N | 1:37:A:PHE:CA | 1:37:A:PHE:C  | 1:38:A:ILE:N | 7        | 1.86          |
| (1,181) | 1:46:A:GLY:C | 1:47:A:ILE:N  | 1:47:A:ILE:CA | 1:47:A:ILE:C | 8        | 1.85          |
| (1,264) | 1:67:B:ALA:N | 1:67:B:ALA:CA | 1:67:B:ALA:C  | 1:68:B:MET:N | 8        | 1.82          |
| (1,181) | 1:46:A:GLY:C | 1:47:A:ILE:N  | 1:47:A:ILE:CA | 1:47:A:ILE:C | 4        | 1.82          |
| (1,107) | 1:28:A:SER:N | 1:28:A:SER:CA | 1:28:A:SER:C  | 1:29:A:LEU:N | 8        | 1.82          |
| (1,152) | 1:39:B:ALA:N | 1:39:B:ALA:CA | 1:39:B:ALA:C  | 1:40:B:LEU:N | 8        | 1.81          |
| (1,1)   | 1:1:A:MET:N  | 1:1:A:MET:CA  | 1:1:A:MET:C   | 1:2:A:GLY:N  | 5        | 1.81          |
| (1,23)  | 1:6:A:PRO:C  | 1:7:A:LEU:N   | 1:7:A:LEU:CA  | 1:7:A:LEU:C  | 4        | 1.8           |
| (1,108) | 1:28:B:SER:N | 1:28:B:SER:CA | 1:28:B:SER:C  | 1:29:B:LEU:N | 8        | 1.79          |
| (1,220) | 1:56:B:VAL:N | 1:56:B:VAL:CA | 1:56:B:VAL:C  | 1:57:B:GLY:N | 1        | 1.78          |
| (1,293) | 1:74:A:ALA:C | 1:75:A:HIS:N  | 1:75:A:HIS:CA | 1:75:A:HIS:C | 3        | 1.76          |
| (1,282) | 1:71:B:GLY:C | 1:72:B:ILE:N  | 1:72:B:ILE:CA | 1:72:B:ILE:C | 1        | 1.75          |
| (1,86)  | 1:22:B:GLU:C | 1:23:B:HIS:N  | 1:23:B:HIS:CA | 1:23:B:HIS:C | 10       | 1.75          |
| (1,281) | 1:71:A:GLY:C | 1:72:A:ILE:N  | 1:72:A:ILE:CA | 1:72:A:ILE:C | 1        | 1.74          |
| (1,280) | 1:71:B:GLY:N | 1:71:B:GLY:CA | 1:71:B:GLY:C  | 1:72:B:ILE:N | 1        | 1.73          |
| (1,63)  | 1:17:A:TYR:N | 1:17:A:TYR:CA | 1:17:A:TYR:C  | 1:18:A:VAL:N | 8        | 1.73          |
| (1,24)  | 1:6:B:PRO:C  | 1:7:B:LEU:N   | 1:7:B:LEU:CA  | 1:7:B:LEU:C  | 4        | 1.73          |
| (1,64)  | 1:17:B:TYR:N | 1:17:B:TYR:CA | 1:17:B:TYR:C  | 1:18:B:VAL:N | 9        | 1.72          |
| (1,63)  | 1:17:A:TYR:N | 1:17:A:TYR:CA | 1:17:A:TYR:C  | 1:18:A:VAL:N | 9        | 1.72          |
| (1,279) | 1:71:A:GLY:N | 1:71:A:GLY:CA | 1:71:A:GLY:C  | 1:72:A:ILE:N | 9        | 1.71          |
| (1,197) | 1:50:A:LYS:C | 1:51:A:ASN:N  | 1:51:A:ASN:CA | 1:51:A:ASN:C | 8        | 1.71          |
| (1,182) | 1:46:B:GLY:C | 1:47:B:ILE:N  | 1:47:B:ILE:CA | 1:47:B:ILE:C | 8        | 1.71          |
| (1,64)  | 1:17:B:TYR:N | 1:17:B:TYR:CA | 1:17:B:TYR:C  | 1:18:B:VAL:N | 5        | 1.71          |
| (1,151) | 1:39:A:ALA:N | 1:39:A:ALA:CA | 1:39:A:ALA:C  | 1:40:A:LEU:N | 1        | 1.7           |

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| Key     | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Model ID | Violation (°) |
|---------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,38)  | 1:10:B:MET:N | 1:10:B:MET:CA | 1:10:B:MET:C  | 1:11:B:PRO:N | 6        | 1.7           |
| (1,37)  | 1:10:A:MET:N | 1:10:A:MET:CA | 1:10:A:MET:C  | 1:11:A:PRO:N | 6        | 1.7           |
| (1,280) | 1:71:B:GLY:N | 1:71:B:GLY:CA | 1:71:B:GLY:C  | 1:72:B:ILE:N | 9        | 1.69          |
| (1,85)  | 1:22:A:GLU:C | 1:23:A:HIS:N  | 1:23:A:HIS:CA | 1:23:A:HIS:C | 10       | 1.69          |
| (1,279) | 1:71:A:GLY:N | 1:71:A:GLY:CA | 1:71:A:GLY:C  | 1:72:A:ILE:N | 1        | 1.67          |
| (1,218) | 1:55:B:TRP:C | 1:56:B:VAL:N  | 1:56:B:VAL:CA | 1:56:B:VAL:C | 9        | 1.67          |
| (1,104) | 1:27:B:LEU:N | 1:27:B:LEU:CA | 1:27:B:LEU:C  | 1:28:B:SER:N | 5        | 1.66          |
| (1,64)  | 1:17:B:TYR:N | 1:17:B:TYR:CA | 1:17:B:TYR:C  | 1:18:B:VAL:N | 8        | 1.65          |
| (1,282) | 1:71:B:GLY:C | 1:72:B:ILE:N  | 1:72:B:ILE:CA | 1:72:B:ILE:C | 5        | 1.64          |
| (1,6)   | 1:2:B:GLY:N  | 1:2:B:GLY:CA  | 1:2:B:GLY:C   | 1:3:B:LEU:N  | 8        | 1.64          |
| (1,220) | 1:56:B:VAL:N | 1:56:B:VAL:CA | 1:56:B:VAL:C  | 1:57:B:GLY:N | 7        | 1.63          |
| (1,219) | 1:56:A:VAL:N | 1:56:A:VAL:CA | 1:56:A:VAL:C  | 1:57:A:GLY:N | 7        | 1.63          |
| (1,103) | 1:27:A:LEU:N | 1:27:A:LEU:CA | 1:27:A:LEU:C  | 1:28:A:SER:N | 5        | 1.63          |
| (1,87)  | 1:23:A:HIS:N | 1:23:A:HIS:CA | 1:23:A:HIS:C  | 1:24:A:ALA:N | 9        | 1.63          |
| (1,190) | 1:48:B:TYR:C | 1:49:B:HIS:N  | 1:49:B:HIS:CA | 1:49:B:HIS:C | 3        | 1.62          |
| (1,5)   | 1:2:A:GLY:N  | 1:2:A:GLY:CA  | 1:2:A:GLY:C   | 1:3:A:LEU:N  | 8        | 1.62          |
| (1,217) | 1:55:A:TRP:C | 1:56:A:VAL:N  | 1:56:A:VAL:CA | 1:56:A:VAL:C | 9        | 1.61          |
| (1,144) | 1:37:B:PHE:N | 1:37:B:PHE:CA | 1:37:B:PHE:C  | 1:38:B:ILE:N | 7        | 1.61          |
| (1,88)  | 1:23:B:HIS:N | 1:23:B:HIS:CA | 1:23:B:HIS:C  | 1:24:B:ALA:N | 9        | 1.6           |
| (1,42)  | 1:11:B:PRO:C | 1:12:B:GLN:N  | 1:12:B:GLN:CA | 1:12:B:GLN:C | 4        | 1.6           |
| (1,87)  | 1:23:A:HIS:N | 1:23:A:HIS:CA | 1:23:A:HIS:C  | 1:24:A:ALA:N | 2        | 1.59          |
| (1,70)  | 1:18:B:VAL:C | 1:19:B:SER:N  | 1:19:B:SER:CA | 1:19:B:SER:C | 9        | 1.59          |
| (1,308) | 1:78:B:GLY:N | 1:78:B:GLY:CA | 1:78:B:GLY:C  | 1:79:B:THR:N | 4        | 1.58          |
| (1,263) | 1:67:A:ALA:N | 1:67:A:ALA:CA | 1:67:A:ALA:C  | 1:68:A:MET:N | 7        | 1.58          |
| (1,189) | 1:48:A:TYR:C | 1:49:A:HIS:N  | 1:49:A:HIS:CA | 1:49:A:HIS:C | 3        | 1.58          |
| (1,88)  | 1:23:B:HIS:N | 1:23:B:HIS:CA | 1:23:B:HIS:C  | 1:24:B:ALA:N | 2        | 1.58          |
| (1,192) | 1:49:B:HIS:N | 1:49:B:HIS:CA | 1:49:B:HIS:C  | 1:50:B:LYS:N | 9        | 1.57          |
| (1,191) | 1:49:A:HIS:N | 1:49:A:HIS:CA | 1:49:A:HIS:C  | 1:50:A:LYS:N | 9        | 1.57          |
| (1,63)  | 1:17:A:TYR:N | 1:17:A:TYR:CA | 1:17:A:TYR:C  | 1:18:A:VAL:N | 5        | 1.57          |
| (1,261) | 1:66:A:VAL:C | 1:67:A:ALA:N  | 1:67:A:ALA:CA | 1:67:A:ALA:C | 1        | 1.56          |
| (1,110) | 1:28:B:SER:C | 1:29:B:LEU:N  | 1:29:B:LEU:CA | 1:29:B:LEU:C | 5        | 1.55          |
| (1,72)  | 1:19:B:SER:N | 1:19:B:SER:CA | 1:19:B:SER:C  | 1:20:B:HIS:N | 9        | 1.55          |
| (1,71)  | 1:19:A:SER:N | 1:19:A:SER:CA | 1:19:A:SER:C  | 1:20:A:HIS:N | 9        | 1.55          |
| (1,262) | 1:66:B:VAL:C | 1:67:B:ALA:N  | 1:67:B:ALA:CA | 1:67:B:ALA:C | 1        | 1.53          |
| (1,43)  | 1:12:A:GLN:N | 1:12:A:GLN:CA | 1:12:A:GLN:C  | 1:13:A:LEU:N | 10       | 1.52          |
| (1,198) | 1:50:B:LYS:C | 1:51:B:ASN:N  | 1:51:B:ASN:CA | 1:51:B:ASN:C | 8        | 1.5           |
| (1,69)  | 1:18:A:VAL:C | 1:19:A:SER:N  | 1:19:A:SER:CA | 1:19:A:SER:C | 9        | 1.5           |
| (1,307) | 1:78:A:GLY:N | 1:78:A:GLY:CA | 1:78:A:GLY:C  | 1:79:A:THR:N | 5        | 1.49          |
| (1,143) | 1:37:A:PHE:N | 1:37:A:PHE:CA | 1:37:A:PHE:C  | 1:38:A:ILE:N | 1        | 1.49          |
| (1,279) | 1:71:A:GLY:N | 1:71:A:GLY:CA | 1:71:A:GLY:C  | 1:72:A:ILE:N | 7        | 1.48          |
| (1,177) | 1:45:A:TYR:C | 1:46:A:GLY:N  | 1:46:A:GLY:CA | 1:46:A:GLY:C | 6        | 1.48          |
| (1,134) | 1:34:B:LEU:C | 1:35:B:TYR:N  | 1:35:B:TYR:CA | 1:35:B:TYR:C | 2        | 1.48          |
| (1,308) | 1:78:B:GLY:N | 1:78:B:GLY:CA | 1:78:B:GLY:C  | 1:79:B:THR:N | 5        | 1.47          |
| (1,192) | 1:49:B:HIS:N | 1:49:B:HIS:CA | 1:49:B:HIS:C  | 1:50:B:LYS:N | 7        | 1.47          |
| (1,41)  | 1:11:A:PRO:C | 1:12:A:GLN:N  | 1:12:A:GLN:CA | 1:12:A:GLN:C | 4        | 1.46          |
| (1,280) | 1:71:B:GLY:N | 1:71:B:GLY:CA | 1:71:B:GLY:C  | 1:72:B:ILE:N | 7        | 1.45          |
| (1,133) | 1:34:A:LEU:C | 1:35:A:TYR:N  | 1:35:A:TYR:CA | 1:35:A:TYR:C | 2        | 1.45          |
| (1,180) | 1:46:B:GLY:N | 1:46:B:GLY:CA | 1:46:B:GLY:C  | 1:47:B:ILE:N | 8        | 1.44          |
| (1,41)  | 1:11:A:PRO:C | 1:12:A:GLN:N  | 1:12:A:GLN:CA | 1:12:A:GLN:C | 9        | 1.44          |
| (1,281) | 1:71:A:GLY:C | 1:72:A:ILE:N  | 1:72:A:ILE:CA | 1:72:A:ILE:C | 5        | 1.43          |
| (1,144) | 1:37:B:PHE:N | 1:37:B:PHE:CA | 1:37:B:PHE:C  | 1:38:B:ILE:N | 1        | 1.43          |

Continued on next page...

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| Key     | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Model ID | Violation (°) |
|---------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,109) | 1:28:A:SER:C | 1:29:A:LEU:N  | 1:29:A:LEU:CA | 1:29:A:LEU:C | 5        | 1.43          |
| (1,44)  | 1:12:B:GLN:N | 1:12:B:GLN:CA | 1:12:B:GLN:C  | 1:13:B:LEU:N | 10       | 1.43          |
| (1,191) | 1:49:A:HIS:N | 1:49:A:HIS:CA | 1:49:A:HIS:C  | 1:50:A:LYS:N | 7        | 1.41          |
| (1,307) | 1:78:A:GLY:N | 1:78:A:GLY:CA | 1:78:A:GLY:C  | 1:79:A:THR:N | 4        | 1.4           |
| (1,282) | 1:71:B:GLY:C | 1:72:B:ILE:N  | 1:72:B:ILE:CA | 1:72:B:ILE:C | 7        | 1.4           |
| (1,179) | 1:46:A:GLY:N | 1:46:A:GLY:CA | 1:46:A:GLY:C  | 1:47:A:ILE:N | 8        | 1.4           |
| (1,42)  | 1:11:B:PRO:C | 1:12:B:GLN:N  | 1:12:B:GLN:CA | 1:12:B:GLN:C | 9        | 1.4           |
| (1,264) | 1:67:B:ALA:N | 1:67:B:ALA:CA | 1:67:B:ALA:C  | 1:68:B:MET:N | 7        | 1.39          |
| (1,230) | 1:58:B:ASN:C | 1:59:B:CYS:N  | 1:59:B:CYS:CA | 1:59:B:CYS:C | 7        | 1.39          |
| (1,49)  | 1:13:A:LEU:C | 1:14:A:TYR:N  | 1:14:A:TYR:CA | 1:14:A:TYR:C | 7        | 1.39          |
| (1,179) | 1:46:A:GLY:N | 1:46:A:GLY:CA | 1:46:A:GLY:C  | 1:47:A:ILE:N | 4        | 1.38          |
| (1,178) | 1:45:B:TYR:C | 1:46:B:GLY:N  | 1:46:B:GLY:CA | 1:46:B:GLY:C | 6        | 1.38          |
| (1,60)  | 1:16:B:LEU:N | 1:16:B:LEU:CA | 1:16:B:LEU:C  | 1:17:B:TYR:N | 5        | 1.37          |
| (1,50)  | 1:13:B:LEU:C | 1:14:B:TYR:N  | 1:14:B:TYR:CA | 1:14:B:TYR:C | 7        | 1.36          |
| (1,307) | 1:78:A:GLY:N | 1:78:A:GLY:CA | 1:78:A:GLY:C  | 1:79:A:THR:N | 1        | 1.35          |
| (1,281) | 1:71:A:GLY:C | 1:72:A:ILE:N  | 1:72:A:ILE:CA | 1:72:A:ILE:C | 7        | 1.34          |
| (1,167) | 1:43:A:THR:N | 1:43:A:THR:CA | 1:43:A:THR:C  | 1:44:A:ILE:N | 8        | 1.34          |
| (1,229) | 1:58:A:ASN:C | 1:59:A:CYS:N  | 1:59:A:CYS:CA | 1:59:A:CYS:C | 7        | 1.33          |
| (1,107) | 1:28:A:SER:N | 1:28:A:SER:CA | 1:28:A:SER:C  | 1:29:A:LEU:N | 2        | 1.32          |
| (1,98)  | 1:25:B:LEU:C | 1:26:B:GLY:N  | 1:26:B:GLY:CA | 1:26:B:GLY:C | 9        | 1.32          |
| (1,69)  | 1:18:A:VAL:C | 1:19:A:SER:N  | 1:19:A:SER:CA | 1:19:A:SER:C | 6        | 1.31          |
| (1,24)  | 1:6:B:PRO:C  | 1:7:B:LEU:N   | 1:7:B:LEU:CA  | 1:7:B:LEU:C  | 1        | 1.31          |
| (1,24)  | 1:6:B:PRO:C  | 1:7:B:LEU:N   | 1:7:B:LEU:CA  | 1:7:B:LEU:C  | 9        | 1.31          |
| (1,263) | 1:67:A:ALA:N | 1:67:A:ALA:CA | 1:67:A:ALA:C  | 1:68:A:MET:N | 6        | 1.3           |
| (1,59)  | 1:16:A:LEU:N | 1:16:A:LEU:CA | 1:16:A:LEU:C  | 1:17:A:TYR:N | 5        | 1.3           |
| (1,23)  | 1:6:A:PRO:C  | 1:7:A:LEU:N   | 1:7:A:LEU:CA  | 1:7:A:LEU:C  | 1        | 1.3           |
| (1,308) | 1:78:B:GLY:N | 1:78:B:GLY:CA | 1:78:B:GLY:C  | 1:79:B:THR:N | 1        | 1.29          |
| (1,97)  | 1:25:A:LEU:C | 1:26:A:GLY:N  | 1:26:A:GLY:CA | 1:26:A:GLY:C | 8        | 1.29          |
| (1,264) | 1:67:B:ALA:N | 1:67:B:ALA:CA | 1:67:B:ALA:C  | 1:68:B:MET:N | 6        | 1.28          |
| (1,229) | 1:58:A:ASN:C | 1:59:A:CYS:N  | 1:59:A:CYS:CA | 1:59:A:CYS:C | 8        | 1.28          |
| (1,121) | 1:31:A:THR:C | 1:32:A:TRP:N  | 1:32:A:TRP:CA | 1:32:A:TRP:C | 2        | 1.28          |
| (1,23)  | 1:6:A:PRO:C  | 1:7:A:LEU:N   | 1:7:A:LEU:CA  | 1:7:A:LEU:C  | 9        | 1.27          |
| (1,198) | 1:50:B:LYS:C | 1:51:B:ASN:N  | 1:51:B:ASN:CA | 1:51:B:ASN:C | 5        | 1.26          |
| (1,122) | 1:31:B:THR:C | 1:32:B:TRP:N  | 1:32:B:TRP:CA | 1:32:B:TRP:C | 2        | 1.26          |
| (1,98)  | 1:25:B:LEU:C | 1:26:B:GLY:N  | 1:26:B:GLY:CA | 1:26:B:GLY:C | 8        | 1.26          |
| (1,70)  | 1:18:B:VAL:C | 1:19:B:SER:N  | 1:19:B:SER:CA | 1:19:B:SER:C | 6        | 1.26          |
| (1,232) | 1:59:B:CYS:N | 1:59:B:CYS:CA | 1:59:B:CYS:C  | 1:60:B:LEU:N | 10       | 1.22          |
| (1,97)  | 1:25:A:LEU:C | 1:26:A:GLY:N  | 1:26:A:GLY:CA | 1:26:A:GLY:C | 9        | 1.22          |
| (1,47)  | 1:13:A:LEU:N | 1:13:A:LEU:CA | 1:13:A:LEU:C  | 1:14:A:TYR:N | 6        | 1.22          |
| (1,6)   | 1:2:B:GLY:N  | 1:2:B:GLY:CA  | 1:2:B:GLY:C   | 1:3:B:LEU:N  | 2        | 1.22          |
| (1,303) | 1:77:A:GLY:N | 1:77:A:GLY:CA | 1:77:A:GLY:C  | 1:78:A:GLY:N | 4        | 1.21          |
| (1,231) | 1:59:A:CYS:N | 1:59:A:CYS:CA | 1:59:A:CYS:C  | 1:60:A:LEU:N | 10       | 1.2           |
| (1,59)  | 1:16:A:LEU:N | 1:16:A:LEU:CA | 1:16:A:LEU:C  | 1:17:A:TYR:N | 2        | 1.2           |
| (1,197) | 1:50:A:LYS:C | 1:51:A:ASN:N  | 1:51:A:ASN:CA | 1:51:A:ASN:C | 5        | 1.19          |
| (1,108) | 1:28:B:SER:N | 1:28:B:SER:CA | 1:28:B:SER:C  | 1:29:B:LEU:N | 2        | 1.18          |
| (1,48)  | 1:13:B:LEU:N | 1:13:B:LEU:CA | 1:13:B:LEU:C  | 1:14:B:TYR:N | 6        | 1.18          |
| (1,182) | 1:46:B:GLY:C | 1:47:B:ILE:N  | 1:47:B:ILE:CA | 1:47:B:ILE:C | 5        | 1.17          |
| (1,168) | 1:43:B:THR:N | 1:43:B:THR:CA | 1:43:B:THR:C  | 1:44:B:ILE:N | 8        | 1.17          |
| (1,42)  | 1:11:B:PRO:C | 1:12:B:GLN:N  | 1:12:B:GLN:CA | 1:12:B:GLN:C | 6        | 1.17          |
| (1,41)  | 1:11:A:PRO:C | 1:12:A:GLN:N  | 1:12:A:GLN:CA | 1:12:A:GLN:C | 6        | 1.17          |
| (1,26)  | 1:7:B:LEU:N  | 1:7:B:LEU:CA  | 1:7:B:LEU:C   | 1:8:B:ALA:N  | 1        | 1.17          |

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| Key     | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Model ID | Violation (°) |
|---------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,52)  | 1:14:B:TYR:N | 1:14:B:TYR:CA | 1:14:B:TYR:C  | 1:15:B:LYS:N | 10       | 1.16          |
| (1,275) | 1:70:A:VAL:N | 1:70:A:VAL:CA | 1:70:A:VAL:C  | 1:71:A:GLY:N | 8        | 1.15          |
| (1,191) | 1:49:A:HIS:N | 1:49:A:HIS:CA | 1:49:A:HIS:C  | 1:50:A:LYS:N | 10       | 1.15          |
| (1,89)  | 1:23:A:HIS:C | 1:24:A:ALA:N  | 1:24:A:ALA:CA | 1:24:A:ALA:C | 2        | 1.15          |
| (1,63)  | 1:17:A:TYR:N | 1:17:A:TYR:CA | 1:17:A:TYR:C  | 1:18:A:VAL:N | 4        | 1.15          |
| (1,60)  | 1:16:B:LEU:N | 1:16:B:LEU:CA | 1:16:B:LEU:C  | 1:17:B:TYR:N | 2        | 1.15          |
| (1,51)  | 1:14:A:TYR:N | 1:14:A:TYR:CA | 1:14:A:TYR:C  | 1:15:A:LYS:N | 10       | 1.15          |
| (1,25)  | 1:7:A:LEU:N  | 1:7:A:LEU:CA  | 1:7:A:LEU:C   | 1:8:A:ALA:N  | 1        | 1.15          |
| (1,230) | 1:58:B:ASN:C | 1:59:B:CYS:N  | 1:59:B:CYS:CA | 1:59:B:CYS:C | 8        | 1.14          |
| (1,181) | 1:46:A:GLY:C | 1:47:A:ILE:N  | 1:47:A:ILE:CA | 1:47:A:ILE:C | 5        | 1.14          |
| (1,162) | 1:41:B:LEU:C | 1:42:B:TRP:N  | 1:42:B:TRP:CA | 1:42:B:TRP:C | 6        | 1.14          |
| (1,277) | 1:70:A:VAL:C | 1:71:A:GLY:N  | 1:71:A:GLY:CA | 1:71:A:GLY:C | 7        | 1.12          |
| (1,49)  | 1:13:A:LEU:C | 1:14:A:TYR:N  | 1:14:A:TYR:CA | 1:14:A:TYR:C | 6        | 1.11          |
| (1,192) | 1:49:B:HIS:N | 1:49:B:HIS:CA | 1:49:B:HIS:C  | 1:50:B:LYS:N | 10       | 1.1           |
| (1,161) | 1:41:A:LEU:C | 1:42:A:TRP:N  | 1:42:A:TRP:CA | 1:42:A:TRP:C | 6        | 1.1           |
| (1,23)  | 1:6:A:PRO:C  | 1:7:A:LEU:N   | 1:7:A:LEU:CA  | 1:7:A:LEU:C  | 7        | 1.1           |
| (1,304) | 1:77:B:GLY:N | 1:77:B:GLY:CA | 1:77:B:GLY:C  | 1:78:B:GLY:N | 4        | 1.09          |
| (1,195) | 1:50:A:LYS:N | 1:50:A:LYS:CA | 1:50:A:LYS:C  | 1:51:A:ASN:N | 6        | 1.09          |
| (1,276) | 1:70:B:VAL:N | 1:70:B:VAL:CA | 1:70:B:VAL:C  | 1:71:B:GLY:N | 4        | 1.08          |
| (1,43)  | 1:12:A:GLN:N | 1:12:A:GLN:CA | 1:12:A:GLN:C  | 1:13:A:LEU:N | 7        | 1.08          |
| (1,188) | 1:48:B:TYR:N | 1:48:B:TYR:CA | 1:48:B:TYR:C  | 1:49:B:HIS:N | 8        | 1.07          |
| (1,64)  | 1:17:B:TYR:N | 1:17:B:TYR:CA | 1:17:B:TYR:C  | 1:18:B:VAL:N | 4        | 1.07          |
| (1,278) | 1:70:B:VAL:C | 1:71:B:GLY:N  | 1:71:B:GLY:CA | 1:71:B:GLY:C | 7        | 1.06          |
| (1,90)  | 1:23:B:HIS:C | 1:24:B:ALA:N  | 1:24:B:ALA:CA | 1:24:B:ALA:C | 2        | 1.06          |
| (1,70)  | 1:18:B:VAL:C | 1:19:B:SER:N  | 1:19:B:SER:CA | 1:19:B:SER:C | 4        | 1.06          |
| (1,50)  | 1:13:B:LEU:C | 1:14:B:TYR:N  | 1:14:B:TYR:CA | 1:14:B:TYR:C | 6        | 1.06          |
| (1,24)  | 1:6:B:PRO:C  | 1:7:B:LEU:N   | 1:7:B:LEU:CA  | 1:7:B:LEU:C  | 7        | 1.06          |
| (1,194) | 1:49:B:HIS:C | 1:50:B:LYS:N  | 1:50:B:LYS:CA | 1:50:B:LYS:C | 2        | 1.05          |
| (1,82)  | 1:21:B:SER:C | 1:22:B:GLU:N  | 1:22:B:GLU:CA | 1:22:B:GLU:C | 9        | 1.05          |
| (1,5)   | 1:2:A:GLY:N  | 1:2:A:GLY:CA  | 1:2:A:GLY:C   | 1:3:A:LEU:N  | 2        | 1.05          |
| (1,255) | 1:65:A:TYR:N | 1:65:A:TYR:CA | 1:65:A:TYR:C  | 1:66:A:VAL:N | 7        | 1.04          |
| (1,193) | 1:49:A:HIS:C | 1:50:A:LYS:N  | 1:50:A:LYS:CA | 1:50:A:LYS:C | 2        | 1.04          |
| (1,187) | 1:48:A:TYR:N | 1:48:A:TYR:CA | 1:48:A:TYR:C  | 1:49:A:HIS:N | 8        | 1.04          |
| (1,69)  | 1:18:A:VAL:C | 1:19:A:SER:N  | 1:19:A:SER:CA | 1:19:A:SER:C | 4        | 1.04          |
| (1,198) | 1:50:B:LYS:C | 1:51:B:ASN:N  | 1:51:B:ASN:CA | 1:51:B:ASN:C | 9        | 1.03          |
| (1,310) | 1:78:B:GLY:C | 1:79:B:THR:N  | 1:79:B:THR:CA | 1:79:B:THR:C | 9        | 1.02          |
| (1,262) | 1:66:B:VAL:C | 1:67:B:ALA:N  | 1:67:B:ALA:CA | 1:67:B:ALA:C | 6        | 1.02          |
| (1,256) | 1:65:B:TYR:N | 1:65:B:TYR:CA | 1:65:B:TYR:C  | 1:66:B:VAL:N | 7        | 1.02          |
| (1,229) | 1:58:A:ASN:C | 1:59:A:CYS:N  | 1:59:A:CYS:CA | 1:59:A:CYS:C | 6        | 1.02          |
| (1,197) | 1:50:A:LYS:C | 1:51:A:ASN:N  | 1:51:A:ASN:CA | 1:51:A:ASN:C | 9        | 1.02          |
| (1,196) | 1:50:B:LYS:N | 1:50:B:LYS:CA | 1:50:B:LYS:C  | 1:51:B:ASN:N | 8        | 1.02          |
| (1,70)  | 1:18:B:VAL:C | 1:19:B:SER:N  | 1:19:B:SER:CA | 1:19:B:SER:C | 8        | 1.02          |
| (1,261) | 1:66:A:VAL:C | 1:67:A:ALA:N  | 1:67:A:ALA:CA | 1:67:A:ALA:C | 6        | 1.01          |
| (1,220) | 1:56:B:VAL:N | 1:56:B:VAL:CA | 1:56:B:VAL:C  | 1:57:B:GLY:N | 2        | 1.01          |
| (1,81)  | 1:21:A:SER:C | 1:22:A:GLU:N  | 1:22:A:GLU:CA | 1:22:A:GLU:C | 9        | 1.01          |
| (1,7)   | 1:2:A:GLY:C  | 1:3:A:LEU:N   | 1:3:A:LEU:CA  | 1:3:A:LEU:C  | 10       | 1.0           |