



# Full wwPDB NMR Structure Validation Report ⓘ

Mar 26, 2026 – 04:18 PM UTC

PDB ID : 2N78 / pdb\_00002n78  
BMRB ID : 26649  
Title : NMR structure of IF1 from Pseudomonas aeruginosa  
Authors : Zhang, Y.  
Deposited on : 2015-09-04

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

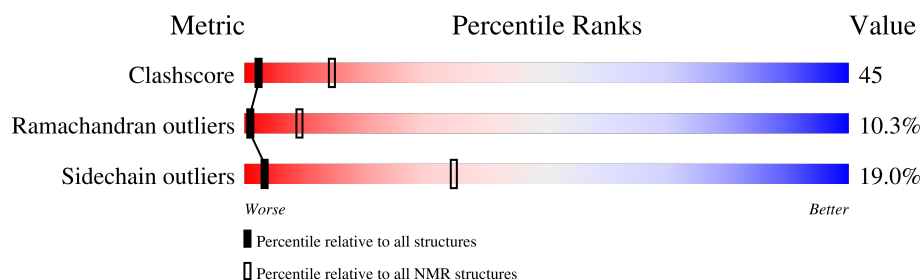
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 80%.

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     | 72     | <div> <div></div> <div>22%</div> <div>46%</div> <div>25%</div> <div>7%</div> </div> |

## 2 Ensemble composition and analysis

This entry contains 15 models. Model 7 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:6-A:72 (67)         | 1.21              | 7            |

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

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

The models can be grouped into 4 clusters and 2 single-model clusters were found.

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

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

There is only 1 type of molecule in this entry. The entry contains 1171 atoms, of which 590 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Translation initiation factor IF-1.

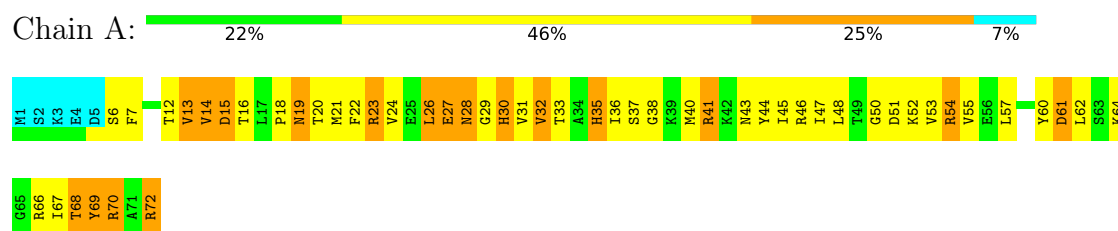
| Mol | Chain | Residues | Atoms |     |     |     |     |   | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|-------|
| 1   | A     | 72       | Total | C   | H   | N   | O   | S | 0     |
|     |       |          | 1171  | 362 | 590 | 105 | 110 | 4 |       |

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

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

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

- Molecule 1: Translation initiation factor IF-1

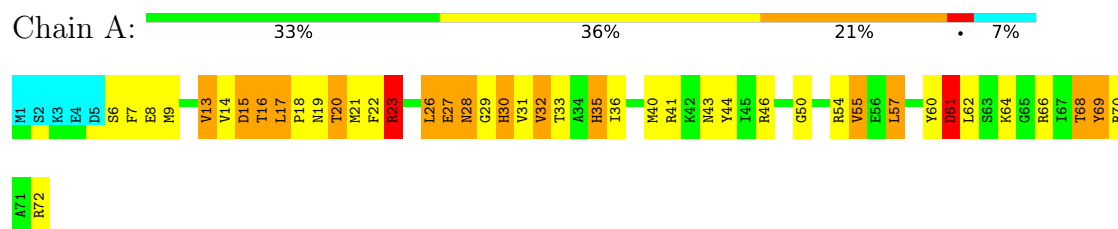


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

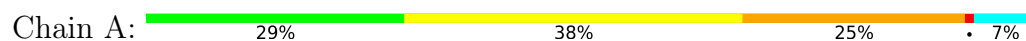
#### 4.2.1 Score per residue for model 1

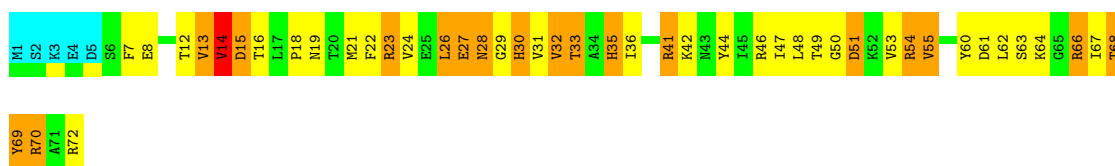
- Molecule 1: Translation initiation factor IF-1



#### 4.2.2 Score per residue for model 2

- Molecule 1: Translation initiation factor IF-1

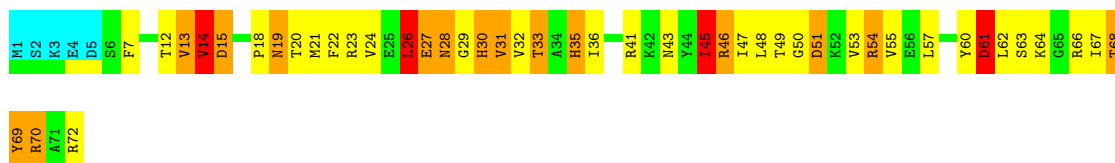




### 4.2.3 Score per residue for model 3

- Molecule 1: Translation initiation factor IF-1

Chain A: 29% 38% 21% 6% 7%



### 4.2.4 Score per residue for model 4

- Molecule 1: Translation initiation factor IF-1

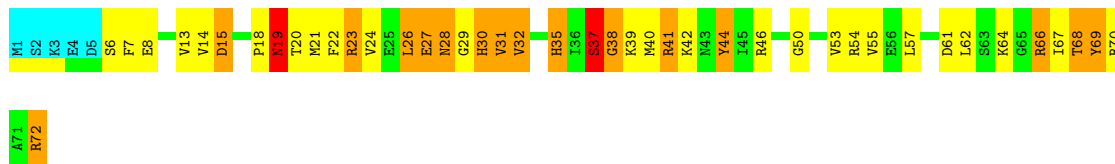
Chain A: 32% 31% 26% 7%



### 4.2.5 Score per residue for model 5

- Molecule 1: Translation initiation factor IF-1

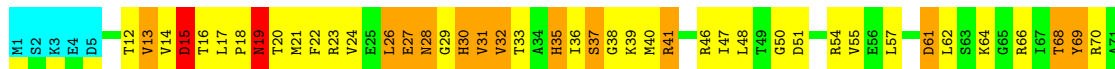
Chain A: 33% 35% 22% 7%



### 4.2.6 Score per residue for model 6

- Molecule 1: Translation initiation factor IF-1

Chain A: 32% 39% 19% 7%



R72

#### 4.2.7 Score per residue for model 7 (medoid)

- Molecule 1: Translation initiation factor IF-1

Chain A: 28% 40% 24% 7%



T68  
Y69  
R70  
A71  
R72

#### 4.2.8 Score per residue for model 8

- Molecule 1: Translation initiation factor IF-1

Chain A: 26% 39% 24% 7%

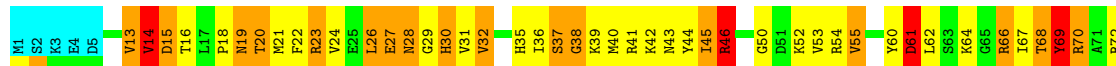


I67  
T68  
Y69  
R70  
A71  
R72

#### 4.2.9 Score per residue for model 9

- Molecule 1: Translation initiation factor IF-1

Chain A: 31% 33% 24% 6% 7%



#### 4.2.10 Score per residue for model 10

- Molecule 1: Translation initiation factor IF-1

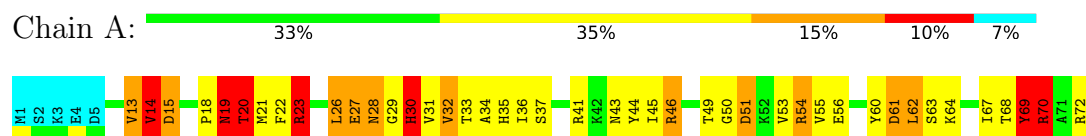
Chain A: 25% 31% 31% 7% 7%



I67  
T68  
Y69  
R70  
A71  
R72

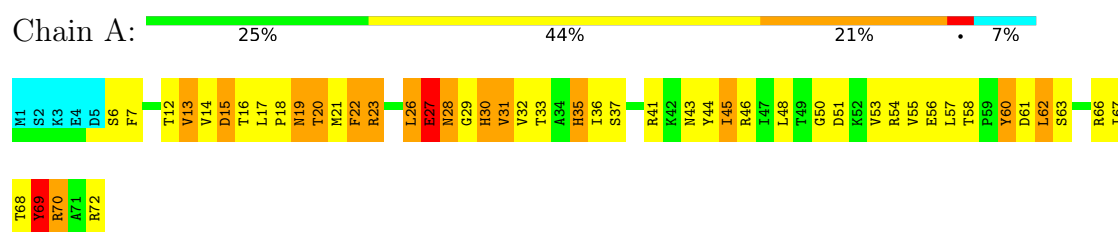
### 4.2.11 Score per residue for model 11

- Molecule 1: Translation initiation factor IF-1



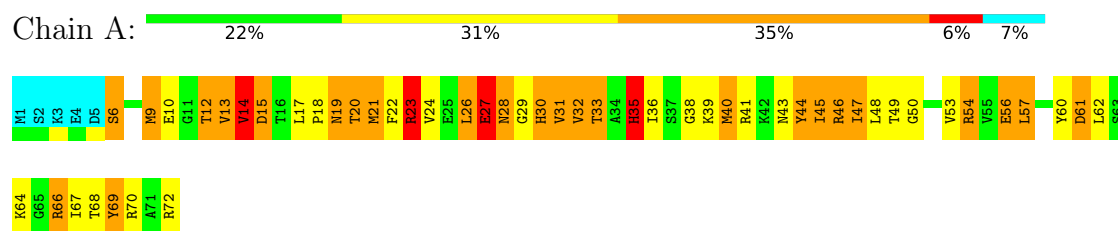
### 4.2.12 Score per residue for model 12

- Molecule 1: Translation initiation factor IF-1



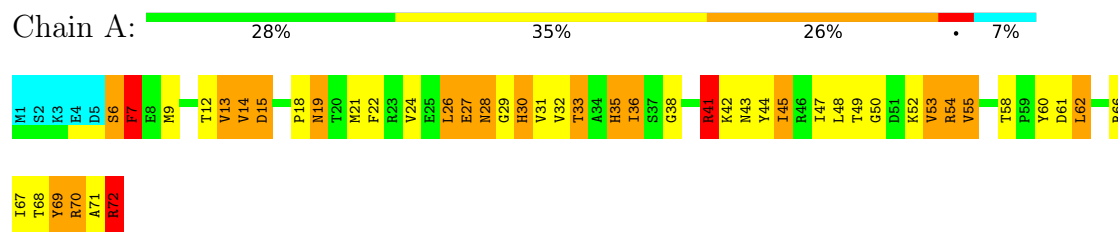
### 4.2.13 Score per residue for model 13

- Molecule 1: Translation initiation factor IF-1



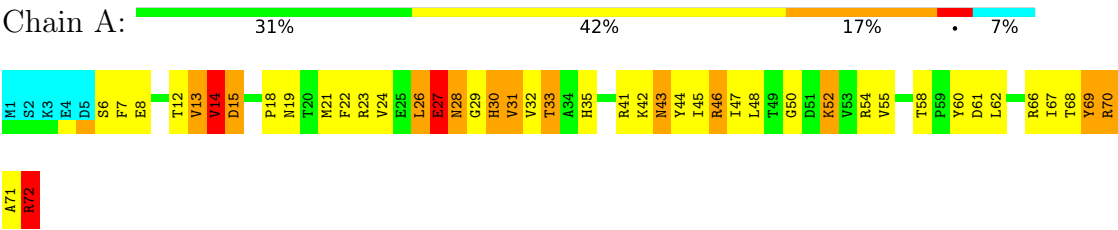
### 4.2.14 Score per residue for model 14

- Molecule 1: Translation initiation factor IF-1



4.2.15 Score per residue for model 15

● Molecule 1: Translation initiation factor IF-1



## 5 Refinement protocol and experimental data overview

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

Of the 50 calculated structures, 15 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 solution |         |
| X-PLOR NIH    | refinement         |         |

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

|                                              |                |
|----------------------------------------------|----------------|
| Chemical shift file(s)                       | working_cs.cif |
| Number of chemical shift lists               | 1              |
| Total number of shifts                       | 799            |
| Number of shifts mapped to atoms             | 799            |
| Number of unparsed shifts                    | 0              |
| Number of shifts with mapping errors         | 0              |
| Number of shifts with mapping warnings       | 0              |
| Assignment completeness (well-defined parts) | 80%            |

## 6 Model quality

### 6.1 Standard geometry

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

| Mol | Chain | Bond lengths |                      | Bond angles |                      |
|-----|-------|--------------|----------------------|-------------|----------------------|
|     |       | RMSZ         | #Z>5                 | RMSZ        | #Z>5                 |
| 1   | A     | 1.66±0.01    | 5±1/549 ( 1.0± 0.1%) | 1.63±0.02   | 4±1/737 ( 0.6± 0.1%) |
| All | All   | 1.66         | 82/8235 ( 1.0%)      | 1.63        | 63/11055 ( 0.6%)     |

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

| Mol | Chain | Chirality | Planarity |
|-----|-------|-----------|-----------|
| 1   | A     | 0.0±0.0   | 6.4±0.6   |
| All | All   | 0         | 96        |

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

| Mol | Chain | Res | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) | Models |       |
|-----|-------|-----|------|---------|--------|-------------|----------|--------|-------|
|     |       |     |      |         |        |             |          | Worst  | Total |
| 1   | A     | 30  | HIS  | CG-ND1  | -11.99 | 1.25        | 1.38     | 14     | 15    |
| 1   | A     | 35  | HIS  | CG-ND1  | -11.99 | 1.25        | 1.38     | 4      | 15    |
| 1   | A     | 13  | VAL  | N-CA    | 6.83   | 1.55        | 1.46     | 13     | 14    |
| 1   | A     | 30  | HIS  | N-CA    | 5.54   | 1.52        | 1.45     | 7      | 3     |
| 1   | A     | 30  | HIS  | ND1-CE1 | -5.45  | 1.27        | 1.32     | 7      | 15    |
| 1   | A     | 35  | HIS  | ND1-CE1 | -5.41  | 1.27        | 1.32     | 15     | 15    |
| 1   | A     | 69  | TYR  | N-CA    | 5.32   | 1.53        | 1.46     | 9      | 4     |
| 1   | A     | 24  | VAL  | C-N     | -5.16  | 1.26        | 1.33     | 10     | 1     |

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

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) | Models |       |
|-----|-------|-----|------|-------------|-------|-------------|----------|--------|-------|
|     |       |     |      |             |       |             |          | Worst  | Total |
| 1   | A     | 26  | LEU  | N-CA-C      | -7.88 | 101.86      | 112.26   | 6      | 15    |
| 1   | A     | 35  | HIS  | CE1-NE2-CD2 | -7.58 | 101.42      | 109.00   | 7      | 15    |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) | Models |       |
|-----|-------|-----|------|-------------|-------|-------------|----------|--------|-------|
|     |       |     |      |             |       |             |          | Worst  | Total |
| 1   | A     | 30  | HIS  | CE1-NE2-CD2 | -7.51 | 101.48      | 109.00   | 6      | 15    |
| 1   | A     | 13  | VAL  | N-CA-C      | 6.18  | 115.62      | 106.85   | 7      | 11    |
| 1   | A     | 44  | TYR  | CB-CA-C     | -5.43 | 108.73      | 115.89   | 7      | 1     |
| 1   | A     | 30  | HIS  | CA-CB-CG    | -5.35 | 108.45      | 113.80   | 7      | 1     |
| 1   | A     | 13  | VAL  | CB-CA-C     | -5.17 | 104.81      | 111.53   | 7      | 3     |
| 1   | A     | 22  | PHE  | CA-CB-CG    | -5.15 | 108.65      | 113.80   | 12     | 1     |
| 1   | A     | 53  | VAL  | N-CA-CB     | -5.13 | 106.70      | 112.45   | 14     | 1     |

There are no chirality outliers.

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

| Mol | Chain | Res | Type | Group     | Models (Total) |
|-----|-------|-----|------|-----------|----------------|
| 1   | A     | 70  | ARG  | Sidechain | 15             |
| 1   | A     | 23  | ARG  | Sidechain | 14             |
| 1   | A     | 41  | ARG  | Sidechain | 14             |
| 1   | A     | 54  | ARG  | Sidechain | 14             |
| 1   | A     | 46  | ARG  | Sidechain | 13             |
| 1   | A     | 66  | ARG  | Sidechain | 13             |
| 1   | A     | 72  | ARG  | Sidechain | 13             |

## 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     | 541   | 554      | 554      | 49±5    |
| All | All   | 8115  | 8310     | 8310     | 740     |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 45.

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

| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:62:LEU:HD12 | 1:A:62:LEU:H    | 1.00     | 1.16        | 4      | 8     |
| 1:A:48:LEU:H    | 1:A:48:LEU:HD23 | 0.97     | 1.17        | 2      | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:47:ILE:N    | 1:A:47:ILE:HD12 | 0.88     | 1.84        | 13     | 1     |
| 1:A:27:GLU:C    | 1:A:29:GLY:H    | 0.86     | 1.79        | 8      | 15    |
| 1:A:32:VAL:HG12 | 1:A:33:THR:H    | 0.76     | 1.39        | 12     | 13    |
| 1:A:32:VAL:HG12 | 1:A:33:THR:N    | 0.75     | 1.96        | 12     | 11    |
| 1:A:40:MET:SD   | 1:A:41:ARG:N    | 0.73     | 2.61        | 13     | 1     |
| 1:A:54:ARG:CZ   | 1:A:69:TYR:CD2  | 0.73     | 2.72        | 14     | 1     |
| 1:A:43:ASN:C    | 1:A:44:TYR:CD1  | 0.73     | 2.67        | 15     | 2     |
| 1:A:26:LEU:O    | 1:A:28:ASN:N    | 0.72     | 2.23        | 13     | 15    |
| 1:A:27:GLU:C    | 1:A:29:GLY:N    | 0.71     | 2.47        | 8      | 15    |
| 1:A:24:VAL:HG11 | 1:A:55:VAL:HG21 | 0.71     | 1.61        | 5      | 5     |
| 1:A:48:LEU:HD23 | 1:A:48:LEU:N    | 0.71     | 1.99        | 2      | 2     |
| 1:A:26:LEU:C    | 1:A:28:ASN:H    | 0.70     | 1.94        | 4      | 15    |
| 1:A:21:MET:C    | 1:A:22:PHE:CD1  | 0.70     | 2.69        | 2      | 11    |
| 1:A:19:ASN:HD22 | 1:A:19:ASN:N    | 0.69     | 1.84        | 11     | 2     |
| 1:A:53:VAL:HG12 | 1:A:70:ARG:HB3  | 0.69     | 1.64        | 3      | 6     |
| 1:A:7:PHE:N     | 1:A:7:PHE:CD1   | 0.69     | 2.60        | 10     | 2     |
| 1:A:62:LEU:H    | 1:A:62:LEU:CD1  | 0.69     | 1.96        | 4      | 5     |
| 1:A:51:ASP:N    | 1:A:51:ASP:OD1  | 0.68     | 2.26        | 4      | 3     |
| 1:A:18:PRO:C    | 1:A:19:ASN:ND2  | 0.68     | 2.52        | 11     | 2     |
| 1:A:19:ASN:C    | 1:A:21:MET:SD   | 0.68     | 2.77        | 13     | 1     |
| 1:A:26:LEU:HD12 | 1:A:32:VAL:CG2  | 0.67     | 2.18        | 4      | 9     |
| 1:A:47:ILE:N    | 1:A:47:ILE:CD1  | 0.66     | 2.57        | 13     | 1     |
| 1:A:41:ARG:NH2  | 1:A:70:ARG:NH2  | 0.66     | 2.43        | 14     | 1     |
| 1:A:47:ILE:HD11 | 1:A:51:ASP:OD2  | 0.66     | 1.91        | 2      | 1     |
| 1:A:47:ILE:O    | 1:A:47:ILE:HG23 | 0.66     | 1.90        | 8      | 2     |
| 1:A:43:ASN:C    | 1:A:45:ILE:N    | 0.66     | 2.53        | 9      | 2     |
| 1:A:32:VAL:CG1  | 1:A:33:THR:N    | 0.65     | 2.59        | 15     | 5     |
| 1:A:21:MET:C    | 1:A:22:PHE:CG   | 0.65     | 2.74        | 12     | 13    |
| 1:A:26:LEU:C    | 1:A:28:ASN:N    | 0.65     | 2.54        | 7      | 15    |
| 1:A:17:LEU:CD1  | 1:A:22:PHE:C    | 0.64     | 2.70        | 13     | 2     |
| 1:A:48:LEU:H    | 1:A:48:LEU:CD2  | 0.64     | 2.01        | 2      | 1     |
| 1:A:26:LEU:HD12 | 1:A:32:VAL:HG23 | 0.64     | 1.68        | 4      | 4     |
| 1:A:15:ASP:OD1  | 1:A:23:ARG:NH2  | 0.64     | 2.31        | 9      | 1     |
| 1:A:40:MET:SD   | 1:A:40:MET:N    | 0.63     | 2.71        | 10     | 2     |
| 1:A:35:HIS:CD2  | 1:A:36:ILE:H    | 0.63     | 2.11        | 2      | 3     |
| 1:A:6:SER:C     | 1:A:7:PHE:CG    | 0.63     | 2.76        | 10     | 1     |
| 1:A:19:ASN:N    | 1:A:19:ASN:ND2  | 0.63     | 2.46        | 11     | 2     |
| 1:A:43:ASN:C    | 1:A:45:ILE:H    | 0.63     | 2.02        | 9      | 2     |
| 1:A:72:ARG:CD   | 1:A:72:ARG:C    | 0.62     | 2.73        | 14     | 2     |
| 1:A:13:VAL:O    | 1:A:50:GLY:N    | 0.62     | 2.32        | 7      | 15    |
| 1:A:62:LEU:C    | 1:A:64:LYS:H    | 0.61     | 2.01        | 1      | 11    |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:6:SER:OG    | 1:A:7:PHE:N     | 0.61     | 2.34        | 5      | 2     |
| 1:A:45:ILE:O    | 1:A:45:ILE:HG22 | 0.61     | 1.94        | 10     | 2     |
| 1:A:62:LEU:C    | 1:A:64:LYS:N    | 0.61     | 2.57        | 1      | 11    |
| 1:A:28:ASN:HD22 | 1:A:28:ASN:C    | 0.60     | 2.03        | 10     | 1     |
| 1:A:20:THR:C    | 1:A:21:MET:SD   | 0.60     | 2.84        | 13     | 1     |
| 1:A:35:HIS:CD2  | 1:A:35:HIS:C    | 0.60     | 2.79        | 6      | 2     |
| 1:A:27:GLU:OE1  | 1:A:28:ASN:N    | 0.60     | 2.34        | 13     | 1     |
| 1:A:27:GLU:CD   | 1:A:27:GLU:N    | 0.60     | 2.60        | 13     | 1     |
| 1:A:53:VAL:HG12 | 1:A:70:ARG:CB   | 0.60     | 2.27        | 4      | 5     |
| 1:A:36:ILE:O    | 1:A:36:ILE:HG23 | 0.60     | 1.97        | 13     | 5     |
| 1:A:70:ARG:HE   | 1:A:72:ARG:NH2  | 0.60     | 1.95        | 2      | 1     |
| 1:A:62:LEU:HD12 | 1:A:62:LEU:N    | 0.60     | 2.01        | 4      | 5     |
| 1:A:53:VAL:HG12 | 1:A:70:ARG:HA   | 0.59     | 1.73        | 14     | 2     |
| 1:A:28:ASN:C    | 1:A:28:ASN:ND2  | 0.59     | 2.60        | 10     | 1     |
| 1:A:18:PRO:C    | 1:A:19:ASN:CG   | 0.59     | 2.70        | 9      | 8     |
| 1:A:15:ASP:OD2  | 1:A:23:ARG:NE   | 0.59     | 2.34        | 12     | 2     |
| 1:A:17:LEU:N    | 1:A:17:LEU:CD2  | 0.59     | 2.66        | 10     | 1     |
| 1:A:58:THR:O    | 1:A:61:ASP:N    | 0.59     | 2.36        | 14     | 4     |
| 1:A:42:LYS:C    | 1:A:44:TYR:H    | 0.58     | 2.04        | 15     | 2     |
| 1:A:57:LEU:H    | 1:A:57:LEU:HD12 | 0.58     | 1.57        | 6      | 1     |
| 1:A:35:HIS:CD2  | 1:A:36:ILE:N    | 0.58     | 2.72        | 1      | 4     |
| 1:A:32:VAL:CG1  | 1:A:33:THR:H    | 0.58     | 2.11        | 12     | 5     |
| 1:A:41:ARG:HH21 | 1:A:70:ARG:NH2  | 0.58     | 1.94        | 14     | 1     |
| 1:A:60:TYR:CD1  | 1:A:60:TYR:N    | 0.58     | 2.67        | 12     | 2     |
| 1:A:35:HIS:N    | 1:A:35:HIS:CD2  | 0.58     | 2.72        | 13     | 2     |
| 1:A:15:ASP:OD2  | 1:A:23:ARG:NH1  | 0.57     | 2.37        | 2      | 1     |
| 1:A:27:GLU:C    | 1:A:27:GLU:CD   | 0.57     | 2.72        | 6      | 1     |
| 1:A:40:MET:CG   | 1:A:41:ARG:N    | 0.57     | 2.67        | 6      | 2     |
| 1:A:61:ASP:N    | 1:A:61:ASP:OD1  | 0.57     | 2.35        | 3      | 2     |
| 1:A:22:PHE:CD1  | 1:A:22:PHE:N    | 0.57     | 2.72        | 7      | 10    |
| 1:A:12:THR:O    | 1:A:24:VAL:HG23 | 0.57     | 2.00        | 7      | 5     |
| 1:A:48:LEU:HD22 | 1:A:48:LEU:N    | 0.57     | 2.15        | 7      | 1     |
| 1:A:67:ILE:O    | 1:A:68:THR:HG23 | 0.57     | 2.00        | 3      | 6     |
| 1:A:40:MET:O    | 1:A:44:TYR:N    | 0.56     | 2.39        | 5      | 2     |
| 1:A:68:THR:O    | 1:A:69:TYR:CB   | 0.56     | 2.54        | 3      | 15    |
| 1:A:53:VAL:HG21 | 1:A:67:ILE:HG12 | 0.56     | 1.77        | 12     | 4     |
| 1:A:8:GLU:CB    | 1:A:54:ARG:NH1  | 0.56     | 2.69        | 1      | 1     |
| 1:A:46:ARG:C    | 1:A:47:ILE:HD12 | 0.56     | 2.26        | 13     | 1     |
| 1:A:15:ASP:OD1  | 1:A:15:ASP:C    | 0.56     | 2.48        | 6      | 1     |
| 1:A:52:LYS:O    | 1:A:71:ALA:N    | 0.56     | 2.37        | 8      | 4     |
| 1:A:7:PHE:CE2   | 1:A:57:LEU:HD12 | 0.55     | 2.37        | 1      | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:27:GLU:O    | 1:A:29:GLY:N    | 0.55     | 2.39        | 3      | 15    |
| 1:A:9:MET:SD    | 1:A:10:GLU:N    | 0.55     | 2.79        | 13     | 1     |
| 1:A:17:LEU:N    | 1:A:17:LEU:HD22 | 0.55     | 2.17        | 10     | 1     |
| 1:A:37:SER:C    | 1:A:39:LYS:N    | 0.55     | 2.64        | 5      | 3     |
| 1:A:47:ILE:CG1  | 1:A:70:ARG:NH2  | 0.55     | 2.69        | 7      | 1     |
| 1:A:56:GLU:OE1  | 1:A:66:ARG:NH1  | 0.55     | 2.40        | 8      | 1     |
| 1:A:6:SER:OG    | 1:A:58:THR:C    | 0.55     | 2.50        | 10     | 1     |
| 1:A:18:PRO:O    | 1:A:21:MET:SD   | 0.54     | 2.65        | 8      | 1     |
| 1:A:15:ASP:OD1  | 1:A:17:LEU:CD2  | 0.54     | 2.55        | 6      | 2     |
| 1:A:19:ASN:O    | 1:A:21:MET:SD   | 0.54     | 2.66        | 13     | 1     |
| 1:A:61:ASP:O    | 1:A:63:SER:N    | 0.54     | 2.41        | 10     | 3     |
| 1:A:15:ASP:CG   | 1:A:23:ARG:NH2  | 0.54     | 2.66        | 9      | 1     |
| 1:A:7:PHE:HB3   | 1:A:57:LEU:HD12 | 0.54     | 1.78        | 12     | 2     |
| 1:A:37:SER:O    | 1:A:39:LYS:N    | 0.54     | 2.41        | 9      | 2     |
| 1:A:43:ASN:C    | 1:A:44:TYR:CG   | 0.54     | 2.86        | 15     | 1     |
| 1:A:18:PRO:O    | 1:A:19:ASN:CB   | 0.53     | 2.56        | 8      | 15    |
| 1:A:56:GLU:OE1  | 1:A:56:GLU:C    | 0.53     | 2.51        | 13     | 1     |
| 1:A:8:GLU:N     | 1:A:8:GLU:CD    | 0.53     | 2.67        | 1      | 1     |
| 1:A:43:ASN:O    | 1:A:44:TYR:CG   | 0.53     | 2.61        | 15     | 4     |
| 1:A:35:HIS:CE1  | 1:A:36:ILE:O    | 0.53     | 2.61        | 10     | 2     |
| 1:A:48:LEU:C    | 1:A:48:LEU:HD13 | 0.53     | 2.27        | 13     | 1     |
| 1:A:58:THR:C    | 1:A:60:TYR:N    | 0.53     | 2.66        | 14     | 4     |
| 1:A:20:THR:O    | 1:A:35:HIS:CD2  | 0.53     | 2.62        | 3      | 1     |
| 1:A:72:ARG:H    | 1:A:72:ARG:CD   | 0.53     | 2.17        | 4      | 1     |
| 1:A:61:ASP:C    | 1:A:63:SER:N    | 0.52     | 2.63        | 10     | 4     |
| 1:A:51:ASP:O    | 1:A:53:VAL:HG13 | 0.52     | 2.04        | 4      | 2     |
| 1:A:37:SER:OG   | 1:A:38:GLY:N    | 0.52     | 2.42        | 7      | 1     |
| 1:A:48:LEU:C    | 1:A:48:LEU:HD12 | 0.52     | 2.29        | 14     | 1     |
| 1:A:35:HIS:ND1  | 1:A:36:ILE:O    | 0.52     | 2.42        | 4      | 1     |
| 1:A:53:VAL:HG12 | 1:A:70:ARG:CA   | 0.52     | 2.35        | 14     | 1     |
| 1:A:14:VAL:HG13 | 1:A:49:THR:HG22 | 0.52     | 1.79        | 4      | 3     |
| 1:A:48:LEU:N    | 1:A:48:LEU:CD2  | 0.52     | 2.72        | 7      | 2     |
| 1:A:43:ASN:O    | 1:A:45:ILE:N    | 0.52     | 2.43        | 9      | 2     |
| 1:A:26:LEU:C    | 1:A:30:HIS:O    | 0.52     | 2.53        | 14     | 15    |
| 1:A:13:VAL:C    | 1:A:14:VAL:CG2  | 0.52     | 2.83        | 13     | 6     |
| 1:A:44:TYR:CD1  | 1:A:44:TYR:N    | 0.52     | 2.72        | 7      | 1     |
| 1:A:70:ARG:N    | 1:A:70:ARG:CD   | 0.52     | 2.73        | 15     | 1     |
| 1:A:16:THR:O    | 1:A:16:THR:HG23 | 0.51     | 2.06        | 12     | 2     |
| 1:A:60:TYR:C    | 1:A:61:ASP:CG   | 0.51     | 2.77        | 3      | 1     |
| 1:A:68:THR:O    | 1:A:68:THR:HG23 | 0.51     | 2.06        | 14     | 2     |
| 1:A:38:GLY:O    | 1:A:41:ARG:N    | 0.51     | 2.44        | 4      | 3     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:15:ASP:OD1  | 1:A:16:THR:N    | 0.51     | 2.44        | 12     | 2     |
| 1:A:36:ILE:HD11 | 1:A:39:LYS:HB2  | 0.51     | 1.82        | 9      | 1     |
| 1:A:10:GLU:CG   | 1:A:54:ARG:NE   | 0.50     | 2.74        | 8      | 1     |
| 1:A:18:PRO:O    | 1:A:19:ASN:CG   | 0.50     | 2.54        | 6      | 9     |
| 1:A:15:ASP:HB3  | 1:A:23:ARG:CB   | 0.50     | 2.37        | 1      | 7     |
| 1:A:61:ASP:O    | 1:A:64:LYS:N    | 0.50     | 2.43        | 2      | 6     |
| 1:A:15:ASP:CG   | 1:A:23:ARG:HH21 | 0.50     | 2.15        | 9      | 1     |
| 1:A:56:GLU:OE1  | 1:A:57:LEU:N    | 0.50     | 2.44        | 13     | 1     |
| 1:A:58:THR:O    | 1:A:60:TYR:N    | 0.50     | 2.45        | 14     | 3     |
| 1:A:15:ASP:HB3  | 1:A:23:ARG:H    | 0.49     | 1.67        | 5      | 6     |
| 1:A:43:ASN:HD22 | 1:A:43:ASN:N    | 0.49     | 2.04        | 3      | 1     |
| 1:A:47:ILE:O    | 1:A:47:ILE:CG2  | 0.49     | 2.60        | 8      | 1     |
| 1:A:54:ARG:N    | 1:A:69:TYR:O    | 0.49     | 2.44        | 11     | 2     |
| 1:A:43:ASN:O    | 1:A:44:TYR:CB   | 0.49     | 2.61        | 13     | 2     |
| 1:A:19:ASN:C    | 1:A:20:THR:OG1  | 0.49     | 2.55        | 9      | 3     |
| 1:A:19:ASN:O    | 1:A:20:THR:CB   | 0.49     | 2.61        | 8      | 8     |
| 1:A:42:LYS:O    | 1:A:44:TYR:CE1  | 0.49     | 2.65        | 7      | 1     |
| 1:A:62:LEU:O    | 1:A:64:LYS:N    | 0.49     | 2.45        | 8      | 10    |
| 1:A:6:SER:OG    | 1:A:59:PRO:N    | 0.49     | 2.46        | 10     | 1     |
| 1:A:9:MET:N     | 1:A:55:VAL:O    | 0.49     | 2.46        | 1      | 2     |
| 1:A:53:VAL:HB   | 1:A:67:ILE:HG23 | 0.49     | 1.85        | 8      | 4     |
| 1:A:12:THR:C    | 1:A:24:VAL:HG23 | 0.49     | 2.33        | 6      | 5     |
| 1:A:24:VAL:HG11 | 1:A:55:VAL:CG2  | 0.49     | 2.35        | 5      | 3     |
| 1:A:45:ILE:O    | 1:A:45:ILE:CG2  | 0.48     | 2.61        | 13     | 2     |
| 1:A:21:MET:O    | 1:A:22:PHE:CG   | 0.48     | 2.67        | 12     | 2     |
| 1:A:57:LEU:HD12 | 1:A:57:LEU:N    | 0.48     | 2.22        | 6      | 1     |
| 1:A:43:ASN:O    | 1:A:44:TYR:C    | 0.48     | 2.57        | 11     | 2     |
| 1:A:10:GLU:OE1  | 1:A:10:GLU:N    | 0.48     | 2.44        | 8      | 1     |
| 1:A:47:ILE:CG2  | 1:A:51:ASP:CG   | 0.47     | 2.87        | 3      | 1     |
| 1:A:30:HIS:ND1  | 1:A:31:VAL:N    | 0.47     | 2.62        | 6      | 1     |
| 1:A:9:MET:O     | 1:A:55:VAL:N    | 0.47     | 2.41        | 7      | 1     |
| 1:A:31:VAL:C    | 1:A:32:VAL:CG2  | 0.47     | 2.87        | 2      | 12    |
| 1:A:19:ASN:OD1  | 1:A:21:MET:SD   | 0.47     | 2.72        | 6      | 1     |
| 1:A:36:ILE:O    | 1:A:36:ILE:CG2  | 0.47     | 2.63        | 13     | 2     |
| 1:A:27:GLU:C    | 1:A:27:GLU:OE1  | 0.47     | 2.58        | 6      | 1     |
| 1:A:37:SER:C    | 1:A:39:LYS:H    | 0.47     | 2.18        | 9      | 3     |
| 1:A:7:PHE:CD1   | 1:A:7:PHE:N     | 0.47     | 2.83        | 1      | 1     |
| 1:A:14:VAL:HG13 | 1:A:49:THR:CG2  | 0.47     | 2.40        | 2      | 1     |
| 1:A:62:LEU:CD1  | 1:A:62:LEU:H    | 0.47     | 2.20        | 14     | 3     |
| 1:A:14:VAL:O    | 1:A:15:ASP:CG   | 0.47     | 2.58        | 3      | 4     |
| 1:A:48:LEU:HD12 | 1:A:48:LEU:N    | 0.47     | 2.24        | 3      | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:20:THR:CG2  | 1:A:35:HIS:NE2  | 0.47     | 2.78        | 4      | 1     |
| 1:A:60:TYR:O    | 1:A:61:ASP:CB   | 0.46     | 2.64        | 9      | 3     |
| 1:A:20:THR:O    | 1:A:21:MET:SD   | 0.46     | 2.73        | 10     | 1     |
| 1:A:13:VAL:C    | 1:A:14:VAL:HG22 | 0.46     | 2.35        | 13     | 3     |
| 1:A:38:GLY:O    | 1:A:42:LYS:N    | 0.46     | 2.49        | 14     | 1     |
| 1:A:17:LEU:HD12 | 1:A:22:PHE:C    | 0.46     | 2.35        | 1      | 2     |
| 1:A:15:ASP:CB   | 1:A:23:ARG:CB   | 0.46     | 2.94        | 9      | 4     |
| 1:A:43:ASN:O    | 1:A:43:ASN:ND2  | 0.46     | 2.49        | 15     | 1     |
| 1:A:38:GLY:C    | 1:A:40:MET:N    | 0.46     | 2.71        | 4      | 4     |
| 1:A:62:LEU:CD1  | 1:A:62:LEU:N    | 0.46     | 2.73        | 5      | 1     |
| 1:A:18:PRO:O    | 1:A:21:MET:CG   | 0.46     | 2.63        | 8      | 1     |
| 1:A:56:GLU:OE1  | 1:A:56:GLU:CA   | 0.46     | 2.63        | 12     | 1     |
| 1:A:48:LEU:N    | 1:A:48:LEU:CD1  | 0.46     | 2.78        | 3      | 1     |
| 1:A:36:ILE:HD11 | 1:A:40:MET:HB3  | 0.46     | 1.87        | 13     | 1     |
| 1:A:23:ARG:HH11 | 1:A:31:VAL:CG2  | 0.46     | 2.24        | 11     | 1     |
| 1:A:44:TYR:O    | 1:A:45:ILE:C    | 0.45     | 2.59        | 14     | 4     |
| 1:A:44:TYR:O    | 1:A:44:TYR:CD2  | 0.45     | 2.69        | 11     | 1     |
| 1:A:62:LEU:HD12 | 1:A:63:SER:H    | 0.45     | 1.70        | 12     | 1     |
| 1:A:60:TYR:O    | 1:A:61:ASP:CG   | 0.45     | 2.59        | 14     | 6     |
| 1:A:38:GLY:O    | 1:A:39:LYS:C    | 0.45     | 2.58        | 9      | 6     |
| 1:A:43:ASN:O    | 1:A:44:TYR:CD1  | 0.45     | 2.69        | 11     | 2     |
| 1:A:62:LEU:CD1  | 1:A:63:SER:H    | 0.45     | 2.24        | 12     | 1     |
| 1:A:42:LYS:C    | 1:A:44:TYR:N    | 0.45     | 2.70        | 15     | 3     |
| 1:A:60:TYR:HB2  | 1:A:62:LEU:HD11 | 0.45     | 1.87        | 7      | 1     |
| 1:A:27:GLU:OE1  | 1:A:27:GLU:N    | 0.45     | 2.49        | 13     | 1     |
| 1:A:35:HIS:CD2  | 1:A:35:HIS:O    | 0.45     | 2.69        | 5      | 2     |
| 1:A:40:MET:O    | 1:A:43:ASN:N    | 0.45     | 2.50        | 10     | 1     |
| 1:A:61:ASP:O    | 1:A:61:ASP:CG   | 0.45     | 2.59        | 7      | 1     |
| 1:A:36:ILE:HD11 | 1:A:40:MET:HG2  | 0.45     | 1.88        | 10     | 1     |
| 1:A:24:VAL:HG13 | 1:A:24:VAL:O    | 0.44     | 2.12        | 8      | 1     |
| 1:A:71:ALA:O    | 1:A:72:ARG:C    | 0.44     | 2.60        | 8      | 1     |
| 1:A:70:ARG:CD   | 1:A:70:ARG:C    | 0.44     | 2.91        | 11     | 1     |
| 1:A:27:GLU:N    | 1:A:27:GLU:OE2  | 0.44     | 2.51        | 12     | 1     |
| 1:A:61:ASP:O    | 1:A:62:LEU:C    | 0.44     | 2.59        | 11     | 9     |
| 1:A:10:GLU:O    | 1:A:26:LEU:CD2  | 0.44     | 2.65        | 8      | 1     |
| 1:A:66:ARG:CG   | 1:A:67:ILE:N    | 0.44     | 2.78        | 4      | 1     |
| 1:A:47:ILE:HG12 | 1:A:70:ARG:NH2  | 0.44     | 2.28        | 7      | 1     |
| 1:A:61:ASP:C    | 1:A:63:SER:H    | 0.44     | 2.20        | 10     | 1     |
| 1:A:12:THR:CG2  | 1:A:14:VAL:CG2  | 0.44     | 2.96        | 13     | 1     |
| 1:A:70:ARG:CG   | 1:A:70:ARG:HH11 | 0.44     | 2.26        | 11     | 1     |
| 1:A:45:ILE:HG23 | 1:A:46:ARG:N    | 0.44     | 2.28        | 3      | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:40:MET:O    | 1:A:43:ASN:CG   | 0.44     | 2.61        | 9      | 1     |
| 1:A:54:ARG:NH2  | 1:A:69:TYR:CG   | 0.43     | 2.86        | 7      | 1     |
| 1:A:15:ASP:OD1  | 1:A:17:LEU:HD23 | 0.43     | 2.13        | 6      | 1     |
| 1:A:19:ASN:O    | 1:A:20:THR:CG2  | 0.43     | 2.67        | 5      | 1     |
| 1:A:47:ILE:HG13 | 1:A:70:ARG:NH2  | 0.43     | 2.28        | 7      | 1     |
| 1:A:15:ASP:CB   | 1:A:23:ARG:HB3  | 0.43     | 2.44        | 10     | 3     |
| 1:A:66:ARG:HG3  | 1:A:67:ILE:N    | 0.43     | 2.28        | 4      | 1     |
| 1:A:8:GLU:OE1   | 1:A:54:ARG:CZ   | 0.43     | 2.66        | 2      | 1     |
| 1:A:40:MET:O    | 1:A:41:ARG:C    | 0.43     | 2.61        | 10     | 1     |
| 1:A:56:GLU:CD   | 1:A:56:GLU:N    | 0.43     | 2.76        | 11     | 1     |
| 1:A:31:VAL:O    | 1:A:31:VAL:CG1  | 0.43     | 2.66        | 10     | 1     |
| 1:A:48:LEU:HD22 | 1:A:49:THR:N    | 0.43     | 2.29        | 13     | 1     |
| 1:A:62:LEU:H    | 1:A:62:LEU:HD12 | 0.43     | 1.73        | 14     | 2     |
| 1:A:10:GLU:HG3  | 1:A:54:ARG:NE   | 0.43     | 2.29        | 8      | 1     |
| 1:A:45:ILE:O    | 1:A:46:ARG:C    | 0.43     | 2.62        | 15     | 2     |
| 1:A:60:TYR:CD1  | 1:A:60:TYR:C    | 0.42     | 2.94        | 1      | 1     |
| 1:A:67:ILE:O    | 1:A:68:THR:CG2  | 0.42     | 2.67        | 11     | 6     |
| 1:A:36:ILE:O    | 1:A:37:SER:C    | 0.42     | 2.61        | 12     | 2     |
| 1:A:8:GLU:HB3   | 1:A:54:ARG:NH1  | 0.42     | 2.29        | 1      | 1     |
| 1:A:43:ASN:ND2  | 1:A:45:ILE:HD12 | 0.42     | 2.29        | 4      | 1     |
| 1:A:46:ARG:NH1  | 1:A:46:ARG:CG   | 0.42     | 2.82        | 8      | 1     |
| 1:A:62:LEU:N    | 1:A:62:LEU:CD1  | 0.42     | 2.75        | 8      | 1     |
| 1:A:17:LEU:CD1  | 1:A:33:THR:HG23 | 0.42     | 2.44        | 12     | 1     |
| 1:A:15:ASP:CB   | 1:A:23:ARG:HE   | 0.42     | 2.27        | 13     | 1     |
| 1:A:72:ARG:N    | 1:A:72:ARG:HD3  | 0.42     | 2.28        | 8      | 1     |
| 1:A:31:VAL:C    | 1:A:32:VAL:HG23 | 0.42     | 2.38        | 15     | 1     |
| 1:A:72:ARG:C    | 1:A:72:ARG:CD   | 0.42     | 2.93        | 15     | 1     |
| 1:A:19:ASN:C    | 1:A:20:THR:HG1  | 0.42     | 2.22        | 8      | 1     |
| 1:A:10:GLU:HG2  | 1:A:54:ARG:NH1  | 0.42     | 2.29        | 13     | 1     |
| 1:A:45:ILE:HG22 | 1:A:46:ARG:N    | 0.42     | 2.30        | 11     | 1     |
| 1:A:38:GLY:O    | 1:A:40:MET:N    | 0.42     | 2.53        | 4      | 2     |
| 1:A:22:PHE:O    | 1:A:34:ALA:N    | 0.42     | 2.53        | 11     | 1     |
| 1:A:48:LEU:O    | 1:A:51:ASP:CG   | 0.41     | 2.63        | 6      | 1     |
| 1:A:54:ARG:HH21 | 1:A:69:TYR:CB   | 0.41     | 2.27        | 7      | 1     |
| 1:A:36:ILE:HG12 | 1:A:37:SER:N    | 0.41     | 2.31        | 8      | 1     |
| 1:A:7:PHE:CD2   | 1:A:8:GLU:N     | 0.41     | 2.87        | 15     | 1     |
| 1:A:48:LEU:O    | 1:A:51:ASP:OD1  | 0.41     | 2.39        | 4      | 1     |
| 1:A:54:ARG:NH1  | 1:A:69:TYR:CD2  | 0.41     | 2.88        | 10     | 2     |
| 1:A:14:VAL:CG1  | 1:A:49:THR:HG22 | 0.41     | 2.46        | 3      | 1     |
| 1:A:17:LEU:CD1  | 1:A:33:THR:OG1  | 0.41     | 2.68        | 7      | 1     |
| 1:A:72:ARG:N    | 1:A:72:ARG:HD2  | 0.41     | 2.30        | 15     | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:35:HIS:CG   | 1:A:36:ILE:N    | 0.41     | 2.88        | 2      | 1     |
| 1:A:60:TYR:O    | 1:A:61:ASP:C    | 0.41     | 2.63        | 14     | 1     |
| 1:A:16:THR:C    | 1:A:17:LEU:HD22 | 0.41     | 2.41        | 6      | 1     |
| 1:A:6:SER:O     | 1:A:7:PHE:CB    | 0.41     | 2.69        | 10     | 1     |
| 1:A:43:ASN:N    | 1:A:43:ASN:ND2  | 0.41     | 2.69        | 3      | 1     |
| 1:A:69:TYR:C    | 1:A:69:TYR:CD1  | 0.41     | 2.98        | 14     | 1     |
| 1:A:53:VAL:HG21 | 1:A:67:ILE:HG23 | 0.41     | 1.92        | 7      | 1     |
| 1:A:72:ARG:CD   | 1:A:72:ARG:N    | 0.41     | 2.83        | 15     | 1     |
| 1:A:40:MET:O    | 1:A:44:TYR:CA   | 0.40     | 2.69        | 5      | 1     |
| 1:A:6:SER:O     | 1:A:7:PHE:CD2   | 0.40     | 2.75        | 14     | 1     |
| 1:A:21:MET:O    | 1:A:22:PHE:CD2  | 0.40     | 2.74        | 12     | 1     |
| 1:A:18:PRO:O    | 1:A:19:ASN:ND2  | 0.40     | 2.54        | 7      | 1     |
| 1:A:27:GLU:O    | 1:A:27:GLU:CD   | 0.40     | 2.65        | 14     | 1     |
| 1:A:19:ASN:C    | 1:A:20:THR:HG22 | 0.40     | 2.40        | 5      | 1     |
| 1:A:47:ILE:CD1  | 1:A:70:ARG:HE   | 0.40     | 2.30        | 14     | 1     |

## 6.3 Torsion angles [i](#)

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

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

| Mol | Chain | Analysed       | Favoured     | Allowed      | Outliers    | Percentiles |          |
|-----|-------|----------------|--------------|--------------|-------------|-------------|----------|
| 1   | A     | 66/72 (92%)    | 49±2 (74±3%) | 11±2 (16±3%) | 7±2 (10±3%) | <b>1</b>    | <b>9</b> |
| All | All   | 990/1080 (92%) | 730 (74%)    | 158 (16%)    | 102 (10%)   | <b>1</b>    | <b>9</b> |

All 17 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     | 15  | ASP  | 15             |
| 1   | A     | 27  | GLU  | 15             |
| 1   | A     | 28  | ASN  | 15             |
| 1   | A     | 69  | TYR  | 15             |
| 1   | A     | 61  | ASP  | 8              |
| 1   | A     | 14  | VAL  | 7              |
| 1   | A     | 45  | ILE  | 6              |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 44  | TYR  | 4              |
| 1   | A     | 19  | ASN  | 3              |
| 1   | A     | 20  | THR  | 3              |
| 1   | A     | 37  | SER  | 2              |
| 1   | A     | 38  | GLY  | 2              |
| 1   | A     | 7   | PHE  | 2              |
| 1   | A     | 62  | LEU  | 2              |
| 1   | A     | 46  | ARG  | 1              |
| 1   | A     | 6   | SER  | 1              |
| 1   | A     | 43  | ASN  | 1              |

### 6.3.2 Protein sidechains ⓘ

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

| Mol | Chain | Analysed      | Rotameric    | Outliers     | Percentiles |    |
|-----|-------|---------------|--------------|--------------|-------------|----|
| 1   | A     | 60/65 (92%)   | 49±3 (81±5%) | 11±3 (19±5%) | 3           | 34 |
| All | All   | 900/975 (92%) | 729 (81%)    | 171 (19%)    | 3           | 34 |

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     | 14  | VAL  | 15             |
| 1   | A     | 68  | THR  | 10             |
| 1   | A     | 19  | ASN  | 10             |
| 1   | A     | 55  | VAL  | 9              |
| 1   | A     | 32  | VAL  | 8              |
| 1   | A     | 20  | THR  | 7              |
| 1   | A     | 31  | VAL  | 7              |
| 1   | A     | 33  | THR  | 6              |
| 1   | A     | 16  | THR  | 5              |
| 1   | A     | 61  | ASP  | 5              |
| 1   | A     | 66  | ARG  | 5              |
| 1   | A     | 72  | ARG  | 5              |
| 1   | A     | 51  | ASP  | 4              |
| 1   | A     | 6   | SER  | 4              |
| 1   | A     | 15  | ASP  | 4              |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 52  | LYS  | 4              |
| 1   | A     | 62  | LEU  | 4              |
| 1   | A     | 23  | ARG  | 3              |
| 1   | A     | 57  | LEU  | 3              |
| 1   | A     | 45  | ILE  | 3              |
| 1   | A     | 70  | ARG  | 3              |
| 1   | A     | 47  | ILE  | 3              |
| 1   | A     | 35  | HIS  | 3              |
| 1   | A     | 12  | THR  | 3              |
| 1   | A     | 27  | GLU  | 3              |
| 1   | A     | 41  | ARG  | 2              |
| 1   | A     | 63  | SER  | 2              |
| 1   | A     | 26  | LEU  | 2              |
| 1   | A     | 8   | GLU  | 2              |
| 1   | A     | 37  | SER  | 2              |
| 1   | A     | 60  | TYR  | 2              |
| 1   | A     | 21  | MET  | 2              |
| 1   | A     | 48  | LEU  | 2              |
| 1   | A     | 7   | PHE  | 2              |
| 1   | A     | 9   | MET  | 2              |
| 1   | A     | 24  | VAL  | 2              |
| 1   | A     | 40  | MET  | 2              |
| 1   | A     | 17  | LEU  | 1              |
| 1   | A     | 43  | ASN  | 1              |
| 1   | A     | 44  | TYR  | 1              |
| 1   | A     | 54  | ARG  | 1              |
| 1   | A     | 42  | LYS  | 1              |
| 1   | A     | 53  | VAL  | 1              |
| 1   | A     | 28  | ASN  | 1              |
| 1   | A     | 64  | LYS  | 1              |
| 1   | A     | 30  | HIS  | 1              |
| 1   | A     | 56  | GLU  | 1              |
| 1   | A     | 36  | ILE  | 1              |

### 6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 6.7 Other polymers [i](#)

There are no such molecules in this entry.

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

There are no chain breaks in this entry.

## 7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 80% for the well-defined parts and 78% for the entire structure.

### 7.1 Chemical shift list 1

File name: working\_cs.cif

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

#### 7.1.1 Bookkeeping

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

|                                         |     |
|-----------------------------------------|-----|
| Total number of shifts                  | 799 |
| Number of shifts mapped to atoms        | 799 |
| 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

The following table shows the suggested chemical shift referencing corrections.

| Nucleus                | # values | Correction $\pm$ precision, ppm | Suggested action           |
|------------------------|----------|---------------------------------|----------------------------|
| $^{13}\text{C}_\alpha$ | 71       | $-2.39 \pm 0.32$                | Should be checked          |
| $^{13}\text{C}_\beta$  | 66       | $-3.61 \pm 0.24$                | Should be checked          |
| $^{13}\text{C}'$       | 69       | $0.17 \pm 0.11$                 | None needed ( $< 0.5$ ppm) |
| $^{15}\text{N}$        | 69       | $0.28 \pm 0.39$                 | None needed ( $< 0.5$ ppm) |

#### 7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 80%, i.e. 767 atoms were assigned a chemical shift out of a possible 958. 0 out of 12 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total         | $^1\text{H}$   | $^{13}\text{C}$ | $^{15}\text{N}$ |
|-----------|---------------|----------------|-----------------|-----------------|
| Backbone  | 334/336 (99%) | 137/137 (100%) | 132/134 (99%)   | 65/65 (100%)    |
| Sidechain | 423/561 (75%) | 297/364 (82%)  | 125/169 (74%)   | 1/28 (4%)       |

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|          | Total         | <sup>1</sup> H | <sup>13</sup> C | <sup>15</sup> N |
|----------|---------------|----------------|-----------------|-----------------|
| Aromatic | 10/61 (16%)   | 10/30 (33%)    | 0/29 (0%)       | 0/2 (0%)        |
| Overall  | 767/958 (80%) | 444/531 (84%)  | 257/332 (77%)   | 66/95 (69%)     |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 78%, i.e. 799 atoms were assigned a chemical shift out of a possible 1020. 0 out of 12 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total          | <sup>1</sup> H | <sup>13</sup> C | <sup>15</sup> N |
|-----------|----------------|----------------|-----------------|-----------------|
| Backbone  | 354/361 (98%)  | 145/147 (99%)  | 140/144 (97%)   | 69/70 (99%)     |
| Sidechain | 435/598 (73%)  | 305/387 (79%)  | 129/182 (71%)   | 1/29 (3%)       |
| Aromatic  | 10/61 (16%)    | 10/30 (33%)    | 0/29 (0%)       | 0/2 (0%)        |
| Overall   | 799/1020 (78%) | 460/564 (82%)  | 269/355 (76%)   | 70/101 (69%)    |

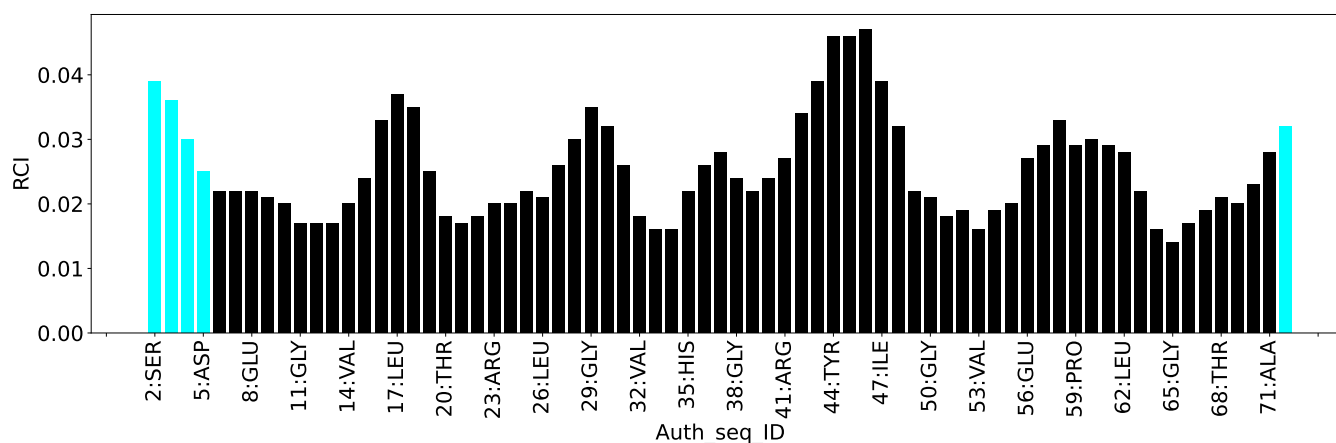
#### 7.1.4 Statistically unusual chemical shifts [i](#)

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 [i](#)

### 8.1 Conformationally restricting restraints [i](#)

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                                | 652   |
| Intra-residue ( $ i-j =0$ )                              | 293   |
| Sequential ( $ i-j =1$ )                                 | 154   |
| Medium range ( $ i-j >1$ and $ i-j <5$ )                 | 30    |
| Long range ( $ i-j \geq 5$ )                             | 142   |
| Inter-chain                                              | 0     |
| Hydrogen bond restraints                                 | 33    |
| Disulfide bond restraints                                | 0     |
| Total dihedral-angle restraints                          | 122   |
| Number of unmapped restraints                            | 0     |
| Number of restraints per residue                         | 10.8  |
| Number of long range restraints per residue <sup>1</sup> | 2.3   |

<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 [i](#)

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 [i](#)

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)  | 23.9                                   | 0.2     |
| 0.2-0.5 (Medium) | 20.7                                   | 0.5     |
| >0.5 (Large)     | 3.5                                    | 0.83    |

### 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)   | 16.9                                   | 9.97    |
| 10.0-20.0 (Medium) | 6.9                                    | 19.97   |
| >20.0 (Large)      | 0.9                                    | 22.74   |

## 9 Distance violation analysis ⓘ

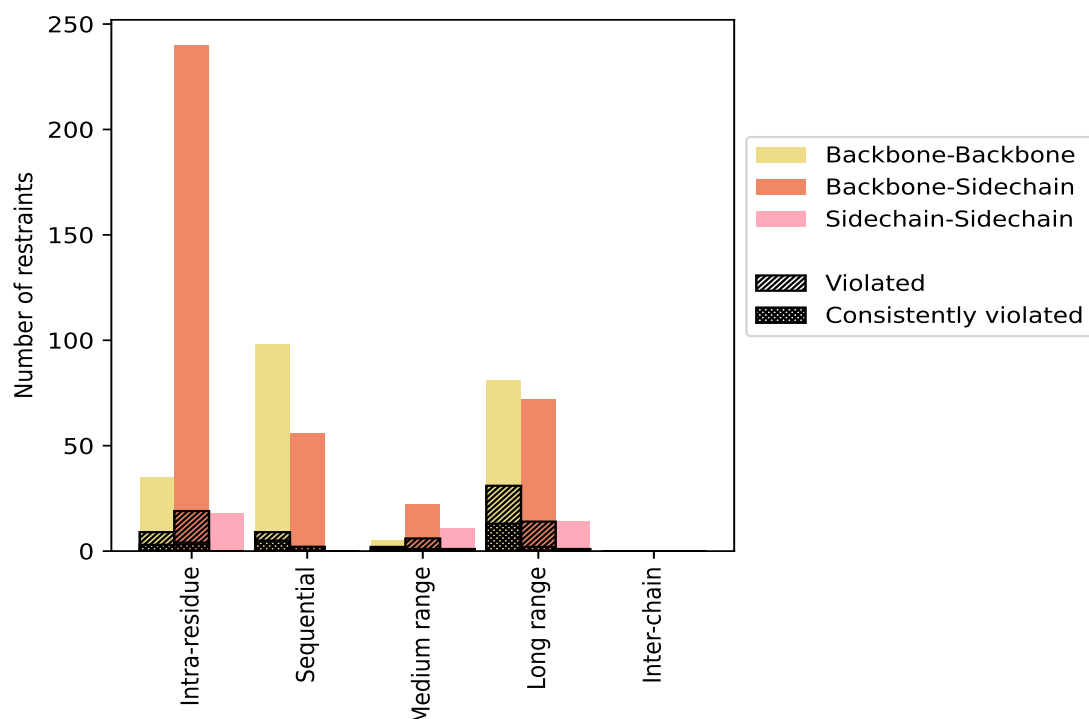
### 9.1 Summary of distance violations ⓘ

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="#">293</a> | <a href="#">44.9</a>  | <a href="#">28</a>    | <a href="#">9.6</a>  | <a href="#">4.3</a>  | <a href="#">7</a>                  | <a href="#">2.4</a> | <a href="#">1.1</a> |
| Backbone-Backbone                                          | 35                  | 5.4                   | 9                     | 25.7                 | 1.4                  | 3                                  | 8.6                 | 0.5                 |
| Backbone-Sidechain                                         | 240                 | 36.8                  | 19                    | 7.9                  | 2.9                  | 4                                  | 1.7                 | 0.6                 |
| Sidechain-Sidechain                                        | 18                  | 2.8                   | 0                     | 0.0                  | 0.0                  | 0                                  | 0.0                 | 0.0                 |
| <a href="#">Sequential ( i-j =1)</a>                       | <a href="#">154</a> | <a href="#">23.6</a>  | <a href="#">11</a>    | <a href="#">7.1</a>  | <a href="#">1.7</a>  | <a href="#">7</a>                  | <a href="#">4.5</a> | <a href="#">1.1</a> |
| Backbone-Backbone                                          | 98                  | 15.0                  | 9                     | 9.2                  | 1.4                  | 5                                  | 5.1                 | 0.8                 |
| Backbone-Sidechain                                         | 56                  | 8.6                   | 2                     | 3.6                  | 0.3                  | 2                                  | 3.6                 | 0.3                 |
| Sidechain-Sidechain                                        | 0                   | 0.0                   | 0                     | 0.0                  | 0.0                  | 0                                  | 0.0                 | 0.0                 |
| <a href="#">Medium range ( i-j &gt;1 &amp;  i-j &lt;5)</a> | <a href="#">30</a>  | <a href="#">4.6</a>   | <a href="#">7</a>     | <a href="#">23.3</a> | <a href="#">1.1</a>  | <a href="#">1</a>                  | <a href="#">3.3</a> | <a href="#">0.2</a> |
| Backbone-Backbone                                          | 5                   | 0.8                   | 2                     | 40.0                 | 0.3                  | 1                                  | 20.0                | 0.2                 |
| Backbone-Sidechain                                         | 14                  | 2.1                   | 4                     | 28.6                 | 0.6                  | 0                                  | 0.0                 | 0.0                 |
| Sidechain-Sidechain                                        | 11                  | 1.7                   | 1                     | 9.1                  | 0.2                  | 0                                  | 0.0                 | 0.0                 |
| <a href="#">Long range ( i-j ≥5)</a>                       | <a href="#">142</a> | <a href="#">21.8</a>  | <a href="#">37</a>    | <a href="#">26.1</a> | <a href="#">5.7</a>  | <a href="#">14</a>                 | <a href="#">9.9</a> | <a href="#">2.1</a> |
| Backbone-Backbone                                          | 81                  | 12.4                  | 31                    | 38.3                 | 4.8                  | 13                                 | 16.0                | 2.0                 |
| Backbone-Sidechain                                         | 47                  | 7.2                   | 5                     | 10.6                 | 0.8                  | 1                                  | 2.1                 | 0.2                 |
| Sidechain-Sidechain                                        | 14                  | 2.1                   | 1                     | 7.1                  | 0.2                  | 0                                  | 0.0                 | 0.0                 |
| <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="#">33</a>  | <a href="#">5.1</a>   | <a href="#">11</a>    | <a href="#">33.3</a> | <a href="#">1.7</a>  | <a href="#">2</a>                  | <a href="#">6.1</a> | <a href="#">0.3</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="#">652</a> | <a href="#">100.0</a> | <a href="#">94</a>    | <a href="#">14.4</a> | <a href="#">14.4</a> | <a href="#">31</a>                 | <a href="#">4.8</a> | <a href="#">4.8</a> |
| Backbone-Backbone                                          | 219                 | 33.6                  | 51                    | 23.3                 | 7.8                  | 22                                 | 10.0                | 3.4                 |
| Backbone-Sidechain                                         | 390                 | 59.8                  | 41                    | 10.5                 | 6.3                  | 9                                  | 2.3                 | 1.4                 |
| Sidechain-Sidechain                                        | 43                  | 6.6                   | 2                     | 4.7                  | 0.3                  | 0                                  | 0.0                 | 0.0                 |

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

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



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

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

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

| Model ID | Number of violations |                 |                 |                 |                 |       | Mean (Å) | Max (Å) | SD <sup>6</sup> (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
|          | IR <sup>1</sup>      | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total |          |         |                     |            |
| 1        | 11                   | 8               | 5               | 26              | 0               | 50    | 0.24     | 0.69    | 0.13                | 0.19       |
| 2        | 16                   | 9               | 4               | 23              | 0               | 52    | 0.23     | 0.83    | 0.15                | 0.18       |
| 3        | 11                   | 7               | 3               | 25              | 0               | 46    | 0.25     | 0.74    | 0.15                | 0.22       |
| 4        | 13                   | 8               | 4               | 26              | 0               | 51    | 0.25     | 0.73    | 0.13                | 0.21       |
| 5        | 15                   | 8               | 3               | 22              | 0               | 48    | 0.24     | 0.65    | 0.13                | 0.2        |
| 6        | 13                   | 7               | 3               | 25              | 0               | 48    | 0.25     | 0.67    | 0.14                | 0.2        |
| 7        | 12                   | 9               | 4               | 27              | 0               | 52    | 0.24     | 0.75    | 0.16                | 0.18       |
| 8        | 15                   | 9               | 4               | 25              | 0               | 53    | 0.25     | 0.72    | 0.14                | 0.2        |
| 9        | 13                   | 9               | 5               | 22              | 0               | 49    | 0.24     | 0.73    | 0.13                | 0.2        |
| 10       | 13                   | 8               | 4               | 30              | 0               | 55    | 0.24     | 0.76    | 0.15                | 0.19       |

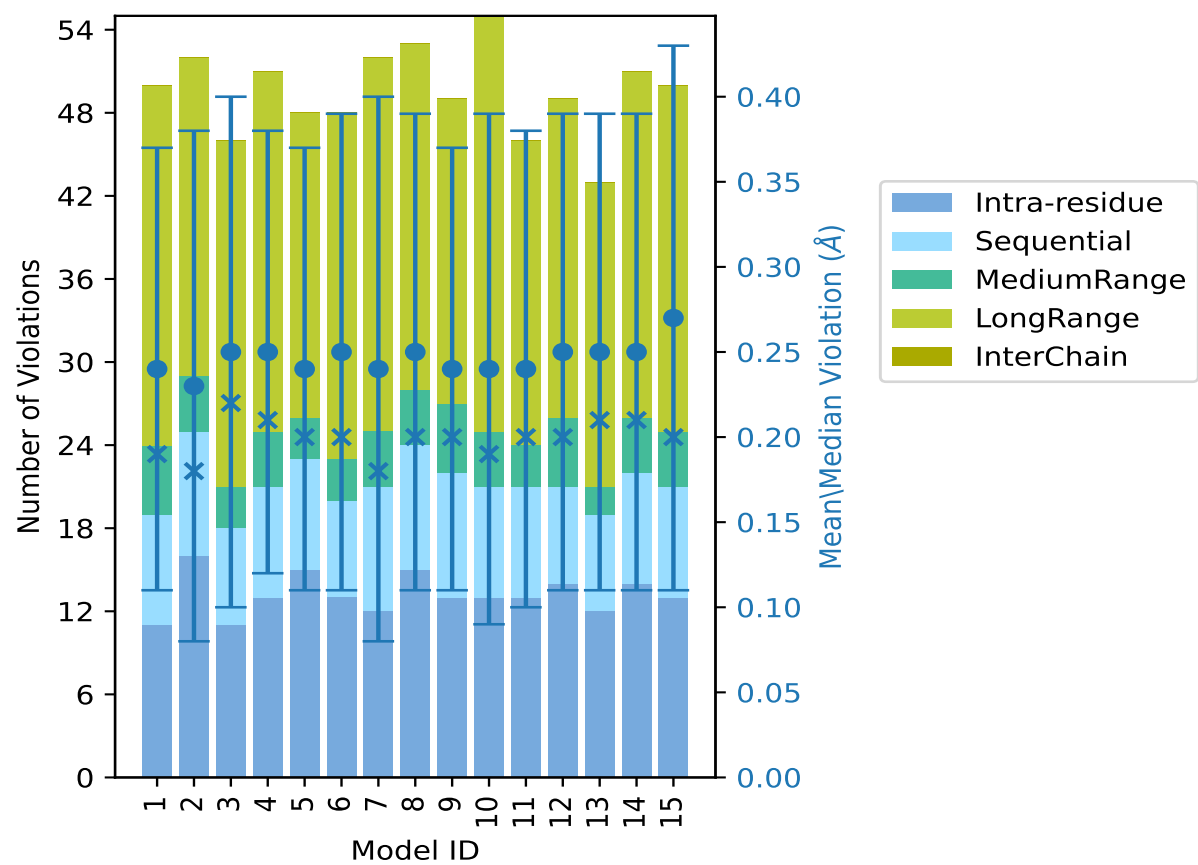
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| Model ID | Number of violations |                 |                 |                 |                 |       | Mean (Å) | Max (Å) | SD <sup>6</sup> (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
|          | IR <sup>1</sup>      | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total |          |         |                     |            |
| 11       | 13                   | 8               | 3               | 22              | 0               | 46    | 0.24     | 0.78    | 0.14                | 0.2        |
| 12       | 14                   | 7               | 5               | 23              | 0               | 49    | 0.25     | 0.72    | 0.14                | 0.2        |
| 13       | 12                   | 7               | 2               | 22              | 0               | 43    | 0.25     | 0.79    | 0.14                | 0.21       |
| 14       | 14                   | 8               | 4               | 25              | 0               | 51    | 0.25     | 0.67    | 0.14                | 0.21       |
| 15       | 13                   | 8               | 4               | 25              | 0               | 50    | 0.27     | 0.75    | 0.16                | 0.2        |

<sup>1</sup>Intra-residue restraints, <sup>2</sup>Sequential restraints, <sup>3</sup>Medium range restraints, <sup>4</sup>Long range restraints, <sup>5</sup>Inter-chain restraints, <sup>6</sup>Standard deviation

9.2.1 Bar graph : Distance Violation statistics for each model ⓘ



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

### 9.3 Distance violation statistics for the ensemble

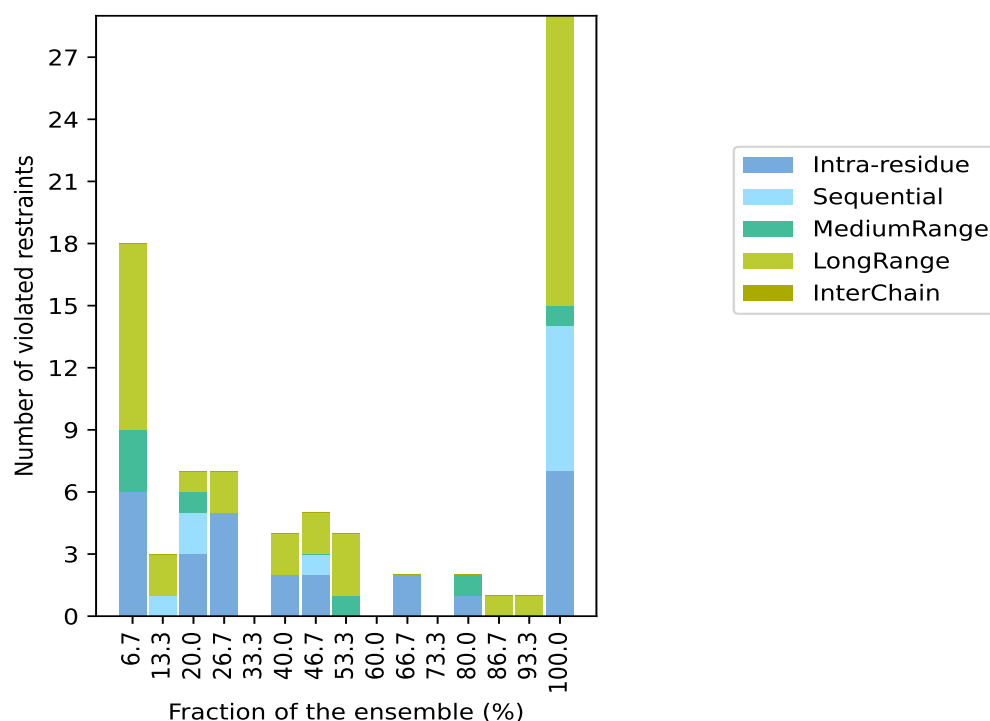
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 536(IR:265, SQ:143, MR:23, LR:105, IC:0) restraints are not 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>       | %     |
| 6                             | 0               | 3               | 9               | 0               | 18    | 1                        | 6.7   |
| 0                             | 1               | 0               | 2               | 0               | 3     | 2                        | 13.3  |
| 3                             | 2               | 1               | 1               | 0               | 7     | 3                        | 20.0  |
| 5                             | 0               | 0               | 2               | 0               | 7     | 4                        | 26.7  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 5                        | 33.3  |
| 2                             | 0               | 0               | 2               | 0               | 4     | 6                        | 40.0  |
| 2                             | 1               | 0               | 2               | 0               | 5     | 7                        | 46.7  |
| 0                             | 0               | 1               | 3               | 0               | 4     | 8                        | 53.3  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 9                        | 60.0  |
| 2                             | 0               | 0               | 0               | 0               | 2     | 10                       | 66.7  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 11                       | 73.3  |
| 1                             | 0               | 1               | 0               | 0               | 2     | 12                       | 80.0  |
| 0                             | 0               | 0               | 1               | 0               | 1     | 13                       | 86.7  |
| 0                             | 0               | 0               | 1               | 0               | 1     | 14                       | 93.3  |
| 7                             | 7               | 1               | 14              | 0               | 29    | 15                       | 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

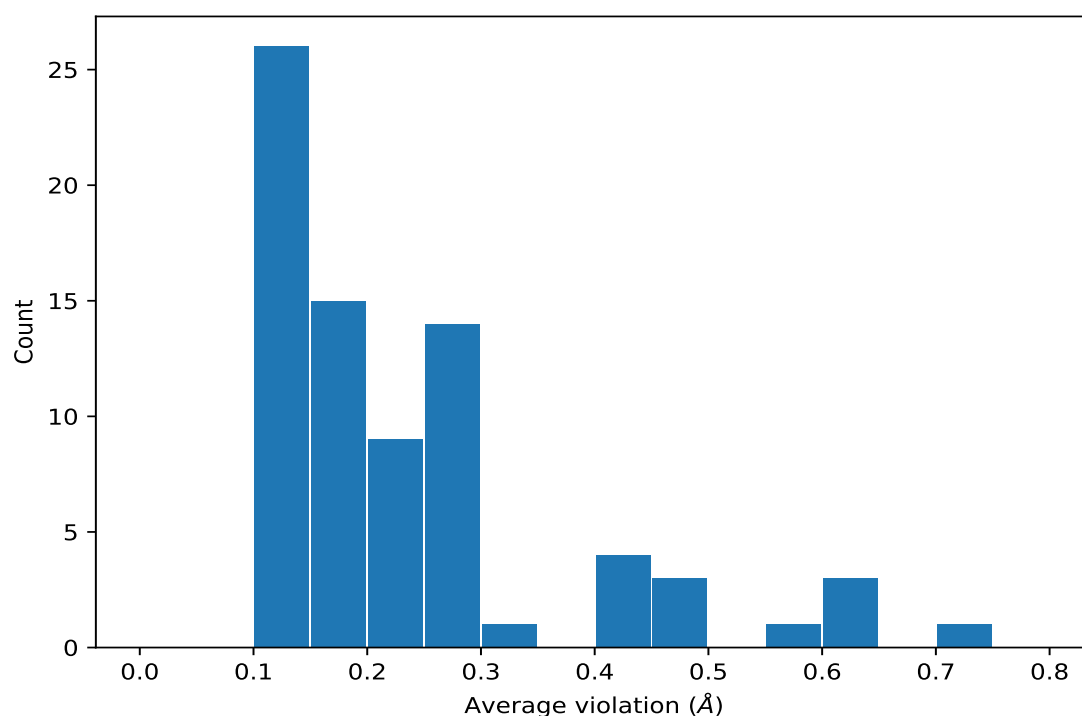
### 9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



## 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) |
|---------|---------------|---------------|---------------------|----------|---------------------|------------|
| (1,26)  | 1:13:A:VAL:H  | 1:52:A:LYS:HA | 15                  | 0.72     | 0.04                | 0.72       |
| (1,233) | 1:49:A:THR:HA | 1:13:A:VAL:HB | 15                  | 0.57     | 0.05                | 0.57       |
| (1,173) | 1:68:A:THR:H  | 1:69:A:TYR:H  | 15                  | 0.49     | 0.02                | 0.49       |
| (1,175) | 1:69:A:TYR:H  | 1:68:A:THR:H  | 15                  | 0.49     | 0.02                | 0.49       |
| (1,210) | 1:32:A:VAL:HA | 1:32:A:VAL:HB | 15                  | 0.46     | 0.01                | 0.46       |
| (1,74)  | 1:30:A:HIS:H  | 1:26:A:LEU:H  | 15                  | 0.33     | 0.05                | 0.35       |
| (4,18)  | 1:17:A:LEU:O  | 1:21:A:MET:H  | 15                  | 0.3      | 0.02                | 0.29       |
| (1,137) | 1:54:A:ARG:H  | 1:69:A:TYR:H  | 15                  | 0.29     | 0.04                | 0.28       |
| (1,176) | 1:69:A:TYR:H  | 1:54:A:ARG:H  | 15                  | 0.29     | 0.04                | 0.28       |
| (1,30)  | 1:14:A:VAL:H  | 1:14:A:VAL:HB | 15                  | 0.28     | 0.09                | 0.27       |
| (4,33)  | 1:64:A:LYS:O  | 1:58:A:THR:H  | 15                  | 0.27     | 0.05                | 0.26       |
| (1,194) | 1:16:A:THR:HA | 1:22:A:PHE:HA | 15                  | 0.26     | 0.06                | 0.27       |
| (1,204) | 1:25:A:GLU:HA | 1:31:A:VAL:HA | 15                  | 0.26     | 0.04                | 0.27       |
| (1,209) | 1:31:A:VAL:HA | 1:25:A:GLU:HA | 15                  | 0.26     | 0.04                | 0.27       |
| (1,84)  | 1:33:A:THR:H  | 1:32:A:VAL:HB | 15                  | 0.26     | 0.13                | 0.24       |
| (1,52)  | 1:22:A:PHE:H  | 1:34:A:ALA:H  | 15                  | 0.25     | 0.15                | 0.17       |

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| Key     | Atom-1        | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|---------------|-----------------|---------------------|----------|---------------------|------------|
| (1,27)  | 1:14:A:VAL:H  | 1:15:A:ASP:H    | 15                  | 0.25     | 0.03                | 0.24       |
| (1,34)  | 1:15:A:ASP:H  | 1:14:A:VAL:H    | 15                  | 0.25     | 0.03                | 0.24       |
| (1,214) | 1:33:A:THR:HA | 1:33:A:THR:HB   | 15                  | 0.22     | 0.03                | 0.23       |
| (1,62)  | 1:24:A:VAL:H  | 1:32:A:VAL:H    | 15                  | 0.22     | 0.04                | 0.21       |
| (1,77)  | 1:32:A:VAL:H  | 1:24:A:VAL:H    | 15                  | 0.22     | 0.04                | 0.21       |
| (1,257) | 1:66:A:ARG:HA | 1:34:A:ALA:HA   | 15                  | 0.21     | 0.04                | 0.22       |
| (1,167) | 1:66:A:ARG:H  | 1:57:A:LEU:HA   | 15                  | 0.21     | 0.05                | 0.21       |
| (1,129) | 1:53:A:VAL:H  | 1:12:A:THR:HA   | 15                  | 0.19     | 0.05                | 0.17       |
| (1,164) | 1:65:A:GLY:H  | 1:34:A:ALA:HA   | 15                  | 0.18     | 0.02                | 0.18       |
| (1,36)  | 1:15:A:ASP:H  | 1:14:A:VAL:HB   | 15                  | 0.17     | 0.03                | 0.17       |
| (1,70)  | 1:28:A:ASN:H  | 1:27:A:GLU:H    | 15                  | 0.15     | 0.02                | 0.16       |
| (1,51)  | 1:22:A:PHE:H  | 1:22:A:PHE:HA   | 15                  | 0.15     | 0.01                | 0.15       |
| (1,180) | 1:71:A:ALA:H  | 1:71:A:ALA:HA   | 15                  | 0.15     | 0.01                | 0.15       |
| (1,140) | 1:55:A:VAL:H  | 1:55:A:VAL:HA   | 15                  | 0.15     | 0.01                | 0.15       |
| (1,258) | 1:67:A:ILE:HA | 1:67:A:ILE:HB   | 15                  | 0.13     | 0.01                | 0.13       |
| (1,170) | 1:67:A:ILE:H  | 1:36:A:ILE:HA   | 14                  | 0.22     | 0.07                | 0.18       |
| (4,28)  | 1:52:A:LYS:H  | 1:71:A:ALA:O    | 14                  | 0.21     | 0.06                | 0.22       |
| (1,255) | 1:64:A:LYS:HA | 1:32:A:VAL:HA   | 13                  | 0.16     | 0.04                | 0.17       |
| (3,27)  | 1:30:A:HIS:HA | 1:32:A:VAL:HG11 | 12                  | 0.43     | 0.2                 | 0.35       |
| (3,27)  | 1:30:A:HIS:HA | 1:32:A:VAL:HG12 | 12                  | 0.43     | 0.2                 | 0.35       |
| (3,27)  | 1:30:A:HIS:HA | 1:32:A:VAL:HG13 | 12                  | 0.43     | 0.2                 | 0.35       |
| (1,179) | 1:70:A:ARG:H  | 1:70:A:ARG:HA   | 12                  | 0.13     | 0.02                | 0.12       |
| (1,61)  | 1:24:A:VAL:H  | 1:24:A:VAL:HB   | 10                  | 0.23     | 0.15                | 0.16       |
| (1,68)  | 1:26:A:LEU:H  | 1:26:A:LEU:HG   | 10                  | 0.14     | 0.01                | 0.14       |
| (2,60)  | 1:34:A:ALA:H  | 1:24:A:VAL:HG21 | 8                   | 0.61     | 0.13                | 0.6        |
| (2,60)  | 1:34:A:ALA:H  | 1:24:A:VAL:HG22 | 8                   | 0.61     | 0.13                | 0.6        |
| (2,60)  | 1:34:A:ALA:H  | 1:24:A:VAL:HG23 | 8                   | 0.61     | 0.13                | 0.6        |
| (4,16)  | 1:15:A:ASP:O  | 1:23:A:ARG:H    | 8                   | 0.19     | 0.04                | 0.18       |
| (2,186) | 1:25:A:GLU:HA | 1:23:A:ARG:HG3  | 8                   | 0.18     | 0.04                | 0.18       |
| (1,65)  | 1:25:A:GLU:H  | 1:12:A:THR:H    | 8                   | 0.14     | 0.03                | 0.14       |
| (1,253) | 1:63:A:SER:HA | 1:32:A:VAL:HA   | 8                   | 0.14     | 0.03                | 0.14       |
| (1,32)  | 1:14:A:VAL:H  | 1:24:A:VAL:HA   | 7                   | 0.18     | 0.08                | 0.15       |
| (4,6)   | 1:7:A:PHE:H   | 1:57:A:LEU:O    | 7                   | 0.18     | 0.05                | 0.17       |
| (1,54)  | 1:23:A:ARG:H  | 1:15:A:ASP:H    | 7                   | 0.16     | 0.03                | 0.16       |
| (4,15)  | 1:14:A:VAL:H  | 1:23:A:ARG:O    | 7                   | 0.15     | 0.02                | 0.14       |
| (1,115) | 1:45:A:ILE:H  | 1:45:A:ILE:HA   | 7                   | 0.14     | 0.02                | 0.14       |
| (1,158) | 1:62:A:LEU:H  | 1:62:A:LEU:HG   | 7                   | 0.14     | 0.02                | 0.14       |
| (1,33)  | 1:15:A:ASP:H  | 1:16:A:THR:H    | 7                   | 0.13     | 0.02                | 0.12       |
| (1,260) | 1:68:A:THR:HA | 1:68:A:THR:HB   | 6                   | 0.16     | 0.01                | 0.16       |
| (1,125) | 1:50:A:GLY:H  | 1:13:A:VAL:HB   | 6                   | 0.14     | 0.02                | 0.15       |
| (1,169) | 1:67:A:ILE:H  | 1:35:A:HIS:H    | 6                   | 0.12     | 0.01                | 0.12       |
| (1,108) | 1:42:A:LYS:H  | 1:42:A:LYS:HA   | 6                   | 0.12     | 0.01                | 0.11       |

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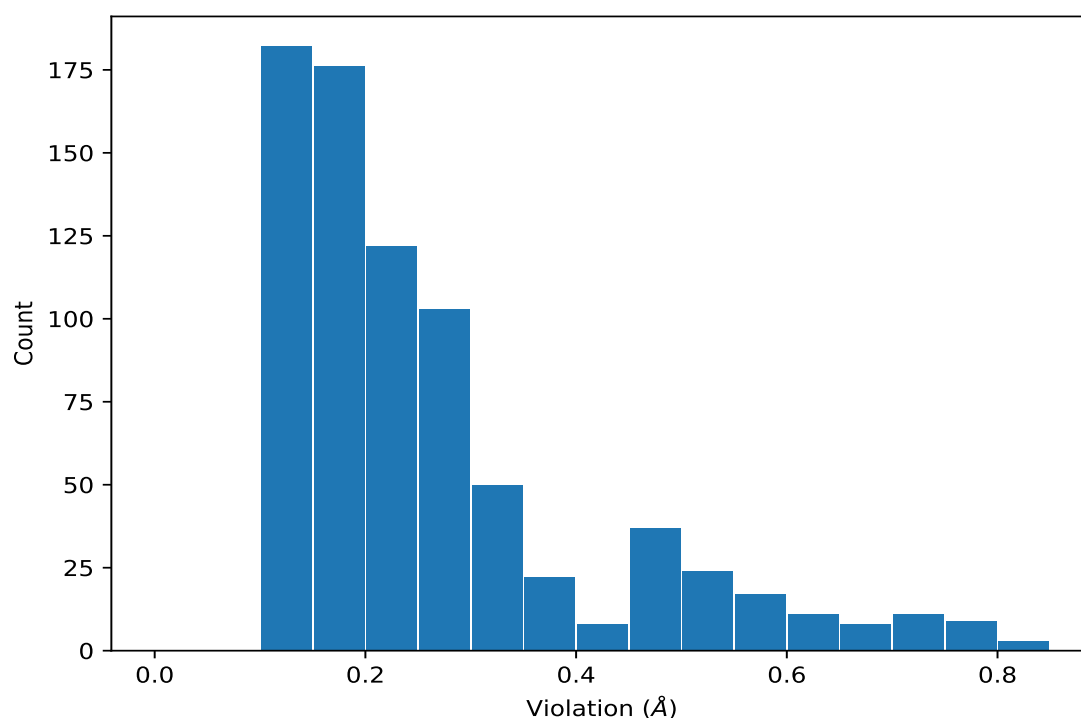
| Key     | Atom-1        | Atom-2        | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|---------------|---------------|---------------------|----------|---------------------|------------|
| (1,121) | 1:47:A:ILE:H  | 1:47:A:ILE:HB | 4                   | 0.3      | 0.23                | 0.2        |
| (1,252) | 1:62:A:LEU:HA | 1:62:A:LEU:HG | 4                   | 0.18     | 0.01                | 0.18       |
| (1,201) | 1:23:A:ARG:HA | 1:17:A:LEU:HG | 4                   | 0.16     | 0.05                | 0.15       |
| (1,4)   | 1:7:A:PHE:H   | 1:56:A:GLU:HA | 4                   | 0.14     | 0.03                | 0.14       |
| (1,208) | 1:31:A:VAL:HA | 1:31:A:VAL:HB | 4                   | 0.14     | 0.02                | 0.14       |
| (1,231) | 1:48:A:LEU:HA | 1:48:A:LEU:HG | 4                   | 0.12     | 0.01                | 0.12       |
| (1,97)  | 1:37:A:SER:H  | 1:37:A:SER:HA | 4                   | 0.12     | 0.02                | 0.12       |
| (1,196) | 1:17:A:LEU:HA | 1:17:A:LEU:HG | 3                   | 0.4      | 0.2                 | 0.54       |
| (1,116) | 1:45:A:ILE:H  | 1:44:A:TYR:HA | 3                   | 0.27     | 0.13                | 0.29       |
| (1,228) | 1:44:A:TYR:HA | 1:43:A:ASN:HA | 3                   | 0.2      | 0.07                | 0.22       |
| (1,112) | 1:44:A:TYR:H  | 1:42:A:LYS:H  | 3                   | 0.19     | 0.07                | 0.18       |
| (1,117) | 1:45:A:ILE:H  | 1:45:A:ILE:HB | 3                   | 0.16     | 0.06                | 0.14       |
| (1,53)  | 1:22:A:PHE:H  | 1:35:A:HIS:HA | 3                   | 0.13     | 0.02                | 0.14       |
| (1,114) | 1:44:A:TYR:H  | 1:44:A:TYR:HA | 3                   | 0.11     | 0.0                 | 0.11       |
| (1,45)  | 1:20:A:THR:H  | 1:21:A:MET:H  | 2                   | 0.16     | 0.04                | 0.16       |
| (4,14)  | 1:13:A:VAL:H  | 1:51:A:ASP:O  | 2                   | 0.14     | 0.02                | 0.14       |
| (4,12)  | 1:12:A:THR:H  | 1:25:A:GLU:O  | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,188) | 1:13:A:VAL:HA | 1:24:A:VAL:HA | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,202) | 1:24:A:VAL:HA | 1:13:A:VAL:HA | 2                   | 0.11     | 0.0                 | 0.11       |

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

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

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

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



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

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

| Key    | Atom-1        | Atom-2          | Model ID | Violation (Å) |
|--------|---------------|-----------------|----------|---------------|
| (2,60) | 1:34:A:ALA:H  | 1:24:A:VAL:HG21 | 2        | 0.83          |
| (2,60) | 1:34:A:ALA:H  | 1:24:A:VAL:HG22 | 2        | 0.83          |
| (2,60) | 1:34:A:ALA:H  | 1:24:A:VAL:HG23 | 2        | 0.83          |
| (1,26) | 1:13:A:VAL:H  | 1:52:A:LYS:HA   | 13       | 0.79          |
| (1,26) | 1:13:A:VAL:H  | 1:52:A:LYS:HA   | 11       | 0.78          |
| (1,26) | 1:13:A:VAL:H  | 1:52:A:LYS:HA   | 10       | 0.76          |
| (3,27) | 1:30:A:HIS:HA | 1:32:A:VAL:HG11 | 7        | 0.75          |
| (3,27) | 1:30:A:HIS:HA | 1:32:A:VAL:HG12 | 7        | 0.75          |
| (3,27) | 1:30:A:HIS:HA | 1:32:A:VAL:HG13 | 7        | 0.75          |
| (3,27) | 1:30:A:HIS:HA | 1:32:A:VAL:HG11 | 15       | 0.75          |
| (3,27) | 1:30:A:HIS:HA | 1:32:A:VAL:HG12 | 15       | 0.75          |
| (3,27) | 1:30:A:HIS:HA | 1:32:A:VAL:HG13 | 15       | 0.75          |
| (2,60) | 1:34:A:ALA:H  | 1:24:A:VAL:HG21 | 3        | 0.74          |
| (2,60) | 1:34:A:ALA:H  | 1:24:A:VAL:HG22 | 3        | 0.74          |
| (2,60) | 1:34:A:ALA:H  | 1:24:A:VAL:HG23 | 3        | 0.74          |
| (1,26) | 1:13:A:VAL:H  | 1:52:A:LYS:HA   | 4        | 0.73          |

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| Key     | Atom-1        | Atom-2          | Model ID | Violation (Å) |
|---------|---------------|-----------------|----------|---------------|
| (1,26)  | 1:13:A:VAL:H  | 1:52:A:LYS:HA   | 9        | 0.73          |
| (1,26)  | 1:13:A:VAL:H  | 1:52:A:LYS:HA   | 2        | 0.72          |
| (1,26)  | 1:13:A:VAL:H  | 1:52:A:LYS:HA   | 3        | 0.72          |
| (1,26)  | 1:13:A:VAL:H  | 1:52:A:LYS:HA   | 8        | 0.72          |
| (1,26)  | 1:13:A:VAL:H  | 1:52:A:LYS:HA   | 12       | 0.72          |
| (1,26)  | 1:13:A:VAL:H  | 1:52:A:LYS:HA   | 15       | 0.72          |
| (1,26)  | 1:13:A:VAL:H  | 1:52:A:LYS:HA   | 7        | 0.7           |
| (1,26)  | 1:13:A:VAL:H  | 1:52:A:LYS:HA   | 1        | 0.69          |
| (1,121) | 1:47:A:ILE:H  | 1:47:A:ILE:HB   | 15       | 0.68          |
| (2,60)  | 1:34:A:ALA:H  | 1:24:A:VAL:HG21 | 6        | 0.67          |
| (2,60)  | 1:34:A:ALA:H  | 1:24:A:VAL:HG22 | 6        | 0.67          |
| (2,60)  | 1:34:A:ALA:H  | 1:24:A:VAL:HG23 | 6        | 0.67          |
| (1,26)  | 1:13:A:VAL:H  | 1:52:A:LYS:HA   | 14       | 0.67          |
| (1,233) | 1:49:A:THR:HA | 1:13:A:VAL:HB   | 7        | 0.65          |
| (1,26)  | 1:13:A:VAL:H  | 1:52:A:LYS:HA   | 5        | 0.65          |
| (1,26)  | 1:13:A:VAL:H  | 1:52:A:LYS:HA   | 6        | 0.63          |
| (2,60)  | 1:34:A:ALA:H  | 1:24:A:VAL:HG21 | 7        | 0.62          |
| (2,60)  | 1:34:A:ALA:H  | 1:24:A:VAL:HG22 | 7        | 0.62          |
| (2,60)  | 1:34:A:ALA:H  | 1:24:A:VAL:HG23 | 7        | 0.62          |
| (1,233) | 1:49:A:THR:HA | 1:13:A:VAL:HB   | 14       | 0.62          |
| (3,27)  | 1:30:A:HIS:HA | 1:32:A:VAL:HG11 | 12       | 0.61          |
| (3,27)  | 1:30:A:HIS:HA | 1:32:A:VAL:HG12 | 12       | 0.61          |
| (3,27)  | 1:30:A:HIS:HA | 1:32:A:VAL:HG13 | 12       | 0.61          |
| (1,233) | 1:49:A:THR:HA | 1:13:A:VAL:HB   | 4        | 0.61          |
| (1,233) | 1:49:A:THR:HA | 1:13:A:VAL:HB   | 2        | 0.6           |
| (1,233) | 1:49:A:THR:HA | 1:13:A:VAL:HB   | 9        | 0.6           |
| (3,27)  | 1:30:A:HIS:HA | 1:32:A:VAL:HG11 | 8        | 0.59          |
| (3,27)  | 1:30:A:HIS:HA | 1:32:A:VAL:HG12 | 8        | 0.59          |
| (3,27)  | 1:30:A:HIS:HA | 1:32:A:VAL:HG13 | 8        | 0.59          |
| (1,233) | 1:49:A:THR:HA | 1:13:A:VAL:HB   | 3        | 0.59          |
| (2,60)  | 1:34:A:ALA:H  | 1:24:A:VAL:HG21 | 14       | 0.58          |
| (2,60)  | 1:34:A:ALA:H  | 1:24:A:VAL:HG22 | 14       | 0.58          |
| (2,60)  | 1:34:A:ALA:H  | 1:24:A:VAL:HG23 | 14       | 0.58          |
| (1,233) | 1:49:A:THR:HA | 1:13:A:VAL:HB   | 6        | 0.58          |
| (1,233) | 1:49:A:THR:HA | 1:13:A:VAL:HB   | 1        | 0.57          |
| (1,233) | 1:49:A:THR:HA | 1:13:A:VAL:HB   | 8        | 0.57          |
| (1,61)  | 1:24:A:VAL:H  | 1:24:A:VAL:HB   | 13       | 0.56          |
| (2,60)  | 1:34:A:ALA:H  | 1:24:A:VAL:HG21 | 15       | 0.55          |
| (2,60)  | 1:34:A:ALA:H  | 1:24:A:VAL:HG22 | 15       | 0.55          |
| (2,60)  | 1:34:A:ALA:H  | 1:24:A:VAL:HG23 | 15       | 0.55          |
| (1,233) | 1:49:A:THR:HA | 1:13:A:VAL:HB   | 10       | 0.55          |
| (1,233) | 1:49:A:THR:HA | 1:13:A:VAL:HB   | 12       | 0.55          |

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| Key     | Atom-1        | Atom-2          | Model ID | Violation (Å) |
|---------|---------------|-----------------|----------|---------------|
| (1,233) | 1:49:A:THR:HA | 1:13:A:VAL:HB   | 15       | 0.55          |
| (1,196) | 1:17:A:LEU:HA | 1:17:A:LEU:HG   | 6        | 0.54          |
| (1,196) | 1:17:A:LEU:HA | 1:17:A:LEU:HG   | 10       | 0.54          |
| (1,84)  | 1:33:A:THR:H  | 1:32:A:VAL:HB   | 7        | 0.54          |
| (1,175) | 1:69:A:TYR:H  | 1:68:A:THR:H    | 8        | 0.53          |
| (1,173) | 1:68:A:THR:H  | 1:69:A:TYR:H    | 8        | 0.53          |
| (3,27)  | 1:30:A:HIS:HA | 1:32:A:VAL:HG11 | 10       | 0.52          |
| (3,27)  | 1:30:A:HIS:HA | 1:32:A:VAL:HG12 | 10       | 0.52          |
| (3,27)  | 1:30:A:HIS:HA | 1:32:A:VAL:HG13 | 10       | 0.52          |
| (1,233) | 1:49:A:THR:HA | 1:13:A:VAL:HB   | 11       | 0.52          |
| (1,175) | 1:69:A:TYR:H  | 1:68:A:THR:H    | 2        | 0.51          |
| (1,175) | 1:69:A:TYR:H  | 1:68:A:THR:H    | 4        | 0.51          |
| (1,175) | 1:69:A:TYR:H  | 1:68:A:THR:H    | 9        | 0.51          |
| (1,173) | 1:68:A:THR:H  | 1:69:A:TYR:H    | 2        | 0.51          |
| (1,173) | 1:68:A:THR:H  | 1:69:A:TYR:H    | 4        | 0.51          |
| (1,173) | 1:68:A:THR:H  | 1:69:A:TYR:H    | 9        | 0.51          |
| (1,52)  | 1:22:A:PHE:H  | 1:34:A:ALA:H    | 5        | 0.51          |
| (2,60)  | 1:34:A:ALA:H  | 1:24:A:VAL:HG21 | 4        | 0.5           |
| (2,60)  | 1:34:A:ALA:H  | 1:24:A:VAL:HG22 | 4        | 0.5           |
| (2,60)  | 1:34:A:ALA:H  | 1:24:A:VAL:HG23 | 4        | 0.5           |
| (1,175) | 1:69:A:TYR:H  | 1:68:A:THR:H    | 11       | 0.5           |
| (1,175) | 1:69:A:TYR:H  | 1:68:A:THR:H    | 14       | 0.5           |
| (1,173) | 1:68:A:THR:H  | 1:69:A:TYR:H    | 11       | 0.5           |
| (1,173) | 1:68:A:THR:H  | 1:69:A:TYR:H    | 14       | 0.5           |
| (1,52)  | 1:22:A:PHE:H  | 1:34:A:ALA:H    | 11       | 0.5           |
| (1,233) | 1:49:A:THR:HA | 1:13:A:VAL:HB   | 5        | 0.49          |
| (1,175) | 1:69:A:TYR:H  | 1:68:A:THR:H    | 1        | 0.49          |
| (1,175) | 1:69:A:TYR:H  | 1:68:A:THR:H    | 3        | 0.49          |
| (1,175) | 1:69:A:TYR:H  | 1:68:A:THR:H    | 7        | 0.49          |
| (1,175) | 1:69:A:TYR:H  | 1:68:A:THR:H    | 10       | 0.49          |
| (1,175) | 1:69:A:TYR:H  | 1:68:A:THR:H    | 13       | 0.49          |
| (1,173) | 1:68:A:THR:H  | 1:69:A:TYR:H    | 1        | 0.49          |
| (1,173) | 1:68:A:THR:H  | 1:69:A:TYR:H    | 3        | 0.49          |
| (1,173) | 1:68:A:THR:H  | 1:69:A:TYR:H    | 7        | 0.49          |
| (1,173) | 1:68:A:THR:H  | 1:69:A:TYR:H    | 10       | 0.49          |
| (1,173) | 1:68:A:THR:H  | 1:69:A:TYR:H    | 13       | 0.49          |
| (1,61)  | 1:24:A:VAL:H  | 1:24:A:VAL:HB   | 10       | 0.49          |
| (1,210) | 1:32:A:VAL:HA | 1:32:A:VAL:HB   | 15       | 0.48          |
| (1,175) | 1:69:A:TYR:H  | 1:68:A:THR:H    | 5        | 0.48          |
| (1,175) | 1:69:A:TYR:H  | 1:68:A:THR:H    | 12       | 0.48          |
| (1,173) | 1:68:A:THR:H  | 1:69:A:TYR:H    | 5        | 0.48          |
| (1,173) | 1:68:A:THR:H  | 1:69:A:TYR:H    | 12       | 0.48          |

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| Key     | Atom-1        | Atom-2          | Model ID | Violation (Å) |
|---------|---------------|-----------------|----------|---------------|
| (1,210) | 1:32:A:VAL:HA | 1:32:A:VAL:HB   | 3        | 0.47          |
| (1,210) | 1:32:A:VAL:HA | 1:32:A:VAL:HB   | 7        | 0.47          |
| (1,210) | 1:32:A:VAL:HA | 1:32:A:VAL:HB   | 12       | 0.47          |
| (1,175) | 1:69:A:TYR:H  | 1:68:A:THR:H    | 6        | 0.47          |
| (1,175) | 1:69:A:TYR:H  | 1:68:A:THR:H    | 15       | 0.47          |
| (1,173) | 1:68:A:THR:H  | 1:69:A:TYR:H    | 6        | 0.47          |
| (1,173) | 1:68:A:THR:H  | 1:69:A:TYR:H    | 15       | 0.47          |
| (1,52)  | 1:22:A:PHE:H  | 1:34:A:ALA:H    | 12       | 0.47          |
| (1,233) | 1:49:A:THR:HA | 1:13:A:VAL:HB   | 13       | 0.46          |
| (1,210) | 1:32:A:VAL:HA | 1:32:A:VAL:HB   | 1        | 0.46          |
| (1,210) | 1:32:A:VAL:HA | 1:32:A:VAL:HB   | 6        | 0.46          |
| (1,210) | 1:32:A:VAL:HA | 1:32:A:VAL:HB   | 8        | 0.46          |
| (1,210) | 1:32:A:VAL:HA | 1:32:A:VAL:HB   | 10       | 0.46          |
| (1,210) | 1:32:A:VAL:HA | 1:32:A:VAL:HB   | 11       | 0.46          |
| (1,210) | 1:32:A:VAL:HA | 1:32:A:VAL:HB   | 14       | 0.46          |
| (1,52)  | 1:22:A:PHE:H  | 1:34:A:ALA:H    | 9        | 0.46          |
| (1,210) | 1:32:A:VAL:HA | 1:32:A:VAL:HB   | 4        | 0.45          |
| (1,84)  | 1:33:A:THR:H  | 1:32:A:VAL:HB   | 10       | 0.45          |
| (1,84)  | 1:33:A:THR:H  | 1:32:A:VAL:HB   | 15       | 0.45          |
| (1,30)  | 1:14:A:VAL:H  | 1:14:A:VAL:HB   | 3        | 0.45          |
| (1,210) | 1:32:A:VAL:HA | 1:32:A:VAL:HB   | 2        | 0.44          |
| (1,210) | 1:32:A:VAL:HA | 1:32:A:VAL:HB   | 5        | 0.44          |
| (1,210) | 1:32:A:VAL:HA | 1:32:A:VAL:HB   | 13       | 0.44          |
| (1,210) | 1:32:A:VAL:HA | 1:32:A:VAL:HB   | 9        | 0.43          |
| (1,30)  | 1:14:A:VAL:H  | 1:14:A:VAL:HB   | 15       | 0.43          |
| (1,116) | 1:45:A:ILE:H  | 1:44:A:TYR:HA   | 9        | 0.42          |
| (1,74)  | 1:30:A:HIS:H  | 1:26:A:LEU:H    | 4        | 0.4           |
| (1,74)  | 1:30:A:HIS:H  | 1:26:A:LEU:H    | 14       | 0.4           |
| (1,30)  | 1:14:A:VAL:H  | 1:14:A:VAL:HB   | 6        | 0.39          |
| (3,27)  | 1:30:A:HIS:HA | 1:32:A:VAL:HG11 | 11       | 0.38          |
| (3,27)  | 1:30:A:HIS:HA | 1:32:A:VAL:HG12 | 11       | 0.38          |
| (3,27)  | 1:30:A:HIS:HA | 1:32:A:VAL:HG13 | 11       | 0.38          |
| (2,60)  | 1:34:A:ALA:H  | 1:24:A:VAL:HG21 | 8        | 0.38          |
| (2,60)  | 1:34:A:ALA:H  | 1:24:A:VAL:HG22 | 8        | 0.38          |
| (2,60)  | 1:34:A:ALA:H  | 1:24:A:VAL:HG23 | 8        | 0.38          |
| (1,194) | 1:16:A:THR:HA | 1:22:A:PHE:HA   | 12       | 0.38          |
| (1,176) | 1:69:A:TYR:H  | 1:54:A:ARG:H    | 5        | 0.38          |
| (1,137) | 1:54:A:ARG:H  | 1:69:A:TYR:H    | 5        | 0.38          |
| (1,52)  | 1:22:A:PHE:H  | 1:34:A:ALA:H    | 1        | 0.38          |
| (1,74)  | 1:30:A:HIS:H  | 1:26:A:LEU:H    | 15       | 0.37          |
| (4,33)  | 1:64:A:LYS:O  | 1:58:A:THR:H    | 12       | 0.36          |
| (1,194) | 1:16:A:THR:HA | 1:22:A:PHE:HA   | 5        | 0.36          |

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| Key     | Atom-1        | Atom-2          | Model ID | Violation (Å) |
|---------|---------------|-----------------|----------|---------------|
| (1,74)  | 1:30:A:HIS:H  | 1:26:A:LEU:H    | 6        | 0.36          |
| (1,74)  | 1:30:A:HIS:H  | 1:26:A:LEU:H    | 13       | 0.36          |
| (4,18)  | 1:17:A:LEU:O  | 1:21:A:MET:H    | 5        | 0.35          |
| (1,170) | 1:67:A:ILE:H  | 1:36:A:ILE:HA   | 13       | 0.35          |
| (1,74)  | 1:30:A:HIS:H  | 1:26:A:LEU:H    | 2        | 0.35          |
| (1,74)  | 1:30:A:HIS:H  | 1:26:A:LEU:H    | 8        | 0.35          |
| (1,74)  | 1:30:A:HIS:H  | 1:26:A:LEU:H    | 10       | 0.35          |
| (1,74)  | 1:30:A:HIS:H  | 1:26:A:LEU:H    | 11       | 0.35          |
| (4,33)  | 1:64:A:LYS:O  | 1:58:A:THR:H    | 1        | 0.34          |
| (4,33)  | 1:64:A:LYS:O  | 1:58:A:THR:H    | 7        | 0.34          |
| (4,18)  | 1:17:A:LEU:O  | 1:21:A:MET:H    | 13       | 0.34          |
| (1,176) | 1:69:A:TYR:H  | 1:54:A:ARG:H    | 1        | 0.34          |
| (1,176) | 1:69:A:TYR:H  | 1:54:A:ARG:H    | 8        | 0.34          |
| (1,176) | 1:69:A:TYR:H  | 1:54:A:ARG:H    | 14       | 0.34          |
| (1,170) | 1:67:A:ILE:H  | 1:36:A:ILE:HA   | 9        | 0.34          |
| (1,137) | 1:54:A:ARG:H  | 1:69:A:TYR:H    | 1        | 0.34          |
| (1,137) | 1:54:A:ARG:H  | 1:69:A:TYR:H    | 8        | 0.34          |
| (1,137) | 1:54:A:ARG:H  | 1:69:A:TYR:H    | 14       | 0.34          |
| (1,32)  | 1:14:A:VAL:H  | 1:24:A:VAL:HA   | 12       | 0.34          |
| (4,33)  | 1:64:A:LYS:O  | 1:58:A:THR:H    | 15       | 0.33          |
| (4,28)  | 1:52:A:LYS:H  | 1:71:A:ALA:O    | 13       | 0.33          |
| (1,209) | 1:31:A:VAL:HA | 1:25:A:GLU:HA   | 13       | 0.33          |
| (1,204) | 1:25:A:GLU:HA | 1:31:A:VAL:HA   | 13       | 0.33          |
| (1,30)  | 1:14:A:VAL:H  | 1:14:A:VAL:HB   | 13       | 0.33          |
| (4,33)  | 1:64:A:LYS:O  | 1:58:A:THR:H    | 9        | 0.32          |
| (3,27)  | 1:30:A:HIS:HA | 1:32:A:VAL:HG11 | 4        | 0.32          |
| (3,27)  | 1:30:A:HIS:HA | 1:32:A:VAL:HG12 | 4        | 0.32          |
| (3,27)  | 1:30:A:HIS:HA | 1:32:A:VAL:HG13 | 4        | 0.32          |
| (3,27)  | 1:30:A:HIS:HA | 1:32:A:VAL:HG11 | 14       | 0.32          |
| (3,27)  | 1:30:A:HIS:HA | 1:32:A:VAL:HG12 | 14       | 0.32          |
| (3,27)  | 1:30:A:HIS:HA | 1:32:A:VAL:HG13 | 14       | 0.32          |
| (1,209) | 1:31:A:VAL:HA | 1:25:A:GLU:HA   | 10       | 0.32          |
| (1,204) | 1:25:A:GLU:HA | 1:31:A:VAL:HA   | 10       | 0.32          |
| (1,167) | 1:66:A:ARG:H  | 1:57:A:LEU:HA   | 13       | 0.32          |
| (1,74)  | 1:30:A:HIS:H  | 1:26:A:LEU:H    | 12       | 0.32          |
| (4,18)  | 1:17:A:LEU:O  | 1:21:A:MET:H    | 11       | 0.31          |
| (4,18)  | 1:17:A:LEU:O  | 1:21:A:MET:H    | 15       | 0.31          |
| (1,223) | 1:36:A:ILE:HA | 1:36:A:ILE:HB   | 14       | 0.31          |
| (1,194) | 1:16:A:THR:HA | 1:22:A:PHE:HA   | 1        | 0.31          |
| (1,194) | 1:16:A:THR:HA | 1:22:A:PHE:HA   | 10       | 0.31          |
| (1,176) | 1:69:A:TYR:H  | 1:54:A:ARG:H    | 6        | 0.31          |
| (1,137) | 1:54:A:ARG:H  | 1:69:A:TYR:H    | 6        | 0.31          |

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| Key     | Atom-1        | Atom-2          | Model ID | Violation (Å) |
|---------|---------------|-----------------|----------|---------------|
| (1,84)  | 1:33:A:THR:H  | 1:32:A:VAL:HB   | 4        | 0.31          |
| (1,74)  | 1:30:A:HIS:H  | 1:26:A:LEU:H    | 5        | 0.31          |
| (1,34)  | 1:15:A:ASP:H  | 1:14:A:VAL:H    | 1        | 0.31          |
| (1,27)  | 1:14:A:VAL:H  | 1:15:A:ASP:H    | 1        | 0.31          |
| (4,33)  | 1:64:A:LYS:O  | 1:58:A:THR:H    | 14       | 0.3           |
| (4,18)  | 1:17:A:LEU:O  | 1:21:A:MET:H    | 2        | 0.3           |
| (4,18)  | 1:17:A:LEU:O  | 1:21:A:MET:H    | 3        | 0.3           |
| (4,18)  | 1:17:A:LEU:O  | 1:21:A:MET:H    | 12       | 0.3           |
| (1,176) | 1:69:A:TYR:H  | 1:54:A:ARG:H    | 10       | 0.3           |
| (1,170) | 1:67:A:ILE:H  | 1:36:A:ILE:HA   | 15       | 0.3           |
| (1,137) | 1:54:A:ARG:H  | 1:69:A:TYR:H    | 10       | 0.3           |
| (1,74)  | 1:30:A:HIS:H  | 1:26:A:LEU:H    | 1        | 0.3           |
| (1,34)  | 1:15:A:ASP:H  | 1:14:A:VAL:H    | 5        | 0.3           |
| (1,34)  | 1:15:A:ASP:H  | 1:14:A:VAL:H    | 12       | 0.3           |
| (1,27)  | 1:14:A:VAL:H  | 1:15:A:ASP:H    | 5        | 0.3           |
| (1,27)  | 1:14:A:VAL:H  | 1:15:A:ASP:H    | 12       | 0.3           |
| (4,33)  | 1:64:A:LYS:O  | 1:58:A:THR:H    | 6        | 0.29          |
| (4,18)  | 1:17:A:LEU:O  | 1:21:A:MET:H    | 6        | 0.29          |
| (4,18)  | 1:17:A:LEU:O  | 1:21:A:MET:H    | 14       | 0.29          |
| (1,209) | 1:31:A:VAL:HA | 1:25:A:GLU:HA   | 15       | 0.29          |
| (1,204) | 1:25:A:GLU:HA | 1:31:A:VAL:HA   | 15       | 0.29          |
| (1,121) | 1:47:A:ILE:H  | 1:47:A:ILE:HB   | 8        | 0.29          |
| (1,116) | 1:45:A:ILE:H  | 1:44:A:TYR:HA   | 8        | 0.29          |
| (1,112) | 1:44:A:TYR:H  | 1:42:A:LYS:H    | 9        | 0.29          |
| (1,77)  | 1:32:A:VAL:H  | 1:24:A:VAL:H    | 8        | 0.29          |
| (1,77)  | 1:32:A:VAL:H  | 1:24:A:VAL:H    | 14       | 0.29          |
| (1,74)  | 1:30:A:HIS:H  | 1:26:A:LEU:H    | 9        | 0.29          |
| (1,62)  | 1:24:A:VAL:H  | 1:32:A:VAL:H    | 8        | 0.29          |
| (1,62)  | 1:24:A:VAL:H  | 1:32:A:VAL:H    | 14       | 0.29          |
| (1,34)  | 1:15:A:ASP:H  | 1:14:A:VAL:H    | 8        | 0.29          |
| (1,30)  | 1:14:A:VAL:H  | 1:14:A:VAL:HB   | 7        | 0.29          |
| (1,27)  | 1:14:A:VAL:H  | 1:15:A:ASP:H    | 8        | 0.29          |
| (4,18)  | 1:17:A:LEU:O  | 1:21:A:MET:H    | 1        | 0.28          |
| (4,18)  | 1:17:A:LEU:O  | 1:21:A:MET:H    | 4        | 0.28          |
| (4,18)  | 1:17:A:LEU:O  | 1:21:A:MET:H    | 10       | 0.28          |
| (3,27)  | 1:30:A:HIS:HA | 1:32:A:VAL:HG11 | 3        | 0.28          |
| (3,27)  | 1:30:A:HIS:HA | 1:32:A:VAL:HG12 | 3        | 0.28          |
| (3,27)  | 1:30:A:HIS:HA | 1:32:A:VAL:HG13 | 3        | 0.28          |
| (1,209) | 1:31:A:VAL:HA | 1:25:A:GLU:HA   | 11       | 0.28          |
| (1,209) | 1:31:A:VAL:HA | 1:25:A:GLU:HA   | 14       | 0.28          |
| (1,204) | 1:25:A:GLU:HA | 1:31:A:VAL:HA   | 11       | 0.28          |
| (1,204) | 1:25:A:GLU:HA | 1:31:A:VAL:HA   | 14       | 0.28          |

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| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,194) | 1:16:A:THR:HA | 1:22:A:PHE:HA | 3        | 0.28          |
| (1,194) | 1:16:A:THR:HA | 1:22:A:PHE:HA | 8        | 0.28          |
| (1,176) | 1:69:A:TYR:H  | 1:54:A:ARG:H  | 3        | 0.28          |
| (1,176) | 1:69:A:TYR:H  | 1:54:A:ARG:H  | 7        | 0.28          |
| (1,176) | 1:69:A:TYR:H  | 1:54:A:ARG:H  | 15       | 0.28          |
| (1,137) | 1:54:A:ARG:H  | 1:69:A:TYR:H  | 3        | 0.28          |
| (1,137) | 1:54:A:ARG:H  | 1:69:A:TYR:H  | 7        | 0.28          |
| (1,137) | 1:54:A:ARG:H  | 1:69:A:TYR:H  | 15       | 0.28          |
| (1,84)  | 1:33:A:THR:H  | 1:32:A:VAL:HB | 8        | 0.28          |
| (1,34)  | 1:15:A:ASP:H  | 1:14:A:VAL:H  | 7        | 0.28          |
| (1,30)  | 1:14:A:VAL:H  | 1:14:A:VAL:HB | 1        | 0.28          |
| (1,30)  | 1:14:A:VAL:H  | 1:14:A:VAL:HB | 5        | 0.28          |
| (1,27)  | 1:14:A:VAL:H  | 1:15:A:ASP:H  | 7        | 0.28          |
| (4,28)  | 1:52:A:LYS:H  | 1:71:A:ALA:O  | 5        | 0.27          |
| (4,18)  | 1:17:A:LEU:O  | 1:21:A:MET:H  | 7        | 0.27          |
| (4,18)  | 1:17:A:LEU:O  | 1:21:A:MET:H  | 8        | 0.27          |
| (1,257) | 1:66:A:ARG:HA | 1:34:A:ALA:HA | 2        | 0.27          |
| (1,228) | 1:44:A:TYR:HA | 1:43:A:ASN:HA | 4        | 0.27          |
| (1,214) | 1:33:A:THR:HA | 1:33:A:THR:HB | 9        | 0.27          |
| (1,209) | 1:31:A:VAL:HA | 1:25:A:GLU:HA | 1        | 0.27          |
| (1,209) | 1:31:A:VAL:HA | 1:25:A:GLU:HA | 3        | 0.27          |
| (1,209) | 1:31:A:VAL:HA | 1:25:A:GLU:HA | 5        | 0.27          |
| (1,209) | 1:31:A:VAL:HA | 1:25:A:GLU:HA | 6        | 0.27          |
| (1,204) | 1:25:A:GLU:HA | 1:31:A:VAL:HA | 1        | 0.27          |
| (1,204) | 1:25:A:GLU:HA | 1:31:A:VAL:HA | 3        | 0.27          |
| (1,204) | 1:25:A:GLU:HA | 1:31:A:VAL:HA | 5        | 0.27          |
| (1,204) | 1:25:A:GLU:HA | 1:31:A:VAL:HA | 6        | 0.27          |
| (1,194) | 1:16:A:THR:HA | 1:22:A:PHE:HA | 4        | 0.27          |
| (1,194) | 1:16:A:THR:HA | 1:22:A:PHE:HA | 15       | 0.27          |
| (1,176) | 1:69:A:TYR:H  | 1:54:A:ARG:H  | 4        | 0.27          |
| (1,176) | 1:69:A:TYR:H  | 1:54:A:ARG:H  | 12       | 0.27          |
| (1,167) | 1:66:A:ARG:H  | 1:57:A:LEU:HA | 4        | 0.27          |
| (1,137) | 1:54:A:ARG:H  | 1:69:A:TYR:H  | 4        | 0.27          |
| (1,137) | 1:54:A:ARG:H  | 1:69:A:TYR:H  | 12       | 0.27          |
| (1,77)  | 1:32:A:VAL:H  | 1:24:A:VAL:H  | 4        | 0.27          |
| (1,77)  | 1:32:A:VAL:H  | 1:24:A:VAL:H  | 7        | 0.27          |
| (1,62)  | 1:24:A:VAL:H  | 1:32:A:VAL:H  | 4        | 0.27          |
| (1,62)  | 1:24:A:VAL:H  | 1:32:A:VAL:H  | 7        | 0.27          |
| (1,30)  | 1:14:A:VAL:H  | 1:14:A:VAL:HB | 9        | 0.27          |
| (1,30)  | 1:14:A:VAL:H  | 1:14:A:VAL:HB | 12       | 0.27          |
| (4,33)  | 1:64:A:LYS:O  | 1:58:A:THR:H  | 5        | 0.26          |
| (4,33)  | 1:64:A:LYS:O  | 1:58:A:THR:H  | 8        | 0.26          |

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| Key     | Atom-1        | Atom-2          | Model ID | Violation (Å) |
|---------|---------------|-----------------|----------|---------------|
| (4,18)  | 1:17:A:LEU:O  | 1:21:A:MET:H    | 9        | 0.26          |
| (4,16)  | 1:15:A:ASP:O  | 1:23:A:ARG:H    | 1        | 0.26          |
| (4,6)   | 1:7:A:PHE:H   | 1:57:A:LEU:O    | 10       | 0.26          |
| (1,257) | 1:66:A:ARG:HA | 1:34:A:ALA:HA   | 4        | 0.26          |
| (1,257) | 1:66:A:ARG:HA | 1:34:A:ALA:HA   | 13       | 0.26          |
| (1,214) | 1:33:A:THR:HA | 1:33:A:THR:HB   | 4        | 0.26          |
| (1,176) | 1:69:A:TYR:H  | 1:54:A:ARG:H    | 9        | 0.26          |
| (1,176) | 1:69:A:TYR:H  | 1:54:A:ARG:H    | 11       | 0.26          |
| (1,176) | 1:69:A:TYR:H  | 1:54:A:ARG:H    | 13       | 0.26          |
| (1,170) | 1:67:A:ILE:H  | 1:36:A:ILE:HA   | 4        | 0.26          |
| (1,170) | 1:67:A:ILE:H  | 1:36:A:ILE:HA   | 11       | 0.26          |
| (1,167) | 1:66:A:ARG:H  | 1:57:A:LEU:HA   | 11       | 0.26          |
| (1,137) | 1:54:A:ARG:H  | 1:69:A:TYR:H    | 9        | 0.26          |
| (1,137) | 1:54:A:ARG:H  | 1:69:A:TYR:H    | 11       | 0.26          |
| (1,137) | 1:54:A:ARG:H  | 1:69:A:TYR:H    | 13       | 0.26          |
| (1,129) | 1:53:A:VAL:H  | 1:12:A:THR:HA   | 6        | 0.26          |
| (1,84)  | 1:33:A:THR:H  | 1:32:A:VAL:HB   | 3        | 0.26          |
| (1,34)  | 1:15:A:ASP:H  | 1:14:A:VAL:H    | 4        | 0.26          |
| (1,30)  | 1:14:A:VAL:H  | 1:14:A:VAL:HB   | 10       | 0.26          |
| (1,27)  | 1:14:A:VAL:H  | 1:15:A:ASP:H    | 4        | 0.26          |
| (4,28)  | 1:52:A:LYS:H  | 1:71:A:ALA:O    | 10       | 0.25          |
| (3,27)  | 1:30:A:HIS:HA | 1:32:A:VAL:HG11 | 6        | 0.25          |
| (3,27)  | 1:30:A:HIS:HA | 1:32:A:VAL:HG12 | 6        | 0.25          |
| (3,27)  | 1:30:A:HIS:HA | 1:32:A:VAL:HG13 | 6        | 0.25          |
| (2,186) | 1:25:A:GLU:HA | 1:23:A:ARG:HG3  | 14       | 0.25          |
| (1,214) | 1:33:A:THR:HA | 1:33:A:THR:HB   | 10       | 0.25          |
| (1,214) | 1:33:A:THR:HA | 1:33:A:THR:HB   | 11       | 0.25          |
| (1,194) | 1:16:A:THR:HA | 1:22:A:PHE:HA   | 7        | 0.25          |
| (1,176) | 1:69:A:TYR:H  | 1:54:A:ARG:H    | 2        | 0.25          |
| (1,137) | 1:54:A:ARG:H  | 1:69:A:TYR:H    | 2        | 0.25          |
| (1,117) | 1:45:A:ILE:H  | 1:45:A:ILE:HB   | 10       | 0.25          |
| (1,84)  | 1:33:A:THR:H  | 1:32:A:VAL:HB   | 14       | 0.25          |
| (1,74)  | 1:30:A:HIS:H  | 1:26:A:LEU:H    | 7        | 0.25          |
| (1,34)  | 1:15:A:ASP:H  | 1:14:A:VAL:H    | 15       | 0.25          |
| (1,27)  | 1:14:A:VAL:H  | 1:15:A:ASP:H    | 15       | 0.25          |
| (4,33)  | 1:64:A:LYS:O  | 1:58:A:THR:H    | 3        | 0.24          |
| (4,28)  | 1:52:A:LYS:H  | 1:71:A:ALA:O    | 11       | 0.24          |
| (4,28)  | 1:52:A:LYS:H  | 1:71:A:ALA:O    | 12       | 0.24          |
| (4,16)  | 1:15:A:ASP:O  | 1:23:A:ARG:H    | 9        | 0.24          |
| (1,257) | 1:66:A:ARG:HA | 1:34:A:ALA:HA   | 3        | 0.24          |
| (1,257) | 1:66:A:ARG:HA | 1:34:A:ALA:HA   | 10       | 0.24          |
| (1,255) | 1:64:A:LYS:HA | 1:32:A:VAL:HA   | 12       | 0.24          |

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| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,214) | 1:33:A:THR:HA | 1:33:A:THR:HB | 5        | 0.24          |
| (1,214) | 1:33:A:THR:HA | 1:33:A:THR:HB | 6        | 0.24          |
| (1,209) | 1:31:A:VAL:HA | 1:25:A:GLU:HA | 4        | 0.24          |
| (1,209) | 1:31:A:VAL:HA | 1:25:A:GLU:HA | 9        | 0.24          |
| (1,209) | 1:31:A:VAL:HA | 1:25:A:GLU:HA | 12       | 0.24          |
| (1,204) | 1:25:A:GLU:HA | 1:31:A:VAL:HA | 4        | 0.24          |
| (1,204) | 1:25:A:GLU:HA | 1:31:A:VAL:HA | 9        | 0.24          |
| (1,204) | 1:25:A:GLU:HA | 1:31:A:VAL:HA | 12       | 0.24          |
| (1,194) | 1:16:A:THR:HA | 1:22:A:PHE:HA | 2        | 0.24          |
| (1,194) | 1:16:A:THR:HA | 1:22:A:PHE:HA | 14       | 0.24          |
| (1,167) | 1:66:A:ARG:H  | 1:57:A:LEU:HA | 1        | 0.24          |
| (1,129) | 1:53:A:VAL:H  | 1:12:A:THR:HA | 2        | 0.24          |
| (1,129) | 1:53:A:VAL:H  | 1:12:A:THR:HA | 7        | 0.24          |
| (1,84)  | 1:33:A:THR:H  | 1:32:A:VAL:HB | 12       | 0.24          |
| (1,77)  | 1:32:A:VAL:H  | 1:24:A:VAL:H  | 15       | 0.24          |
| (1,74)  | 1:30:A:HIS:H  | 1:26:A:LEU:H  | 3        | 0.24          |
| (1,62)  | 1:24:A:VAL:H  | 1:32:A:VAL:H  | 15       | 0.24          |
| (1,34)  | 1:15:A:ASP:H  | 1:14:A:VAL:H  | 10       | 0.24          |
| (1,32)  | 1:14:A:VAL:H  | 1:24:A:VAL:HA | 1        | 0.24          |
| (1,27)  | 1:14:A:VAL:H  | 1:15:A:ASP:H  | 10       | 0.24          |
| (4,33)  | 1:64:A:LYS:O  | 1:58:A:THR:H  | 13       | 0.23          |
| (4,28)  | 1:52:A:LYS:H  | 1:71:A:ALA:O  | 3        | 0.23          |
| (4,28)  | 1:52:A:LYS:H  | 1:71:A:ALA:O  | 9        | 0.23          |
| (1,257) | 1:66:A:ARG:HA | 1:34:A:ALA:HA | 6        | 0.23          |
| (1,214) | 1:33:A:THR:HA | 1:33:A:THR:HB | 1        | 0.23          |
| (1,214) | 1:33:A:THR:HA | 1:33:A:THR:HB | 8        | 0.23          |
| (1,129) | 1:53:A:VAL:H  | 1:12:A:THR:HA | 3        | 0.23          |
| (1,129) | 1:53:A:VAL:H  | 1:12:A:THR:HA | 8        | 0.23          |
| (1,77)  | 1:32:A:VAL:H  | 1:24:A:VAL:H  | 3        | 0.23          |
| (1,77)  | 1:32:A:VAL:H  | 1:24:A:VAL:H  | 6        | 0.23          |
| (1,62)  | 1:24:A:VAL:H  | 1:32:A:VAL:H  | 3        | 0.23          |
| (1,62)  | 1:24:A:VAL:H  | 1:32:A:VAL:H  | 6        | 0.23          |
| (1,34)  | 1:15:A:ASP:H  | 1:14:A:VAL:H  | 9        | 0.23          |
| (1,34)  | 1:15:A:ASP:H  | 1:14:A:VAL:H  | 14       | 0.23          |
| (1,27)  | 1:14:A:VAL:H  | 1:15:A:ASP:H  | 9        | 0.23          |
| (1,27)  | 1:14:A:VAL:H  | 1:15:A:ASP:H  | 14       | 0.23          |
| (4,33)  | 1:64:A:LYS:O  | 1:58:A:THR:H  | 2        | 0.22          |
| (4,28)  | 1:52:A:LYS:H  | 1:71:A:ALA:O  | 4        | 0.22          |
| (4,6)   | 1:7:A:PHE:H   | 1:57:A:LEU:O  | 14       | 0.22          |
| (1,257) | 1:66:A:ARG:HA | 1:34:A:ALA:HA | 1        | 0.22          |
| (1,257) | 1:66:A:ARG:HA | 1:34:A:ALA:HA | 5        | 0.22          |
| (1,228) | 1:44:A:TYR:HA | 1:43:A:ASN:HA | 8        | 0.22          |

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| Key     | Atom-1        | Atom-2         | Model ID | Violation (Å) |
|---------|---------------|----------------|----------|---------------|
| (1,214) | 1:33:A:THR:HA | 1:33:A:THR:HB  | 3        | 0.22          |
| (1,214) | 1:33:A:THR:HA | 1:33:A:THR:HB  | 12       | 0.22          |
| (1,214) | 1:33:A:THR:HA | 1:33:A:THR:HB  | 13       | 0.22          |
| (1,209) | 1:31:A:VAL:HA | 1:25:A:GLU:HA  | 2        | 0.22          |
| (1,209) | 1:31:A:VAL:HA | 1:25:A:GLU:HA  | 7        | 0.22          |
| (1,204) | 1:25:A:GLU:HA | 1:31:A:VAL:HA  | 2        | 0.22          |
| (1,204) | 1:25:A:GLU:HA | 1:31:A:VAL:HA  | 7        | 0.22          |
| (1,194) | 1:16:A:THR:HA | 1:22:A:PHE:HA  | 9        | 0.22          |
| (1,167) | 1:66:A:ARG:H  | 1:57:A:LEU:HA  | 5        | 0.22          |
| (1,167) | 1:66:A:ARG:H  | 1:57:A:LEU:HA  | 10       | 0.22          |
| (1,164) | 1:65:A:GLY:H  | 1:34:A:ALA:HA  | 2        | 0.22          |
| (1,129) | 1:53:A:VAL:H  | 1:12:A:THR:HA  | 15       | 0.22          |
| (1,54)  | 1:23:A:ARG:H  | 1:15:A:ASP:H   | 11       | 0.22          |
| (1,36)  | 1:15:A:ASP:H  | 1:14:A:VAL:HB  | 11       | 0.22          |
| (1,34)  | 1:15:A:ASP:H  | 1:14:A:VAL:H   | 3        | 0.22          |
| (1,34)  | 1:15:A:ASP:H  | 1:14:A:VAL:H   | 6        | 0.22          |
| (1,34)  | 1:15:A:ASP:H  | 1:14:A:VAL:H   | 11       | 0.22          |
| (1,34)  | 1:15:A:ASP:H  | 1:14:A:VAL:H   | 13       | 0.22          |
| (1,30)  | 1:14:A:VAL:H  | 1:14:A:VAL:HB  | 14       | 0.22          |
| (1,27)  | 1:14:A:VAL:H  | 1:15:A:ASP:H   | 3        | 0.22          |
| (1,27)  | 1:14:A:VAL:H  | 1:15:A:ASP:H   | 6        | 0.22          |
| (1,27)  | 1:14:A:VAL:H  | 1:15:A:ASP:H   | 11       | 0.22          |
| (1,27)  | 1:14:A:VAL:H  | 1:15:A:ASP:H   | 13       | 0.22          |
| (4,33)  | 1:64:A:LYS:O  | 1:58:A:THR:H   | 10       | 0.21          |
| (2,186) | 1:25:A:GLU:HA | 1:23:A:ARG:HG3 | 7        | 0.21          |
| (1,255) | 1:64:A:LYS:HA | 1:32:A:VAL:HA  | 4        | 0.21          |
| (1,253) | 1:63:A:SER:HA | 1:32:A:VAL:HA  | 8        | 0.21          |
| (1,214) | 1:33:A:THR:HA | 1:33:A:THR:HB  | 15       | 0.21          |
| (1,201) | 1:23:A:ARG:HA | 1:17:A:LEU:HG  | 1        | 0.21          |
| (1,194) | 1:16:A:THR:HA | 1:22:A:PHE:HA  | 13       | 0.21          |
| (1,170) | 1:67:A:ILE:H  | 1:36:A:ILE:HA  | 5        | 0.21          |
| (1,167) | 1:66:A:ARG:H  | 1:57:A:LEU:HA  | 2        | 0.21          |
| (1,167) | 1:66:A:ARG:H  | 1:57:A:LEU:HA  | 3        | 0.21          |
| (1,167) | 1:66:A:ARG:H  | 1:57:A:LEU:HA  | 9        | 0.21          |
| (1,164) | 1:65:A:GLY:H  | 1:34:A:ALA:HA  | 13       | 0.21          |
| (1,129) | 1:53:A:VAL:H  | 1:12:A:THR:HA  | 14       | 0.21          |
| (1,77)  | 1:32:A:VAL:H  | 1:24:A:VAL:H   | 2        | 0.21          |
| (1,62)  | 1:24:A:VAL:H  | 1:32:A:VAL:H   | 2        | 0.21          |
| (1,52)  | 1:22:A:PHE:H  | 1:34:A:ALA:H   | 13       | 0.21          |
| (1,45)  | 1:20:A:THR:H  | 1:21:A:MET:H   | 5        | 0.21          |
| (1,36)  | 1:15:A:ASP:H  | 1:14:A:VAL:HB  | 2        | 0.21          |
| (1,36)  | 1:15:A:ASP:H  | 1:14:A:VAL:HB  | 4        | 0.21          |

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| Key     | Atom-1        | Atom-2          | Model ID | Violation (Å) |
|---------|---------------|-----------------|----------|---------------|
| (1,36)  | 1:15:A:ASP:H  | 1:14:A:VAL:HB   | 10       | 0.21          |
| (1,36)  | 1:15:A:ASP:H  | 1:14:A:VAL:HB   | 14       | 0.21          |
| (1,34)  | 1:15:A:ASP:H  | 1:14:A:VAL:H    | 2        | 0.21          |
| (1,30)  | 1:14:A:VAL:H  | 1:14:A:VAL:HB   | 2        | 0.21          |
| (1,30)  | 1:14:A:VAL:H  | 1:14:A:VAL:HB   | 8        | 0.21          |
| (1,27)  | 1:14:A:VAL:H  | 1:15:A:ASP:H    | 2        | 0.21          |
| (4,33)  | 1:64:A:LYS:O  | 1:58:A:THR:H    | 4        | 0.2           |
| (4,33)  | 1:64:A:LYS:O  | 1:58:A:THR:H    | 11       | 0.2           |
| (4,16)  | 1:15:A:ASP:O  | 1:23:A:ARG:H    | 5        | 0.2           |
| (3,27)  | 1:30:A:HIS:HA | 1:32:A:VAL:HG11 | 1        | 0.2           |
| (3,27)  | 1:30:A:HIS:HA | 1:32:A:VAL:HG12 | 1        | 0.2           |
| (3,27)  | 1:30:A:HIS:HA | 1:32:A:VAL:HG13 | 1        | 0.2           |
| (2,186) | 1:25:A:GLU:HA | 1:23:A:ARG:HG3  | 8        | 0.2           |
| (1,257) | 1:66:A:ARG:HA | 1:34:A:ALA:HA   | 8        | 0.2           |
| (1,257) | 1:66:A:ARG:HA | 1:34:A:ALA:HA   | 9        | 0.2           |
| (1,257) | 1:66:A:ARG:HA | 1:34:A:ALA:HA   | 11       | 0.2           |
| (1,257) | 1:66:A:ARG:HA | 1:34:A:ALA:HA   | 14       | 0.2           |
| (1,255) | 1:64:A:LYS:HA | 1:32:A:VAL:HA   | 14       | 0.2           |
| (1,252) | 1:62:A:LEU:HA | 1:62:A:LEU:HG   | 12       | 0.2           |
| (1,164) | 1:65:A:GLY:H  | 1:34:A:ALA:HA   | 1        | 0.2           |
| (1,164) | 1:65:A:GLY:H  | 1:34:A:ALA:HA   | 4        | 0.2           |
| (1,164) | 1:65:A:GLY:H  | 1:34:A:ALA:HA   | 6        | 0.2           |
| (1,164) | 1:65:A:GLY:H  | 1:34:A:ALA:HA   | 8        | 0.2           |
| (1,77)  | 1:32:A:VAL:H  | 1:24:A:VAL:H    | 5        | 0.2           |
| (1,77)  | 1:32:A:VAL:H  | 1:24:A:VAL:H    | 9        | 0.2           |
| (1,77)  | 1:32:A:VAL:H  | 1:24:A:VAL:H    | 12       | 0.2           |
| (1,62)  | 1:24:A:VAL:H  | 1:32:A:VAL:H    | 5        | 0.2           |
| (1,62)  | 1:24:A:VAL:H  | 1:32:A:VAL:H    | 9        | 0.2           |
| (1,62)  | 1:24:A:VAL:H  | 1:32:A:VAL:H    | 12       | 0.2           |
| (1,61)  | 1:24:A:VAL:H  | 1:24:A:VAL:HB   | 3        | 0.2           |
| (1,30)  | 1:14:A:VAL:H  | 1:14:A:VAL:HB   | 11       | 0.2           |
| (4,28)  | 1:52:A:LYS:H  | 1:71:A:ALA:O    | 8        | 0.19          |
| (4,16)  | 1:15:A:ASP:O  | 1:23:A:ARG:H    | 10       | 0.19          |
| (4,15)  | 1:14:A:VAL:H  | 1:23:A:ARG:O    | 6        | 0.19          |
| (4,6)   | 1:7:A:PHE:H   | 1:57:A:LEU:O    | 7        | 0.19          |
| (1,255) | 1:64:A:LYS:HA | 1:32:A:VAL:HA   | 7        | 0.19          |
| (1,214) | 1:33:A:THR:HA | 1:33:A:THR:HB   | 2        | 0.19          |
| (1,209) | 1:31:A:VAL:HA | 1:25:A:GLU:HA   | 8        | 0.19          |
| (1,204) | 1:25:A:GLU:HA | 1:31:A:VAL:HA   | 8        | 0.19          |
| (1,201) | 1:23:A:ARG:HA | 1:17:A:LEU:HG   | 13       | 0.19          |
| (1,170) | 1:67:A:ILE:H  | 1:36:A:ILE:HA   | 10       | 0.19          |
| (1,65)  | 1:25:A:GLU:H  | 1:12:A:THR:H    | 7        | 0.19          |

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| Key     | Atom-1        | Atom-2          | Model ID | Violation (Å) |
|---------|---------------|-----------------|----------|---------------|
| (1,36)  | 1:15:A:ASP:H  | 1:14:A:VAL:HB   | 9        | 0.19          |
| (1,36)  | 1:15:A:ASP:H  | 1:14:A:VAL:HB   | 13       | 0.19          |
| (4,28)  | 1:52:A:LYS:H  | 1:71:A:ALA:O    | 2        | 0.18          |
| (4,16)  | 1:15:A:ASP:O  | 1:23:A:ARG:H    | 4        | 0.18          |
| (3,27)  | 1:30:A:HIS:HA | 1:32:A:VAL:HG11 | 2        | 0.18          |
| (3,27)  | 1:30:A:HIS:HA | 1:32:A:VAL:HG12 | 2        | 0.18          |
| (3,27)  | 1:30:A:HIS:HA | 1:32:A:VAL:HG13 | 2        | 0.18          |
| (2,186) | 1:25:A:GLU:HA | 1:23:A:ARG:HG3  | 9        | 0.18          |
| (1,255) | 1:64:A:LYS:HA | 1:32:A:VAL:HA   | 3        | 0.18          |
| (1,252) | 1:62:A:LEU:HA | 1:62:A:LEU:HG   | 15       | 0.18          |
| (1,214) | 1:33:A:THR:HA | 1:33:A:THR:HB   | 14       | 0.18          |
| (1,170) | 1:67:A:ILE:H  | 1:36:A:ILE:HA   | 2        | 0.18          |
| (1,167) | 1:66:A:ARG:H  | 1:57:A:LEU:HA   | 7        | 0.18          |
| (1,167) | 1:66:A:ARG:H  | 1:57:A:LEU:HA   | 12       | 0.18          |
| (1,167) | 1:66:A:ARG:H  | 1:57:A:LEU:HA   | 14       | 0.18          |
| (1,164) | 1:65:A:GLY:H  | 1:34:A:ALA:HA   | 9        | 0.18          |
| (1,164) | 1:65:A:GLY:H  | 1:34:A:ALA:HA   | 14       | 0.18          |
| (1,112) | 1:44:A:TYR:H  | 1:42:A:LYS:H    | 15       | 0.18          |
| (1,84)  | 1:33:A:THR:H  | 1:32:A:VAL:HB   | 6        | 0.18          |
| (1,84)  | 1:33:A:THR:H  | 1:32:A:VAL:HB   | 9        | 0.18          |
| (1,77)  | 1:32:A:VAL:H  | 1:24:A:VAL:H    | 1        | 0.18          |
| (1,62)  | 1:24:A:VAL:H  | 1:32:A:VAL:H    | 1        | 0.18          |
| (1,61)  | 1:24:A:VAL:H  | 1:24:A:VAL:HB   | 7        | 0.18          |
| (1,4)   | 1:7:A:PHE:H   | 1:56:A:GLU:HA   | 10       | 0.18          |
| (4,28)  | 1:52:A:LYS:H  | 1:71:A:ALA:O    | 14       | 0.17          |
| (4,15)  | 1:14:A:VAL:H  | 1:23:A:ARG:O    | 15       | 0.17          |
| (4,6)   | 1:7:A:PHE:H   | 1:57:A:LEU:O    | 1        | 0.17          |
| (2,186) | 1:25:A:GLU:HA | 1:23:A:ARG:HG3  | 4        | 0.17          |
| (1,260) | 1:68:A:THR:HA | 1:68:A:THR:HB   | 2        | 0.17          |
| (1,260) | 1:68:A:THR:HA | 1:68:A:THR:HB   | 3        | 0.17          |
| (1,260) | 1:68:A:THR:HA | 1:68:A:THR:HB   | 13       | 0.17          |
| (1,255) | 1:64:A:LYS:HA | 1:32:A:VAL:HA   | 8        | 0.17          |
| (1,255) | 1:64:A:LYS:HA | 1:32:A:VAL:HA   | 15       | 0.17          |
| (1,252) | 1:62:A:LEU:HA | 1:62:A:LEU:HG   | 14       | 0.17          |
| (1,194) | 1:16:A:THR:HA | 1:22:A:PHE:HA   | 6        | 0.17          |
| (1,180) | 1:71:A:ALA:H  | 1:71:A:ALA:HA   | 2        | 0.17          |
| (1,170) | 1:67:A:ILE:H  | 1:36:A:ILE:HA   | 7        | 0.17          |
| (1,170) | 1:67:A:ILE:H  | 1:36:A:ILE:HA   | 8        | 0.17          |
| (1,167) | 1:66:A:ARG:H  | 1:57:A:LEU:HA   | 6        | 0.17          |
| (1,158) | 1:62:A:LEU:H  | 1:62:A:LEU:HG   | 5        | 0.17          |
| (1,129) | 1:53:A:VAL:H  | 1:12:A:THR:HA   | 4        | 0.17          |
| (1,125) | 1:50:A:GLY:H  | 1:13:A:VAL:HB   | 6        | 0.17          |

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| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,84)  | 1:33:A:THR:H  | 1:32:A:VAL:HB | 1        | 0.17          |
| (1,70)  | 1:28:A:ASN:H  | 1:27:A:GLU:H  | 2        | 0.17          |
| (1,70)  | 1:28:A:ASN:H  | 1:27:A:GLU:H  | 3        | 0.17          |
| (1,70)  | 1:28:A:ASN:H  | 1:27:A:GLU:H  | 4        | 0.17          |
| (1,54)  | 1:23:A:ARG:H  | 1:15:A:ASP:H  | 9        | 0.17          |
| (1,54)  | 1:23:A:ARG:H  | 1:15:A:ASP:H  | 14       | 0.17          |
| (1,52)  | 1:22:A:PHE:H  | 1:34:A:ALA:H  | 10       | 0.17          |
| (1,52)  | 1:22:A:PHE:H  | 1:34:A:ALA:H  | 15       | 0.17          |
| (1,51)  | 1:22:A:PHE:H  | 1:22:A:PHE:HA | 1        | 0.17          |
| (1,51)  | 1:22:A:PHE:H  | 1:22:A:PHE:HA | 13       | 0.17          |
| (1,36)  | 1:15:A:ASP:H  | 1:14:A:VAL:HB | 1        | 0.17          |
| (1,36)  | 1:15:A:ASP:H  | 1:14:A:VAL:HB | 8        | 0.17          |
| (4,28)  | 1:52:A:LYS:H  | 1:71:A:ALA:O  | 15       | 0.16          |
| (4,15)  | 1:14:A:VAL:H  | 1:23:A:ARG:O  | 3        | 0.16          |
| (4,14)  | 1:13:A:VAL:H  | 1:51:A:ASP:O  | 11       | 0.16          |
| (4,6)   | 1:7:A:PHE:H   | 1:57:A:LEU:O  | 15       | 0.16          |
| (1,260) | 1:68:A:THR:HA | 1:68:A:THR:HB | 12       | 0.16          |
| (1,255) | 1:64:A:LYS:HA | 1:32:A:VAL:HA | 6        | 0.16          |
| (1,252) | 1:62:A:LEU:HA | 1:62:A:LEU:HG | 7        | 0.16          |
| (1,208) | 1:31:A:VAL:HA | 1:31:A:VAL:HB | 2        | 0.16          |
| (1,194) | 1:16:A:THR:HA | 1:22:A:PHE:HA | 11       | 0.16          |
| (1,180) | 1:71:A:ALA:H  | 1:71:A:ALA:HA | 3        | 0.16          |
| (1,180) | 1:71:A:ALA:H  | 1:71:A:ALA:HA | 4        | 0.16          |
| (1,180) | 1:71:A:ALA:H  | 1:71:A:ALA:HA | 11       | 0.16          |
| (1,180) | 1:71:A:ALA:H  | 1:71:A:ALA:HA | 12       | 0.16          |
| (1,180) | 1:71:A:ALA:H  | 1:71:A:ALA:HA | 13       | 0.16          |
| (1,179) | 1:70:A:ARG:H  | 1:70:A:ARG:HA | 1        | 0.16          |
| (1,164) | 1:65:A:GLY:H  | 1:34:A:ALA:HA | 3        | 0.16          |
| (1,164) | 1:65:A:GLY:H  | 1:34:A:ALA:HA | 5        | 0.16          |
| (1,164) | 1:65:A:GLY:H  | 1:34:A:ALA:HA | 12       | 0.16          |
| (1,164) | 1:65:A:GLY:H  | 1:34:A:ALA:HA | 15       | 0.16          |
| (1,140) | 1:55:A:VAL:H  | 1:55:A:VAL:HA | 8        | 0.16          |
| (1,129) | 1:53:A:VAL:H  | 1:12:A:THR:HA | 1        | 0.16          |
| (1,129) | 1:53:A:VAL:H  | 1:12:A:THR:HA | 9        | 0.16          |
| (1,115) | 1:45:A:ILE:H  | 1:45:A:ILE:HA | 11       | 0.16          |
| (1,115) | 1:45:A:ILE:H  | 1:45:A:ILE:HA | 15       | 0.16          |
| (1,84)  | 1:33:A:THR:H  | 1:32:A:VAL:HB | 5        | 0.16          |
| (1,77)  | 1:32:A:VAL:H  | 1:24:A:VAL:H  | 10       | 0.16          |
| (1,77)  | 1:32:A:VAL:H  | 1:24:A:VAL:H  | 13       | 0.16          |
| (1,70)  | 1:28:A:ASN:H  | 1:27:A:GLU:H  | 1        | 0.16          |
| (1,70)  | 1:28:A:ASN:H  | 1:27:A:GLU:H  | 6        | 0.16          |
| (1,70)  | 1:28:A:ASN:H  | 1:27:A:GLU:H  | 10       | 0.16          |

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| Key     | Atom-1        | Atom-2         | Model ID | Violation (Å) |
|---------|---------------|----------------|----------|---------------|
| (1,70)  | 1:28:A:ASN:H  | 1:27:A:GLU:H   | 13       | 0.16          |
| (1,70)  | 1:28:A:ASN:H  | 1:27:A:GLU:H   | 15       | 0.16          |
| (1,68)  | 1:26:A:LEU:H  | 1:26:A:LEU:HG  | 4        | 0.16          |
| (1,65)  | 1:25:A:GLU:H  | 1:12:A:THR:H   | 4        | 0.16          |
| (1,65)  | 1:25:A:GLU:H  | 1:12:A:THR:H   | 15       | 0.16          |
| (1,62)  | 1:24:A:VAL:H  | 1:32:A:VAL:H   | 10       | 0.16          |
| (1,62)  | 1:24:A:VAL:H  | 1:32:A:VAL:H   | 13       | 0.16          |
| (1,61)  | 1:24:A:VAL:H  | 1:24:A:VAL:HB  | 2        | 0.16          |
| (1,61)  | 1:24:A:VAL:H  | 1:24:A:VAL:HB  | 8        | 0.16          |
| (1,54)  | 1:23:A:ARG:H  | 1:15:A:ASP:H   | 4        | 0.16          |
| (1,52)  | 1:22:A:PHE:H  | 1:34:A:ALA:H   | 2        | 0.16          |
| (1,51)  | 1:22:A:PHE:H  | 1:22:A:PHE:HA  | 4        | 0.16          |
| (1,51)  | 1:22:A:PHE:H  | 1:22:A:PHE:HA  | 5        | 0.16          |
| (1,51)  | 1:22:A:PHE:H  | 1:22:A:PHE:HA  | 10       | 0.16          |
| (1,36)  | 1:15:A:ASP:H  | 1:14:A:VAL:HB  | 12       | 0.16          |
| (1,33)  | 1:15:A:ASP:H  | 1:16:A:THR:H   | 1        | 0.16          |
| (1,33)  | 1:15:A:ASP:H  | 1:16:A:THR:H   | 11       | 0.16          |
| (1,32)  | 1:14:A:VAL:H  | 1:24:A:VAL:HA  | 5        | 0.16          |
| (4,16)  | 1:15:A:ASP:O  | 1:23:A:ARG:H   | 8        | 0.15          |
| (4,2)   | 1:38:A:GLY:O  | 1:42:A:LYS:H   | 9        | 0.15          |
| (2,186) | 1:25:A:GLU:HA | 1:23:A:ARG:HG3 | 1        | 0.15          |
| (1,260) | 1:68:A:THR:HA | 1:68:A:THR:HB  | 11       | 0.15          |
| (1,260) | 1:68:A:THR:HA | 1:68:A:THR:HB  | 15       | 0.15          |
| (1,258) | 1:67:A:ILE:HA | 1:67:A:ILE:HB  | 7        | 0.15          |
| (1,257) | 1:66:A:ARG:HA | 1:34:A:ALA:HA  | 12       | 0.15          |
| (1,255) | 1:64:A:LYS:HA | 1:32:A:VAL:HA  | 10       | 0.15          |
| (1,253) | 1:63:A:SER:HA | 1:32:A:VAL:HA  | 3        | 0.15          |
| (1,253) | 1:63:A:SER:HA | 1:32:A:VAL:HA  | 4        | 0.15          |
| (1,249) | 1:57:A:LEU:HA | 1:57:A:LEU:HG  | 8        | 0.15          |
| (1,214) | 1:33:A:THR:HA | 1:33:A:THR:HB  | 7        | 0.15          |
| (1,180) | 1:71:A:ALA:H  | 1:71:A:ALA:HA  | 1        | 0.15          |
| (1,180) | 1:71:A:ALA:H  | 1:71:A:ALA:HA  | 5        | 0.15          |
| (1,180) | 1:71:A:ALA:H  | 1:71:A:ALA:HA  | 6        | 0.15          |
| (1,180) | 1:71:A:ALA:H  | 1:71:A:ALA:HA  | 10       | 0.15          |
| (1,180) | 1:71:A:ALA:H  | 1:71:A:ALA:HA  | 14       | 0.15          |
| (1,180) | 1:71:A:ALA:H  | 1:71:A:ALA:HA  | 15       | 0.15          |
| (1,179) | 1:70:A:ARG:H  | 1:70:A:ARG:HA  | 6        | 0.15          |
| (1,170) | 1:67:A:ILE:H  | 1:36:A:ILE:HA  | 6        | 0.15          |
| (1,170) | 1:67:A:ILE:H  | 1:36:A:ILE:HA  | 14       | 0.15          |
| (1,164) | 1:65:A:GLY:H  | 1:34:A:ALA:HA  | 7        | 0.15          |
| (1,164) | 1:65:A:GLY:H  | 1:34:A:ALA:HA  | 11       | 0.15          |
| (1,158) | 1:62:A:LEU:H  | 1:62:A:LEU:HG  | 2        | 0.15          |

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| Key     | Atom-1       | Atom-2        | Model ID | Violation (Å) |
|---------|--------------|---------------|----------|---------------|
| (1,158) | 1:62:A:LEU:H | 1:62:A:LEU:HG | 10       | 0.15          |
| (1,140) | 1:55:A:VAL:H | 1:55:A:VAL:HA | 1        | 0.15          |
| (1,140) | 1:55:A:VAL:H | 1:55:A:VAL:HA | 2        | 0.15          |
| (1,140) | 1:55:A:VAL:H | 1:55:A:VAL:HA | 3        | 0.15          |
| (1,140) | 1:55:A:VAL:H | 1:55:A:VAL:HA | 4        | 0.15          |
| (1,140) | 1:55:A:VAL:H | 1:55:A:VAL:HA | 5        | 0.15          |
| (1,140) | 1:55:A:VAL:H | 1:55:A:VAL:HA | 6        | 0.15          |
| (1,140) | 1:55:A:VAL:H | 1:55:A:VAL:HA | 9        | 0.15          |
| (1,140) | 1:55:A:VAL:H | 1:55:A:VAL:HA | 12       | 0.15          |
| (1,140) | 1:55:A:VAL:H | 1:55:A:VAL:HA | 15       | 0.15          |
| (1,129) | 1:53:A:VAL:H | 1:12:A:THR:HA | 11       | 0.15          |
| (1,125) | 1:50:A:GLY:H | 1:13:A:VAL:HB | 4        | 0.15          |
| (1,125) | 1:50:A:GLY:H | 1:13:A:VAL:HB | 15       | 0.15          |
| (1,97)  | 1:37:A:SER:H | 1:37:A:SER:HA | 9        | 0.15          |
| (1,77)  | 1:32:A:VAL:H | 1:24:A:VAL:H  | 11       | 0.15          |
| (1,70)  | 1:28:A:ASN:H | 1:27:A:GLU:H  | 8        | 0.15          |
| (1,70)  | 1:28:A:ASN:H | 1:27:A:GLU:H  | 9        | 0.15          |
| (1,70)  | 1:28:A:ASN:H | 1:27:A:GLU:H  | 12       | 0.15          |
| (1,68)  | 1:26:A:LEU:H | 1:26:A:LEU:HG | 1        | 0.15          |
| (1,68)  | 1:26:A:LEU:H | 1:26:A:LEU:HG | 6        | 0.15          |
| (1,68)  | 1:26:A:LEU:H | 1:26:A:LEU:HG | 9        | 0.15          |
| (1,62)  | 1:24:A:VAL:H | 1:32:A:VAL:H  | 11       | 0.15          |
| (1,61)  | 1:24:A:VAL:H | 1:24:A:VAL:HB | 4        | 0.15          |
| (1,61)  | 1:24:A:VAL:H | 1:24:A:VAL:HB | 14       | 0.15          |
| (1,53)  | 1:22:A:PHE:H | 1:35:A:HIS:HA | 1        | 0.15          |
| (1,52)  | 1:22:A:PHE:H | 1:34:A:ALA:H  | 4        | 0.15          |
| (1,52)  | 1:22:A:PHE:H | 1:34:A:ALA:H  | 8        | 0.15          |
| (1,51)  | 1:22:A:PHE:H | 1:22:A:PHE:HA | 7        | 0.15          |
| (1,51)  | 1:22:A:PHE:H | 1:22:A:PHE:HA | 8        | 0.15          |
| (1,51)  | 1:22:A:PHE:H | 1:22:A:PHE:HA | 9        | 0.15          |
| (1,51)  | 1:22:A:PHE:H | 1:22:A:PHE:HA | 11       | 0.15          |
| (1,51)  | 1:22:A:PHE:H | 1:22:A:PHE:HA | 12       | 0.15          |
| (1,51)  | 1:22:A:PHE:H | 1:22:A:PHE:HA | 14       | 0.15          |
| (1,51)  | 1:22:A:PHE:H | 1:22:A:PHE:HA | 15       | 0.15          |
| (1,36)  | 1:15:A:ASP:H | 1:14:A:VAL:HB | 6        | 0.15          |
| (1,36)  | 1:15:A:ASP:H | 1:14:A:VAL:HB | 7        | 0.15          |
| (1,32)  | 1:14:A:VAL:H | 1:24:A:VAL:HA | 8        | 0.15          |
| (1,32)  | 1:14:A:VAL:H | 1:24:A:VAL:HA | 11       | 0.15          |
| (1,4)   | 1:7:A:PHE:H  | 1:56:A:GLU:HA | 14       | 0.15          |
| (4,28)  | 1:52:A:LYS:H | 1:71:A:ALA:O  | 1        | 0.14          |
| (4,16)  | 1:15:A:ASP:O | 1:23:A:ARG:H  | 12       | 0.14          |
| (4,15)  | 1:14:A:VAL:H | 1:23:A:ARG:O  | 7        | 0.14          |

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| Key     | Atom-1        | Atom-2         | Model ID | Violation (Å) |
|---------|---------------|----------------|----------|---------------|
| (4,15)  | 1:14:A:VAL:H  | 1:23:A:ARG:O   | 14       | 0.14          |
| (2,186) | 1:25:A:GLU:HA | 1:23:A:ARG:HG3 | 5        | 0.14          |
| (2,186) | 1:25:A:GLU:HA | 1:23:A:ARG:HG3 | 12       | 0.14          |
| (1,258) | 1:67:A:ILE:HA | 1:67:A:ILE:HB  | 5        | 0.14          |
| (1,258) | 1:67:A:ILE:HA | 1:67:A:ILE:HB  | 6        | 0.14          |
| (1,257) | 1:66:A:ARG:HA | 1:34:A:ALA:HA  | 15       | 0.14          |
| (1,253) | 1:63:A:SER:HA | 1:32:A:VAL:HA  | 1        | 0.14          |
| (1,246) | 1:55:A:VAL:HB | 1:57:A:LEU:HG  | 12       | 0.14          |
| (1,231) | 1:48:A:LEU:HA | 1:48:A:LEU:HG  | 2        | 0.14          |
| (1,208) | 1:31:A:VAL:HA | 1:31:A:VAL:HB  | 3        | 0.14          |
| (1,208) | 1:31:A:VAL:HA | 1:31:A:VAL:HB  | 5        | 0.14          |
| (1,193) | 1:16:A:THR:HA | 1:16:A:THR:HB  | 10       | 0.14          |
| (1,180) | 1:71:A:ALA:H  | 1:71:A:ALA:HA  | 7        | 0.14          |
| (1,180) | 1:71:A:ALA:H  | 1:71:A:ALA:HA  | 9        | 0.14          |
| (1,179) | 1:70:A:ARG:H  | 1:70:A:ARG:HA  | 5        | 0.14          |
| (1,179) | 1:70:A:ARG:H  | 1:70:A:ARG:HA  | 15       | 0.14          |
| (1,170) | 1:67:A:ILE:H  | 1:36:A:ILE:HA  | 3        | 0.14          |
| (1,170) | 1:67:A:ILE:H  | 1:36:A:ILE:HA  | 12       | 0.14          |
| (1,169) | 1:67:A:ILE:H  | 1:35:A:HIS:H   | 4        | 0.14          |
| (1,167) | 1:66:A:ARG:H  | 1:57:A:LEU:HA  | 8        | 0.14          |
| (1,164) | 1:65:A:GLY:H  | 1:34:A:ALA:HA  | 10       | 0.14          |
| (1,158) | 1:62:A:LEU:H  | 1:62:A:LEU:HG  | 4        | 0.14          |
| (1,140) | 1:55:A:VAL:H  | 1:55:A:VAL:HA  | 7        | 0.14          |
| (1,140) | 1:55:A:VAL:H  | 1:55:A:VAL:HA  | 10       | 0.14          |
| (1,140) | 1:55:A:VAL:H  | 1:55:A:VAL:HA  | 11       | 0.14          |
| (1,140) | 1:55:A:VAL:H  | 1:55:A:VAL:HA  | 13       | 0.14          |
| (1,140) | 1:55:A:VAL:H  | 1:55:A:VAL:HA  | 14       | 0.14          |
| (1,129) | 1:53:A:VAL:H  | 1:12:A:THR:HA  | 10       | 0.14          |
| (1,129) | 1:53:A:VAL:H  | 1:12:A:THR:HA  | 13       | 0.14          |
| (1,125) | 1:50:A:GLY:H  | 1:13:A:VAL:HB  | 14       | 0.14          |
| (1,117) | 1:45:A:ILE:H  | 1:45:A:ILE:HB  | 9        | 0.14          |
| (1,115) | 1:45:A:ILE:H  | 1:45:A:ILE:HA  | 2        | 0.14          |
| (1,115) | 1:45:A:ILE:H  | 1:45:A:ILE:HA  | 4        | 0.14          |
| (1,108) | 1:42:A:LYS:H  | 1:42:A:LYS:HA  | 9        | 0.14          |
| (1,84)  | 1:33:A:THR:H  | 1:32:A:VAL:HB  | 11       | 0.14          |
| (1,76)  | 1:31:A:VAL:H  | 1:31:A:VAL:HB  | 7        | 0.14          |
| (1,70)  | 1:28:A:ASN:H  | 1:27:A:GLU:H   | 5        | 0.14          |
| (1,70)  | 1:28:A:ASN:H  | 1:27:A:GLU:H   | 11       | 0.14          |
| (1,70)  | 1:28:A:ASN:H  | 1:27:A:GLU:H   | 14       | 0.14          |
| (1,68)  | 1:26:A:LEU:H  | 1:26:A:LEU:HG  | 2        | 0.14          |
| (1,68)  | 1:26:A:LEU:H  | 1:26:A:LEU:HG  | 14       | 0.14          |
| (1,65)  | 1:25:A:GLU:H  | 1:12:A:THR:H   | 8        | 0.14          |

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| Key     | Atom-1        | Atom-2         | Model ID | Violation (Å) |
|---------|---------------|----------------|----------|---------------|
| (1,54)  | 1:23:A:ARG:H  | 1:15:A:ASP:H   | 13       | 0.14          |
| (1,53)  | 1:22:A:PHE:H  | 1:35:A:HIS:HA  | 12       | 0.14          |
| (1,52)  | 1:22:A:PHE:H  | 1:34:A:ALA:H   | 3        | 0.14          |
| (1,51)  | 1:22:A:PHE:H  | 1:22:A:PHE:HA  | 3        | 0.14          |
| (1,51)  | 1:22:A:PHE:H  | 1:22:A:PHE:HA  | 6        | 0.14          |
| (4,16)  | 1:15:A:ASP:O  | 1:23:A:ARG:H   | 7        | 0.13          |
| (4,15)  | 1:14:A:VAL:H  | 1:23:A:ARG:O   | 13       | 0.13          |
| (4,6)   | 1:7:A:PHE:H   | 1:57:A:LEU:O   | 12       | 0.13          |
| (2,187) | 1:25:A:GLU:HA | 1:23:A:ARG:HG2 | 10       | 0.13          |
| (1,258) | 1:67:A:ILE:HA | 1:67:A:ILE:HB  | 1        | 0.13          |
| (1,258) | 1:67:A:ILE:HA | 1:67:A:ILE:HB  | 4        | 0.13          |
| (1,258) | 1:67:A:ILE:HA | 1:67:A:ILE:HB  | 8        | 0.13          |
| (1,258) | 1:67:A:ILE:HA | 1:67:A:ILE:HB  | 9        | 0.13          |
| (1,258) | 1:67:A:ILE:HA | 1:67:A:ILE:HB  | 10       | 0.13          |
| (1,258) | 1:67:A:ILE:HA | 1:67:A:ILE:HB  | 13       | 0.13          |
| (1,258) | 1:67:A:ILE:HA | 1:67:A:ILE:HB  | 14       | 0.13          |
| (1,258) | 1:67:A:ILE:HA | 1:67:A:ILE:HB  | 15       | 0.13          |
| (1,257) | 1:66:A:ARG:HA | 1:34:A:ALA:HA  | 7        | 0.13          |
| (1,253) | 1:63:A:SER:HA | 1:32:A:VAL:HA  | 9        | 0.13          |
| (1,231) | 1:48:A:LEU:HA | 1:48:A:LEU:HG  | 12       | 0.13          |
| (1,180) | 1:71:A:ALA:H  | 1:71:A:ALA:HA  | 8        | 0.13          |
| (1,179) | 1:70:A:ARG:H  | 1:70:A:ARG:HA  | 10       | 0.13          |
| (1,167) | 1:66:A:ARG:H  | 1:57:A:LEU:HA  | 15       | 0.13          |
| (1,158) | 1:62:A:LEU:H  | 1:62:A:LEU:HG  | 11       | 0.13          |
| (1,155) | 1:60:A:TYR:H  | 1:58:A:THR:HB  | 1        | 0.13          |
| (1,129) | 1:53:A:VAL:H  | 1:12:A:THR:HA  | 12       | 0.13          |
| (1,115) | 1:45:A:ILE:H  | 1:45:A:ILE:HA  | 5        | 0.13          |
| (1,108) | 1:42:A:LYS:H  | 1:42:A:LYS:HA  | 5        | 0.13          |
| (1,68)  | 1:26:A:LEU:H  | 1:26:A:LEU:HG  | 8        | 0.13          |
| (1,68)  | 1:26:A:LEU:H  | 1:26:A:LEU:HG  | 11       | 0.13          |
| (1,68)  | 1:26:A:LEU:H  | 1:26:A:LEU:HG  | 12       | 0.13          |
| (1,65)  | 1:25:A:GLU:H  | 1:12:A:THR:H   | 3        | 0.13          |
| (1,54)  | 1:23:A:ARG:H  | 1:15:A:ASP:H   | 10       | 0.13          |
| (1,51)  | 1:22:A:PHE:H  | 1:22:A:PHE:HA  | 2        | 0.13          |
| (1,36)  | 1:15:A:ASP:H  | 1:14:A:VAL:HB  | 5        | 0.13          |
| (1,33)  | 1:15:A:ASP:H  | 1:16:A:THR:H   | 7        | 0.13          |
| (1,30)  | 1:14:A:VAL:H  | 1:14:A:VAL:HB  | 4        | 0.13          |
| (1,4)   | 1:7:A:PHE:H   | 1:56:A:GLU:HA  | 8        | 0.13          |
| (4,15)  | 1:14:A:VAL:H  | 1:23:A:ARG:O   | 2        | 0.12          |
| (4,14)  | 1:13:A:VAL:H  | 1:51:A:ASP:O   | 2        | 0.12          |
| (4,6)   | 1:7:A:PHE:H   | 1:57:A:LEU:O   | 8        | 0.12          |
| (1,259) | 1:67:A:ILE:HA | 1:53:A:VAL:HB  | 7        | 0.12          |

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| Key     | Atom-1        | Atom-2         | Model ID | Violation (Å) |
|---------|---------------|----------------|----------|---------------|
| (1,258) | 1:67:A:ILE:HA | 1:67:A:ILE:HB  | 2        | 0.12          |
| (1,258) | 1:67:A:ILE:HA | 1:67:A:ILE:HB  | 3        | 0.12          |
| (1,258) | 1:67:A:ILE:HA | 1:67:A:ILE:HB  | 11       | 0.12          |
| (1,258) | 1:67:A:ILE:HA | 1:67:A:ILE:HB  | 12       | 0.12          |
| (1,255) | 1:64:A:LYS:HA | 1:32:A:VAL:HA  | 5        | 0.12          |
| (1,255) | 1:64:A:LYS:HA | 1:32:A:VAL:HA  | 13       | 0.12          |
| (1,253) | 1:63:A:SER:HA | 1:32:A:VAL:HA  | 6        | 0.12          |
| (1,253) | 1:63:A:SER:HA | 1:32:A:VAL:HA  | 12       | 0.12          |
| (1,231) | 1:48:A:LEU:HA | 1:48:A:LEU:HG  | 13       | 0.12          |
| (1,220) | 1:35:A:HIS:HA | 1:35:A:HIS:HD2 | 5        | 0.12          |
| (1,196) | 1:17:A:LEU:HA | 1:17:A:LEU:HG  | 11       | 0.12          |
| (1,179) | 1:70:A:ARG:H  | 1:70:A:ARG:HA  | 8        | 0.12          |
| (1,179) | 1:70:A:ARG:H  | 1:70:A:ARG:HA  | 9        | 0.12          |
| (1,179) | 1:70:A:ARG:H  | 1:70:A:ARG:HA  | 11       | 0.12          |
| (1,179) | 1:70:A:ARG:H  | 1:70:A:ARG:HA  | 14       | 0.12          |
| (1,169) | 1:67:A:ILE:H  | 1:35:A:HIS:H   | 7        | 0.12          |
| (1,169) | 1:67:A:ILE:H  | 1:35:A:HIS:H   | 9        | 0.12          |
| (1,125) | 1:50:A:GLY:H  | 1:13:A:VAL:HB  | 1        | 0.12          |
| (1,125) | 1:50:A:GLY:H  | 1:13:A:VAL:HB  | 7        | 0.12          |
| (1,115) | 1:45:A:ILE:H  | 1:45:A:ILE:HA  | 8        | 0.12          |
| (1,115) | 1:45:A:ILE:H  | 1:45:A:ILE:HA  | 9        | 0.12          |
| (1,97)  | 1:37:A:SER:H  | 1:37:A:SER:HA  | 2        | 0.12          |
| (1,68)  | 1:26:A:LEU:H  | 1:26:A:LEU:HG  | 5        | 0.12          |
| (1,65)  | 1:25:A:GLU:H  | 1:12:A:THR:H   | 2        | 0.12          |
| (1,65)  | 1:25:A:GLU:H  | 1:12:A:THR:H   | 6        | 0.12          |
| (1,61)  | 1:24:A:VAL:H  | 1:24:A:VAL:HB  | 15       | 0.12          |
| (1,56)  | 1:23:A:ARG:H  | 1:14:A:VAL:H   | 11       | 0.12          |
| (1,52)  | 1:22:A:PHE:H  | 1:34:A:ALA:H   | 6        | 0.12          |
| (1,45)  | 1:20:A:THR:H  | 1:21:A:MET:H   | 15       | 0.12          |
| (1,36)  | 1:15:A:ASP:H  | 1:14:A:VAL:HB  | 3        | 0.12          |
| (1,33)  | 1:15:A:ASP:H  | 1:16:A:THR:H   | 9        | 0.12          |
| (1,33)  | 1:15:A:ASP:H  | 1:16:A:THR:H   | 14       | 0.12          |
| (4,28)  | 1:52:A:LYS:H  | 1:71:A:ALA:O   | 6        | 0.11          |
| (4,26)  | 1:35:A:HIS:O  | 1:67:A:ILE:H   | 10       | 0.11          |
| (4,12)  | 1:12:A:THR:H  | 1:25:A:GLU:O   | 6        | 0.11          |
| (4,12)  | 1:12:A:THR:H  | 1:25:A:GLU:O   | 15       | 0.11          |
| (1,255) | 1:64:A:LYS:HA | 1:32:A:VAL:HA  | 11       | 0.11          |
| (1,253) | 1:63:A:SER:HA | 1:32:A:VAL:HA  | 5        | 0.11          |
| (1,231) | 1:48:A:LEU:HA | 1:48:A:LEU:HG  | 7        | 0.11          |
| (1,228) | 1:44:A:TYR:HA | 1:43:A:ASN:HA  | 2        | 0.11          |
| (1,202) | 1:24:A:VAL:HA | 1:13:A:VAL:HA  | 10       | 0.11          |
| (1,201) | 1:23:A:ARG:HA | 1:17:A:LEU:HG  | 6        | 0.11          |

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| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,201) | 1:23:A:ARG:HA | 1:17:A:LEU:HG | 10       | 0.11          |
| (1,188) | 1:13:A:VAL:HA | 1:24:A:VAL:HA | 10       | 0.11          |
| (1,179) | 1:70:A:ARG:H  | 1:70:A:ARG:HA | 2        | 0.11          |
| (1,179) | 1:70:A:ARG:H  | 1:70:A:ARG:HA | 12       | 0.11          |
| (1,172) | 1:68:A:THR:H  | 1:55:A:VAL:HA | 5        | 0.11          |
| (1,169) | 1:67:A:ILE:H  | 1:35:A:HIS:H  | 1        | 0.11          |
| (1,169) | 1:67:A:ILE:H  | 1:35:A:HIS:H  | 13       | 0.11          |
| (1,169) | 1:67:A:ILE:H  | 1:35:A:HIS:H  | 15       | 0.11          |
| (1,158) | 1:62:A:LEU:H  | 1:62:A:LEU:HG | 13       | 0.11          |
| (1,129) | 1:53:A:VAL:H  | 1:12:A:THR:HA | 5        | 0.11          |
| (1,121) | 1:47:A:ILE:H  | 1:47:A:ILE:HB | 6        | 0.11          |
| (1,114) | 1:44:A:TYR:H  | 1:44:A:TYR:HA | 1        | 0.11          |
| (1,114) | 1:44:A:TYR:H  | 1:44:A:TYR:HA | 12       | 0.11          |
| (1,112) | 1:44:A:TYR:H  | 1:42:A:LYS:H  | 2        | 0.11          |
| (1,108) | 1:42:A:LYS:H  | 1:42:A:LYS:HA | 6        | 0.11          |
| (1,108) | 1:42:A:LYS:H  | 1:42:A:LYS:HA | 8        | 0.11          |
| (1,108) | 1:42:A:LYS:H  | 1:42:A:LYS:HA | 12       | 0.11          |
| (1,106) | 1:41:A:ARG:H  | 1:41:A:ARG:HA | 14       | 0.11          |
| (1,97)  | 1:37:A:SER:H  | 1:37:A:SER:HA | 4        | 0.11          |
| (1,97)  | 1:37:A:SER:H  | 1:37:A:SER:HA | 7        | 0.11          |
| (1,84)  | 1:33:A:THR:H  | 1:32:A:VAL:HB | 2        | 0.11          |
| (1,84)  | 1:33:A:THR:H  | 1:32:A:VAL:HB | 13       | 0.11          |
| (1,70)  | 1:28:A:ASN:H  | 1:27:A:GLU:H  | 7        | 0.11          |
| (1,65)  | 1:25:A:GLU:H  | 1:12:A:THR:H  | 14       | 0.11          |
| (1,61)  | 1:24:A:VAL:H  | 1:24:A:VAL:HB | 6        | 0.11          |
| (1,52)  | 1:22:A:PHE:H  | 1:34:A:ALA:H  | 7        | 0.11          |
| (1,52)  | 1:22:A:PHE:H  | 1:34:A:ALA:H  | 14       | 0.11          |
| (1,36)  | 1:15:A:ASP:H  | 1:14:A:VAL:HB | 15       | 0.11          |
| (1,33)  | 1:15:A:ASP:H  | 1:16:A:THR:H  | 10       | 0.11          |
| (1,32)  | 1:14:A:VAL:H  | 1:24:A:VAL:HA | 9        | 0.11          |
| (1,32)  | 1:14:A:VAL:H  | 1:24:A:VAL:HA | 10       | 0.11          |
| (1,4)   | 1:7:A:PHE:H   | 1:56:A:GLU:HA | 4        | 0.11          |
| (4,30)  | 1:54:A:ARG:H  | 1:69:A:TYR:O  | 7        | 0.1           |
| (1,256) | 1:64:A:LYS:HA | 1:34:A:ALA:HA | 3        | 0.1           |
| (1,255) | 1:64:A:LYS:HA | 1:32:A:VAL:HA | 2        | 0.1           |
| (1,241) | 1:53:A:VAL:HB | 1:67:A:ILE:HB | 7        | 0.1           |
| (1,219) | 1:35:A:HIS:HA | 1:21:A:MET:HA | 10       | 0.1           |
| (1,217) | 1:34:A:ALA:HA | 1:64:A:LYS:HA | 3        | 0.1           |
| (1,208) | 1:31:A:VAL:HA | 1:31:A:VAL:HB | 13       | 0.1           |
| (1,202) | 1:24:A:VAL:HA | 1:13:A:VAL:HA | 1        | 0.1           |
| (1,199) | 1:21:A:MET:HA | 1:35:A:HIS:HA | 10       | 0.1           |
| (1,188) | 1:13:A:VAL:HA | 1:24:A:VAL:HA | 1        | 0.1           |

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| Key     | Atom-1       | Atom-2        | Model ID | Violation (Å) |
|---------|--------------|---------------|----------|---------------|
| (1,179) | 1:70:A:ARG:H | 1:70:A:ARG:HA | 4        | 0.1           |
| (1,158) | 1:62:A:LEU:H | 1:62:A:LEU:HG | 3        | 0.1           |
| (1,121) | 1:47:A:ILE:H | 1:47:A:ILE:HB | 5        | 0.1           |
| (1,117) | 1:45:A:ILE:H | 1:45:A:ILE:HB | 8        | 0.1           |
| (1,116) | 1:45:A:ILE:H | 1:44:A:TYR:HA | 7        | 0.1           |
| (1,114) | 1:44:A:TYR:H | 1:44:A:TYR:HA | 14       | 0.1           |
| (1,108) | 1:42:A:LYS:H | 1:42:A:LYS:HA | 1        | 0.1           |
| (1,54)  | 1:23:A:ARG:H | 1:15:A:ASP:H  | 2        | 0.1           |
| (1,53)  | 1:22:A:PHE:H | 1:35:A:HIS:HA | 10       | 0.1           |
| (1,33)  | 1:15:A:ASP:H | 1:16:A:THR:H  | 2        | 0.1           |
| (1,17)  | 1:11:A:GLY:H | 1:54:A:ARG:HA | 3        | 0.1           |

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

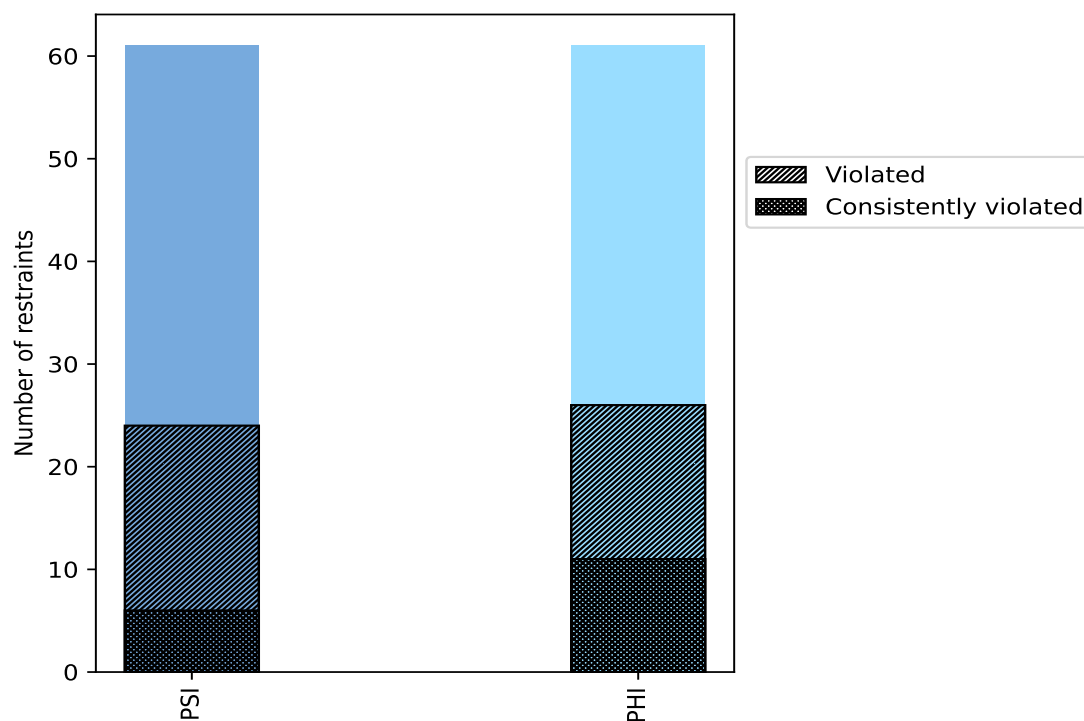
### 10.1 Summary of dihedral-angle violations [i](#)

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        | 61    | 50.0           | 24                    | 39.3           | 19.7           | 6                                  | 9.8            | 4.9            |
| PHI        | 61    | 50.0           | 26                    | 42.6           | 21.3           | 11                                 | 18.0           | 9.0            |
| Total      | 122   | 100.0          | 50                    | 41.0           | 41.0           | 17                                 | 13.9           | 13.9           |

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

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



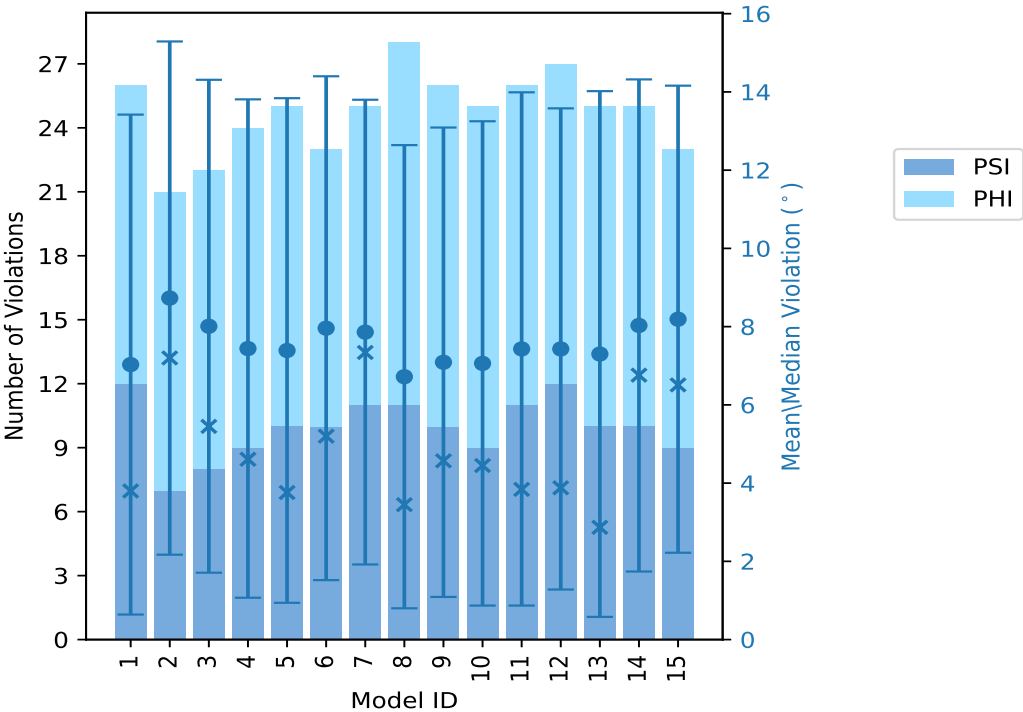
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model ⓘ

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

| Model ID | Number of violations |     |       | Mean (°) | Max (°) | SD (°) | Median (°) |
|----------|----------------------|-----|-------|----------|---------|--------|------------|
|          | PSI                  | PHI | Total |          |         |        |            |
| 1        | 12                   | 14  | 26    | 7.03     | 20.62   | 6.39   | 3.8        |
| 2        | 7                    | 14  | 21    | 8.73     | 21.98   | 6.56   | 7.2        |
| 3        | 8                    | 14  | 22    | 8.01     | 22.57   | 6.3    | 5.45       |
| 4        | 9                    | 15  | 24    | 7.44     | 21.84   | 6.37   | 4.61       |
| 5        | 10                   | 15  | 25    | 7.39     | 22.74   | 6.45   | 3.76       |
| 6        | 10                   | 13  | 23    | 7.96     | 22.42   | 6.44   | 5.2        |
| 7        | 11                   | 14  | 25    | 7.86     | 20.35   | 5.94   | 7.34       |
| 8        | 11                   | 17  | 28    | 6.72     | 21.17   | 5.92   | 3.45       |
| 9        | 10                   | 16  | 26    | 7.09     | 19.33   | 6.0    | 4.57       |
| 10       | 9                    | 16  | 25    | 7.06     | 19.77   | 6.19   | 4.45       |
| 11       | 11                   | 15  | 26    | 7.43     | 21.43   | 6.56   | 3.84       |
| 12       | 12                   | 15  | 27    | 7.43     | 20.41   | 6.15   | 3.88       |
| 13       | 10                   | 15  | 25    | 7.3      | 21.17   | 6.72   | 2.87       |
| 14       | 10                   | 15  | 25    | 8.03     | 21.64   | 6.29   | 6.76       |
| 15       | 9                    | 14  | 23    | 8.19     | 21.18   | 5.97   | 6.51       |

10.2.1 Bar graph : Dihedral violation statistics for each model ⓘ



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

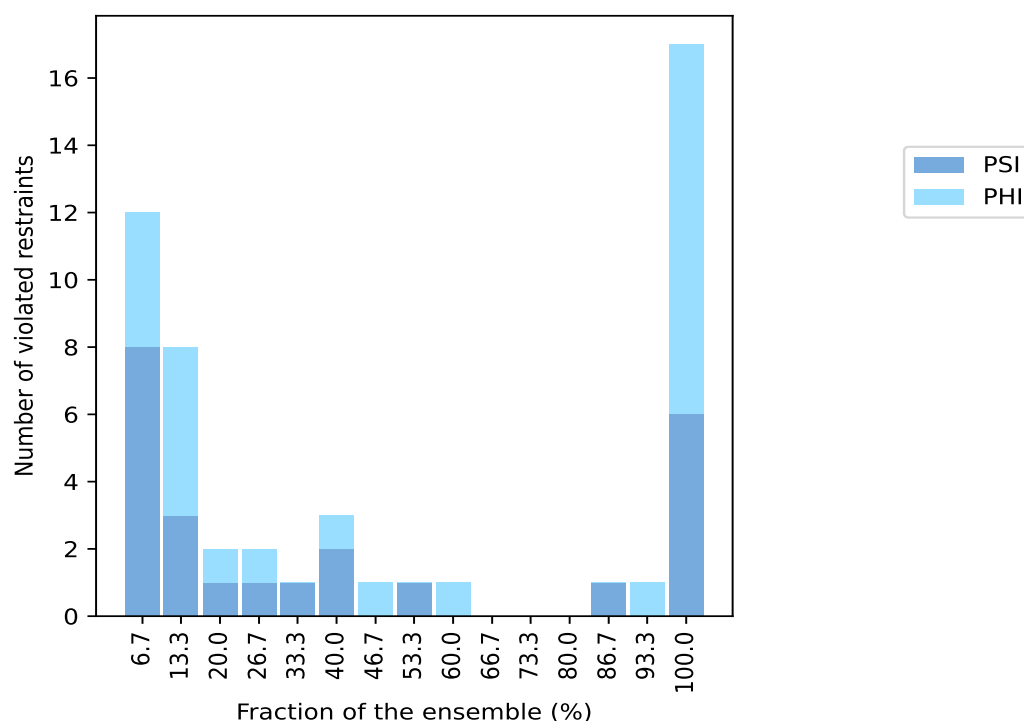
### 10.3 Dihedral-angle violation statistics for the ensemble [i](#)

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>       | %     |
| 8                             | 4   | 12    | 1                        | 6.7   |
| 3                             | 5   | 8     | 2                        | 13.3  |
| 1                             | 1   | 2     | 3                        | 20.0  |
| 1                             | 1   | 2     | 4                        | 26.7  |
| 1                             | 0   | 1     | 5                        | 33.3  |
| 2                             | 1   | 3     | 6                        | 40.0  |
| 0                             | 1   | 1     | 7                        | 46.7  |
| 1                             | 0   | 1     | 8                        | 53.3  |
| 0                             | 1   | 1     | 9                        | 60.0  |
| 0                             | 0   | 0     | 10                       | 66.7  |
| 0                             | 0   | 0     | 11                       | 73.3  |
| 0                             | 0   | 0     | 12                       | 80.0  |
| 1                             | 0   | 1     | 13                       | 86.7  |
| 0                             | 1   | 1     | 14                       | 93.3  |
| 6                             | 11  | 17    | 15                       | 100.0 |

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

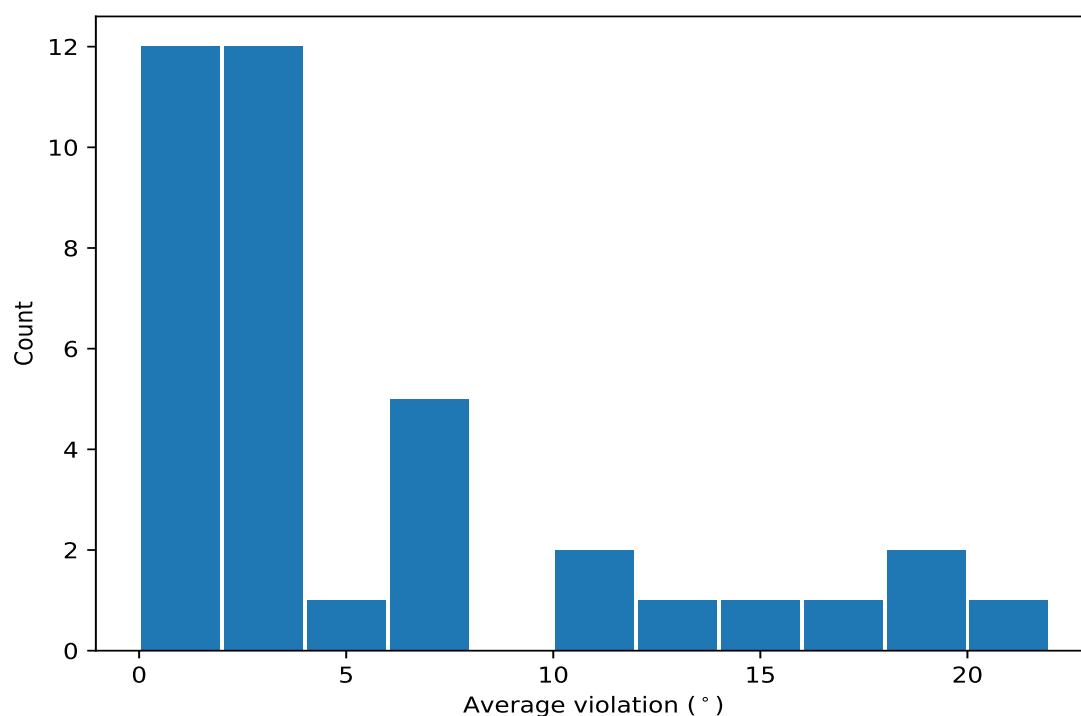
### 10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



## 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 |
|---------|--------------|---------------|---------------|--------------|---------------------|-------|-----------------|--------|
| (1,103) | 1:50:A:GLY:N | 1:50:A:GLY:CA | 1:50:A:GLY:C  | 1:51:A:ASP:N | 15                  | 21.17 | 1.07            | 21.18  |
| (1,81)  | 1:26:A:LEU:N | 1:26:A:LEU:CA | 1:26:A:LEU:C  | 1:27:A:GLU:N | 15                  | 18.69 | 0.69            | 18.75  |
| (1,70)  | 1:14:A:VAL:N | 1:14:A:VAL:CA | 1:14:A:VAL:C  | 1:15:A:ASP:N | 15                  | 18.18 | 1.17            | 18.42  |
| (1,43)  | 1:50:A:GLY:C | 1:51:A:ASP:N  | 1:51:A:ASP:CA | 1:51:A:ASP:C | 15                  | 16.34 | 0.97            | 16.42  |
| (1,21)  | 1:26:A:LEU:C | 1:27:A:GLU:N  | 1:27:A:GLU:CA | 1:27:A:GLU:C | 15                  | 15.19 | 0.41            | 15.12  |
| (1,120) | 1:68:A:THR:N | 1:68:A:THR:CA | 1:68:A:THR:C  | 1:69:A:TYR:N | 15                  | 13.39 | 0.81            | 13.55  |
| (1,13)  | 1:17:A:LEU:C | 1:18:A:PRO:N  | 1:18:A:PRO:CA | 1:18:A:PRO:C | 15                  | 11.99 | 0.54            | 11.96  |
| (1,10)  | 1:14:A:VAL:C | 1:15:A:ASP:N  | 1:15:A:ASP:CA | 1:15:A:ASP:C | 15                  | 11.54 | 1.89            | 11.22  |
| (1,24)  | 1:29:A:GLY:C | 1:30:A:HIS:N  | 1:30:A:HIS:CA | 1:30:A:HIS:C | 15                  | 7.85  | 0.24            | 7.84   |
| (1,23)  | 1:28:A:ASN:C | 1:29:A:GLY:N  | 1:29:A:GLY:CA | 1:29:A:GLY:C | 15                  | 7.31  | 0.47            | 7.2    |
| (1,25)  | 1:30:A:HIS:C | 1:31:A:VAL:N  | 1:31:A:VAL:CA | 1:31:A:VAL:C | 15                  | 6.8   | 0.61            | 6.89   |
| (1,117) | 1:65:A:GLY:N | 1:65:A:GLY:CA | 1:65:A:GLY:C  | 1:66:A:ARG:N | 15                  | 4.77  | 0.71            | 4.75   |
| (1,8)   | 1:12:A:THR:C | 1:13:A:VAL:N  | 1:13:A:VAL:CA | 1:13:A:VAL:C | 15                  | 3.32  | 0.58            | 3.38   |
| (1,59)  | 1:67:A:ILE:C | 1:68:A:THR:N  | 1:68:A:THR:CA | 1:68:A:THR:C | 15                  | 3.18  | 0.98            | 3.16   |
| (1,49)  | 1:56:A:GLU:C | 1:57:A:LEU:N  | 1:57:A:LEU:CA | 1:57:A:LEU:C | 15                  | 3.17  | 0.56            | 3.32   |
| (1,83)  | 1:28:A:ASN:N | 1:28:A:ASN:CA | 1:28:A:ASN:C  | 1:29:A:GLY:N | 15                  | 2.75  | 0.25            | 2.77   |
| (1,58)  | 1:66:A:ARG:C | 1:67:A:ILE:N  | 1:67:A:ILE:CA | 1:67:A:ILE:C | 15                  | 2.13  | 0.6             | 2.08   |
| (1,47)  | 1:54:A:ARG:C | 1:55:A:VAL:N  | 1:55:A:VAL:CA | 1:55:A:VAL:C | 14                  | 1.8   | 0.48            | 1.78   |
| (1,105) | 1:52:A:LYS:N | 1:52:A:LYS:CA | 1:52:A:LYS:C  | 1:53:A:VAL:N | 13                  | 2.8   | 0.76            | 2.69   |
| (1,42)  | 1:49:A:THR:C | 1:50:A:GLY:N  | 1:50:A:GLY:CA | 1:50:A:GLY:C | 9                   | 1.55  | 0.24            | 1.6    |
| (1,104) | 1:51:A:ASP:N | 1:51:A:ASP:CA | 1:51:A:ASP:C  | 1:52:A:LYS:N | 8                   | 3.24  | 0.88            | 3.55   |

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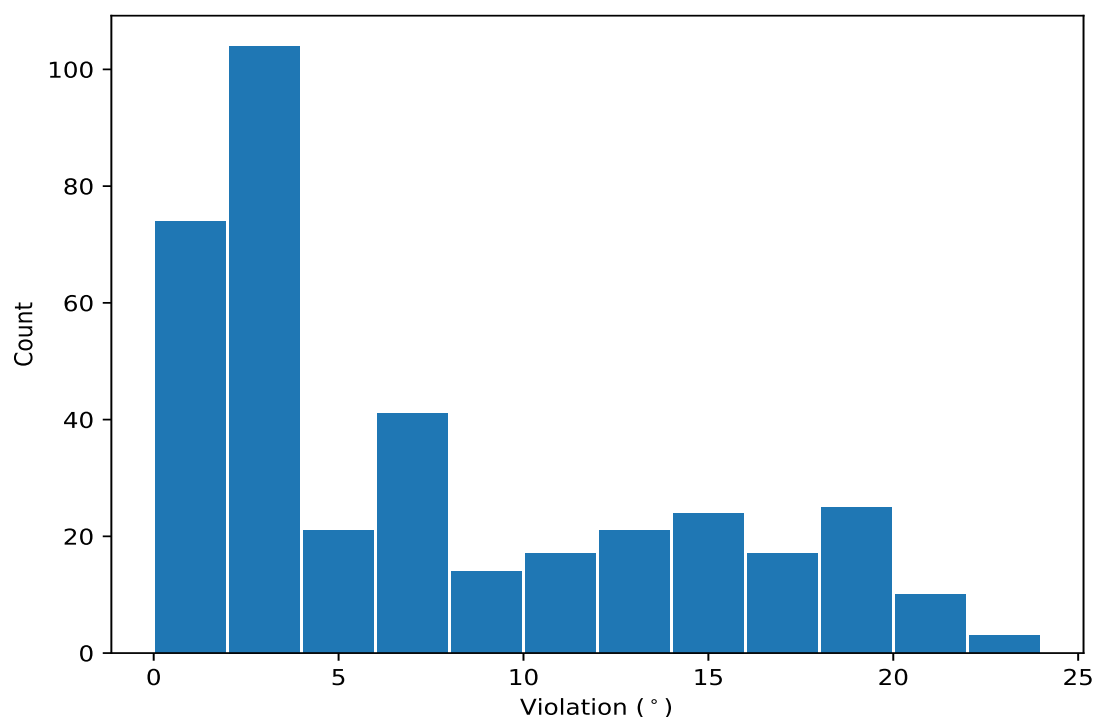
| Key     | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Models <sup>1</sup> | Mean | SD <sup>2</sup> | Median |
|---------|--------------|---------------|---------------|--------------|---------------------|------|-----------------|--------|
| (1,44)  | 1:51:A:ASP:C | 1:52:A:LYS:N  | 1:52:A:LYS:CA | 1:52:A:LYS:C | 7                   | 2.32 | 0.53            | 2.42   |
| (1,54)  | 1:62:A:LEU:C | 1:63:A:SER:N  | 1:63:A:SER:CA | 1:63:A:SER:C | 6                   | 6.4  | 3.52            | 8.4    |
| (1,74)  | 1:18:A:PRO:N | 1:18:A:PRO:CA | 1:18:A:PRO:C  | 1:19:A:ASN:N | 6                   | 2.02 | 0.76            | 1.86   |
| (1,100) | 1:47:A:ILE:N | 1:47:A:ILE:CA | 1:47:A:ILE:C  | 1:48:A:LEU:N | 6                   | 1.66 | 0.41            | 1.62   |
| (1,121) | 1:70:A:ARG:N | 1:70:A:ARG:CA | 1:70:A:ARG:C  | 1:71:A:ALA:N | 5                   | 1.52 | 0.23            | 1.63   |
| (1,114) | 1:62:A:LEU:N | 1:62:A:LEU:CA | 1:62:A:LEU:C  | 1:63:A:SER:N | 4                   | 7.24 | 0.69            | 7.08   |
| (1,40)  | 1:47:A:ILE:C | 1:48:A:LEU:N  | 1:48:A:LEU:CA | 1:48:A:LEU:C | 4                   | 1.48 | 0.3             | 1.57   |
| (1,17)  | 1:22:A:PHE:C | 1:23:A:ARG:N  | 1:23:A:ARG:CA | 1:23:A:ARG:C | 3                   | 3.13 | 0.74            | 3.58   |
| (1,119) | 1:67:A:ILE:N | 1:67:A:ILE:CA | 1:67:A:ILE:C  | 1:68:A:THR:N | 3                   | 1.72 | 0.23            | 1.63   |
| (1,33)  | 1:38:A:GLY:C | 1:39:A:LYS:N  | 1:39:A:LYS:CA | 1:39:A:LYS:C | 2                   | 2.09 | 0.48            | 2.09   |
| (1,93)  | 1:38:A:GLY:N | 1:38:A:GLY:CA | 1:38:A:GLY:C  | 1:39:A:LYS:N | 2                   | 2.06 | 0.35            | 2.06   |
| (1,61)  | 1:70:A:ARG:C | 1:71:A:ALA:N  | 1:71:A:ALA:CA | 1:71:A:ALA:C | 2                   | 1.6  | 0.38            | 1.6    |
| (1,102) | 1:49:A:THR:N | 1:49:A:THR:CA | 1:49:A:THR:C  | 1:50:A:GLY:N | 2                   | 1.58 | 0.3             | 1.58   |
| (1,2)   | 1:6:A:SER:C  | 1:7:A:PHE:N   | 1:7:A:PHE:CA  | 1:7:A:PHE:C  | 2                   | 1.52 | 0.24            | 1.52   |
| (1,19)  | 1:24:A:VAL:C | 1:25:A:GLU:N  | 1:25:A:GLU:CA | 1:25:A:GLU:C | 2                   | 1.42 | 0.4             | 1.42   |
| (1,38)  | 1:45:A:ILE:C | 1:46:A:ARG:N  | 1:46:A:ARG:CA | 1:46:A:ARG:C | 2                   | 1.36 | 0.34            | 1.36   |
| (1,69)  | 1:13:A:VAL:N | 1:13:A:VAL:CA | 1:13:A:VAL:C  | 1:14:A:VAL:N | 2                   | 1.22 | 0.17            | 1.22   |

<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 (°) |
|---------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,103) | 1:50:A:GLY:N | 1:50:A:GLY:CA | 1:50:A:GLY:C  | 1:51:A:ASP:N | 5        | 22.74         |
| (1,103) | 1:50:A:GLY:N | 1:50:A:GLY:CA | 1:50:A:GLY:C  | 1:51:A:ASP:N | 3        | 22.57         |
| (1,103) | 1:50:A:GLY:N | 1:50:A:GLY:CA | 1:50:A:GLY:C  | 1:51:A:ASP:N | 6        | 22.42         |
| (1,103) | 1:50:A:GLY:N | 1:50:A:GLY:CA | 1:50:A:GLY:C  | 1:51:A:ASP:N | 2        | 21.98         |
| (1,103) | 1:50:A:GLY:N | 1:50:A:GLY:CA | 1:50:A:GLY:C  | 1:51:A:ASP:N | 4        | 21.84         |
| (1,103) | 1:50:A:GLY:N | 1:50:A:GLY:CA | 1:50:A:GLY:C  | 1:51:A:ASP:N | 14       | 21.64         |
| (1,103) | 1:50:A:GLY:N | 1:50:A:GLY:CA | 1:50:A:GLY:C  | 1:51:A:ASP:N | 11       | 21.43         |
| (1,103) | 1:50:A:GLY:N | 1:50:A:GLY:CA | 1:50:A:GLY:C  | 1:51:A:ASP:N | 15       | 21.18         |
| (1,103) | 1:50:A:GLY:N | 1:50:A:GLY:CA | 1:50:A:GLY:C  | 1:51:A:ASP:N | 8        | 21.17         |
| (1,103) | 1:50:A:GLY:N | 1:50:A:GLY:CA | 1:50:A:GLY:C  | 1:51:A:ASP:N | 13       | 21.17         |
| (1,103) | 1:50:A:GLY:N | 1:50:A:GLY:CA | 1:50:A:GLY:C  | 1:51:A:ASP:N | 1        | 20.62         |
| (1,103) | 1:50:A:GLY:N | 1:50:A:GLY:CA | 1:50:A:GLY:C  | 1:51:A:ASP:N | 12       | 20.41         |
| (1,81)  | 1:26:A:LEU:N | 1:26:A:LEU:CA | 1:26:A:LEU:C  | 1:27:A:GLU:N | 7        | 20.35         |
| (1,70)  | 1:14:A:VAL:N | 1:14:A:VAL:CA | 1:14:A:VAL:C  | 1:15:A:ASP:N | 11       | 19.97         |
| (1,103) | 1:50:A:GLY:N | 1:50:A:GLY:CA | 1:50:A:GLY:C  | 1:51:A:ASP:N | 10       | 19.77         |
| (1,70)  | 1:14:A:VAL:N | 1:14:A:VAL:CA | 1:14:A:VAL:C  | 1:15:A:ASP:N | 14       | 19.49         |
| (1,81)  | 1:26:A:LEU:N | 1:26:A:LEU:CA | 1:26:A:LEU:C  | 1:27:A:GLU:N | 2        | 19.47         |
| (1,103) | 1:50:A:GLY:N | 1:50:A:GLY:CA | 1:50:A:GLY:C  | 1:51:A:ASP:N | 9        | 19.33         |
| (1,103) | 1:50:A:GLY:N | 1:50:A:GLY:CA | 1:50:A:GLY:C  | 1:51:A:ASP:N | 7        | 19.25         |
| (1,70)  | 1:14:A:VAL:N | 1:14:A:VAL:CA | 1:14:A:VAL:C  | 1:15:A:ASP:N | 2        | 19.23         |
| (1,70)  | 1:14:A:VAL:N | 1:14:A:VAL:CA | 1:14:A:VAL:C  | 1:15:A:ASP:N | 10       | 19.2          |
| (1,81)  | 1:26:A:LEU:N | 1:26:A:LEU:CA | 1:26:A:LEU:C  | 1:27:A:GLU:N | 13       | 19.1          |
| (1,81)  | 1:26:A:LEU:N | 1:26:A:LEU:CA | 1:26:A:LEU:C  | 1:27:A:GLU:N | 12       | 19.05         |
| (1,81)  | 1:26:A:LEU:N | 1:26:A:LEU:CA | 1:26:A:LEU:C  | 1:27:A:GLU:N | 4        | 19.04         |
| (1,81)  | 1:26:A:LEU:N | 1:26:A:LEU:CA | 1:26:A:LEU:C  | 1:27:A:GLU:N | 11       | 19.02         |
| (1,81)  | 1:26:A:LEU:N | 1:26:A:LEU:CA | 1:26:A:LEU:C  | 1:27:A:GLU:N | 8        | 18.91         |
| (1,70)  | 1:14:A:VAL:N | 1:14:A:VAL:CA | 1:14:A:VAL:C  | 1:15:A:ASP:N | 13       | 18.84         |
| (1,70)  | 1:14:A:VAL:N | 1:14:A:VAL:CA | 1:14:A:VAL:C  | 1:15:A:ASP:N | 1        | 18.78         |
| (1,81)  | 1:26:A:LEU:N | 1:26:A:LEU:CA | 1:26:A:LEU:C  | 1:27:A:GLU:N | 14       | 18.75         |
| (1,70)  | 1:14:A:VAL:N | 1:14:A:VAL:CA | 1:14:A:VAL:C  | 1:15:A:ASP:N | 4        | 18.73         |
| (1,81)  | 1:26:A:LEU:N | 1:26:A:LEU:CA | 1:26:A:LEU:C  | 1:27:A:GLU:N | 1        | 18.47         |
| (1,43)  | 1:50:A:GLY:C | 1:51:A:ASP:N  | 1:51:A:ASP:CA | 1:51:A:ASP:C | 5        | 18.45         |
| (1,70)  | 1:14:A:VAL:N | 1:14:A:VAL:CA | 1:14:A:VAL:C  | 1:15:A:ASP:N | 6        | 18.42         |
| (1,81)  | 1:26:A:LEU:N | 1:26:A:LEU:CA | 1:26:A:LEU:C  | 1:27:A:GLU:N | 15       | 18.34         |
| (1,81)  | 1:26:A:LEU:N | 1:26:A:LEU:CA | 1:26:A:LEU:C  | 1:27:A:GLU:N | 5        | 18.33         |
| (1,70)  | 1:14:A:VAL:N | 1:14:A:VAL:CA | 1:14:A:VAL:C  | 1:15:A:ASP:N | 9        | 18.33         |
| (1,81)  | 1:26:A:LEU:N | 1:26:A:LEU:CA | 1:26:A:LEU:C  | 1:27:A:GLU:N | 9        | 18.29         |
| (1,70)  | 1:14:A:VAL:N | 1:14:A:VAL:CA | 1:14:A:VAL:C  | 1:15:A:ASP:N | 12       | 18.14         |
| (1,43)  | 1:50:A:GLY:C | 1:51:A:ASP:N  | 1:51:A:ASP:CA | 1:51:A:ASP:C | 14       | 17.92         |
| (1,81)  | 1:26:A:LEU:N | 1:26:A:LEU:CA | 1:26:A:LEU:C  | 1:27:A:GLU:N | 6        | 17.76         |
| (1,81)  | 1:26:A:LEU:N | 1:26:A:LEU:CA | 1:26:A:LEU:C  | 1:27:A:GLU:N | 10       | 17.74         |
| (1,81)  | 1:26:A:LEU:N | 1:26:A:LEU:CA | 1:26:A:LEU:C  | 1:27:A:GLU:N | 3        | 17.69         |
| (1,70)  | 1:14:A:VAL:N | 1:14:A:VAL:CA | 1:14:A:VAL:C  | 1:15:A:ASP:N | 7        | 17.52         |
| (1,43)  | 1:50:A:GLY:C | 1:51:A:ASP:N  | 1:51:A:ASP:CA | 1:51:A:ASP:C | 6        | 17.07         |
| (1,70)  | 1:14:A:VAL:N | 1:14:A:VAL:CA | 1:14:A:VAL:C  | 1:15:A:ASP:N | 8        | 17.05         |
| (1,70)  | 1:14:A:VAL:N | 1:14:A:VAL:CA | 1:14:A:VAL:C  | 1:15:A:ASP:N | 3        | 17.02         |
| (1,43)  | 1:50:A:GLY:C | 1:51:A:ASP:N  | 1:51:A:ASP:CA | 1:51:A:ASP:C | 1        | 16.72         |

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| Key     | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Model ID | Violation (°) |
|---------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,43)  | 1:50:A:GLY:C | 1:51:A:ASP:N  | 1:51:A:ASP:CA | 1:51:A:ASP:C | 3        | 16.64         |
| (1,43)  | 1:50:A:GLY:C | 1:51:A:ASP:N  | 1:51:A:ASP:CA | 1:51:A:ASP:C | 13       | 16.59         |
| (1,43)  | 1:50:A:GLY:C | 1:51:A:ASP:N  | 1:51:A:ASP:CA | 1:51:A:ASP:C | 8        | 16.57         |
| (1,43)  | 1:50:A:GLY:C | 1:51:A:ASP:N  | 1:51:A:ASP:CA | 1:51:A:ASP:C | 11       | 16.42         |
| (1,21)  | 1:26:A:LEU:C | 1:27:A:GLU:N  | 1:27:A:GLU:CA | 1:27:A:GLU:C | 7        | 16.16         |
| (1,43)  | 1:50:A:GLY:C | 1:51:A:ASP:N  | 1:51:A:ASP:CA | 1:51:A:ASP:C | 12       | 16.08         |
| (1,70)  | 1:14:A:VAL:N | 1:14:A:VAL:CA | 1:14:A:VAL:C  | 1:15:A:ASP:N | 15       | 16.06         |
| (1,43)  | 1:50:A:GLY:C | 1:51:A:ASP:N  | 1:51:A:ASP:CA | 1:51:A:ASP:C | 4        | 16.02         |
| (1,70)  | 1:14:A:VAL:N | 1:14:A:VAL:CA | 1:14:A:VAL:C  | 1:15:A:ASP:N | 5        | 15.99         |
| (1,43)  | 1:50:A:GLY:C | 1:51:A:ASP:N  | 1:51:A:ASP:CA | 1:51:A:ASP:C | 2        | 15.9          |
| (1,21)  | 1:26:A:LEU:C | 1:27:A:GLU:N  | 1:27:A:GLU:CA | 1:27:A:GLU:C | 2        | 15.83         |
| (1,21)  | 1:26:A:LEU:C | 1:27:A:GLU:N  | 1:27:A:GLU:CA | 1:27:A:GLU:C | 13       | 15.57         |
| (1,43)  | 1:50:A:GLY:C | 1:51:A:ASP:N  | 1:51:A:ASP:CA | 1:51:A:ASP:C | 15       | 15.44         |
| (1,43)  | 1:50:A:GLY:C | 1:51:A:ASP:N  | 1:51:A:ASP:CA | 1:51:A:ASP:C | 10       | 15.41         |
| (1,21)  | 1:26:A:LEU:C | 1:27:A:GLU:N  | 1:27:A:GLU:CA | 1:27:A:GLU:C | 12       | 15.36         |
| (1,21)  | 1:26:A:LEU:C | 1:27:A:GLU:N  | 1:27:A:GLU:CA | 1:27:A:GLU:C | 11       | 15.33         |
| (1,10)  | 1:14:A:VAL:C | 1:15:A:ASP:N  | 1:15:A:ASP:CA | 1:15:A:ASP:C | 11       | 15.31         |
| (1,21)  | 1:26:A:LEU:C | 1:27:A:GLU:N  | 1:27:A:GLU:CA | 1:27:A:GLU:C | 6        | 15.24         |
| (1,43)  | 1:50:A:GLY:C | 1:51:A:ASP:N  | 1:51:A:ASP:CA | 1:51:A:ASP:C | 9        | 15.16         |
| (1,21)  | 1:26:A:LEU:C | 1:27:A:GLU:N  | 1:27:A:GLU:CA | 1:27:A:GLU:C | 5        | 15.15         |
| (1,21)  | 1:26:A:LEU:C | 1:27:A:GLU:N  | 1:27:A:GLU:CA | 1:27:A:GLU:C | 4        | 15.12         |
| (1,21)  | 1:26:A:LEU:C | 1:27:A:GLU:N  | 1:27:A:GLU:CA | 1:27:A:GLU:C | 1        | 15.09         |
| (1,21)  | 1:26:A:LEU:C | 1:27:A:GLU:N  | 1:27:A:GLU:CA | 1:27:A:GLU:C | 15       | 15.06         |
| (1,10)  | 1:14:A:VAL:C | 1:15:A:ASP:N  | 1:15:A:ASP:CA | 1:15:A:ASP:C | 13       | 15.01         |
| (1,21)  | 1:26:A:LEU:C | 1:27:A:GLU:N  | 1:27:A:GLU:CA | 1:27:A:GLU:C | 14       | 14.99         |
| (1,21)  | 1:26:A:LEU:C | 1:27:A:GLU:N  | 1:27:A:GLU:CA | 1:27:A:GLU:C | 9        | 14.92         |
| (1,120) | 1:68:A:THR:N | 1:68:A:THR:CA | 1:68:A:THR:C  | 1:69:A:TYR:N | 15       | 14.85         |
| (1,21)  | 1:26:A:LEU:C | 1:27:A:GLU:N  | 1:27:A:GLU:CA | 1:27:A:GLU:C | 3        | 14.81         |
| (1,21)  | 1:26:A:LEU:C | 1:27:A:GLU:N  | 1:27:A:GLU:CA | 1:27:A:GLU:C | 10       | 14.7          |
| (1,43)  | 1:50:A:GLY:C | 1:51:A:ASP:N  | 1:51:A:ASP:CA | 1:51:A:ASP:C | 7        | 14.68         |
| (1,120) | 1:68:A:THR:N | 1:68:A:THR:CA | 1:68:A:THR:C  | 1:69:A:TYR:N | 12       | 14.63         |
| (1,21)  | 1:26:A:LEU:C | 1:27:A:GLU:N  | 1:27:A:GLU:CA | 1:27:A:GLU:C | 8        | 14.56         |
| (1,120) | 1:68:A:THR:N | 1:68:A:THR:CA | 1:68:A:THR:C  | 1:69:A:TYR:N | 6        | 13.95         |
| (1,120) | 1:68:A:THR:N | 1:68:A:THR:CA | 1:68:A:THR:C  | 1:69:A:TYR:N | 1        | 13.9          |
| (1,120) | 1:68:A:THR:N | 1:68:A:THR:CA | 1:68:A:THR:C  | 1:69:A:TYR:N | 7        | 13.83         |
| (1,120) | 1:68:A:THR:N | 1:68:A:THR:CA | 1:68:A:THR:C  | 1:69:A:TYR:N | 13       | 13.78         |
| (1,10)  | 1:14:A:VAL:C | 1:15:A:ASP:N  | 1:15:A:ASP:CA | 1:15:A:ASP:C | 2        | 13.77         |
| (1,120) | 1:68:A:THR:N | 1:68:A:THR:CA | 1:68:A:THR:C  | 1:69:A:TYR:N | 10       | 13.58         |
| (1,120) | 1:68:A:THR:N | 1:68:A:THR:CA | 1:68:A:THR:C  | 1:69:A:TYR:N | 5        | 13.55         |
| (1,120) | 1:68:A:THR:N | 1:68:A:THR:CA | 1:68:A:THR:C  | 1:69:A:TYR:N | 11       | 13.45         |
| (1,13)  | 1:17:A:LEU:C | 1:18:A:PRO:N  | 1:18:A:PRO:CA | 1:18:A:PRO:C | 5        | 13.2          |
| (1,120) | 1:68:A:THR:N | 1:68:A:THR:CA | 1:68:A:THR:C  | 1:69:A:TYR:N | 9        | 13.08         |
| (1,120) | 1:68:A:THR:N | 1:68:A:THR:CA | 1:68:A:THR:C  | 1:69:A:TYR:N | 3        | 12.85         |
| (1,120) | 1:68:A:THR:N | 1:68:A:THR:CA | 1:68:A:THR:C  | 1:69:A:TYR:N | 2        | 12.8          |
| (1,13)  | 1:17:A:LEU:C | 1:18:A:PRO:N  | 1:18:A:PRO:CA | 1:18:A:PRO:C | 9        | 12.55         |
| (1,120) | 1:68:A:THR:N | 1:68:A:THR:CA | 1:68:A:THR:C  | 1:69:A:TYR:N | 14       | 12.53         |
| (1,13)  | 1:17:A:LEU:C | 1:18:A:PRO:N  | 1:18:A:PRO:CA | 1:18:A:PRO:C | 7        | 12.37         |
| (1,13)  | 1:17:A:LEU:C | 1:18:A:PRO:N  | 1:18:A:PRO:CA | 1:18:A:PRO:C | 14       | 12.35         |
| (1,10)  | 1:14:A:VAL:C | 1:15:A:ASP:N  | 1:15:A:ASP:CA | 1:15:A:ASP:C | 14       | 12.27         |
| (1,13)  | 1:17:A:LEU:C | 1:18:A:PRO:N  | 1:18:A:PRO:CA | 1:18:A:PRO:C | 15       | 12.26         |
| (1,13)  | 1:17:A:LEU:C | 1:18:A:PRO:N  | 1:18:A:PRO:CA | 1:18:A:PRO:C | 3        | 12.24         |

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| Key     | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Model ID | Violation (°) |
|---------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,120) | 1:68:A:THR:N | 1:68:A:THR:CA | 1:68:A:THR:C  | 1:69:A:TYR:N | 4        | 12.2          |
| (1,13)  | 1:17:A:LEU:C | 1:18:A:PRO:N  | 1:18:A:PRO:CA | 1:18:A:PRO:C | 2        | 12.02         |
| (1,13)  | 1:17:A:LEU:C | 1:18:A:PRO:N  | 1:18:A:PRO:CA | 1:18:A:PRO:C | 12       | 11.96         |
| (1,10)  | 1:14:A:VAL:C | 1:15:A:ASP:N  | 1:15:A:ASP:CA | 1:15:A:ASP:C | 1        | 11.94         |
| (1,10)  | 1:14:A:VAL:C | 1:15:A:ASP:N  | 1:15:A:ASP:CA | 1:15:A:ASP:C | 6        | 11.93         |
| (1,120) | 1:68:A:THR:N | 1:68:A:THR:CA | 1:68:A:THR:C  | 1:69:A:TYR:N | 8        | 11.91         |
| (1,13)  | 1:17:A:LEU:C | 1:18:A:PRO:N  | 1:18:A:PRO:CA | 1:18:A:PRO:C | 8        | 11.9          |
| (1,13)  | 1:17:A:LEU:C | 1:18:A:PRO:N  | 1:18:A:PRO:CA | 1:18:A:PRO:C | 11       | 11.86         |
| (1,13)  | 1:17:A:LEU:C | 1:18:A:PRO:N  | 1:18:A:PRO:CA | 1:18:A:PRO:C | 1        | 11.78         |
| (1,13)  | 1:17:A:LEU:C | 1:18:A:PRO:N  | 1:18:A:PRO:CA | 1:18:A:PRO:C | 10       | 11.64         |
| (1,13)  | 1:17:A:LEU:C | 1:18:A:PRO:N  | 1:18:A:PRO:CA | 1:18:A:PRO:C | 4        | 11.63         |
| (1,10)  | 1:14:A:VAL:C | 1:15:A:ASP:N  | 1:15:A:ASP:CA | 1:15:A:ASP:C | 9        | 11.33         |
| (1,10)  | 1:14:A:VAL:C | 1:15:A:ASP:N  | 1:15:A:ASP:CA | 1:15:A:ASP:C | 15       | 11.22         |
| (1,13)  | 1:17:A:LEU:C | 1:18:A:PRO:N  | 1:18:A:PRO:CA | 1:18:A:PRO:C | 13       | 11.18         |
| (1,10)  | 1:14:A:VAL:C | 1:15:A:ASP:N  | 1:15:A:ASP:CA | 1:15:A:ASP:C | 12       | 10.99         |
| (1,13)  | 1:17:A:LEU:C | 1:18:A:PRO:N  | 1:18:A:PRO:CA | 1:18:A:PRO:C | 6        | 10.91         |
| (1,10)  | 1:14:A:VAL:C | 1:15:A:ASP:N  | 1:15:A:ASP:CA | 1:15:A:ASP:C | 3        | 10.86         |
| (1,10)  | 1:14:A:VAL:C | 1:15:A:ASP:N  | 1:15:A:ASP:CA | 1:15:A:ASP:C | 10       | 10.29         |
| (1,10)  | 1:14:A:VAL:C | 1:15:A:ASP:N  | 1:15:A:ASP:CA | 1:15:A:ASP:C | 7        | 10.26         |
| (1,10)  | 1:14:A:VAL:C | 1:15:A:ASP:N  | 1:15:A:ASP:CA | 1:15:A:ASP:C | 5        | 9.97          |
| (1,10)  | 1:14:A:VAL:C | 1:15:A:ASP:N  | 1:15:A:ASP:CA | 1:15:A:ASP:C | 4        | 9.8           |
| (1,54)  | 1:62:A:LEU:C | 1:63:A:SER:N  | 1:63:A:SER:CA | 1:63:A:SER:C | 12       | 9.7           |
| (1,54)  | 1:62:A:LEU:C | 1:63:A:SER:N  | 1:63:A:SER:CA | 1:63:A:SER:C | 15       | 8.96          |
| (1,54)  | 1:62:A:LEU:C | 1:63:A:SER:N  | 1:63:A:SER:CA | 1:63:A:SER:C | 7        | 8.4           |
| (1,54)  | 1:62:A:LEU:C | 1:63:A:SER:N  | 1:63:A:SER:CA | 1:63:A:SER:C | 14       | 8.4           |
| (1,114) | 1:62:A:LEU:N | 1:62:A:LEU:CA | 1:62:A:LEU:C  | 1:63:A:SER:N | 12       | 8.29          |
| (1,24)  | 1:29:A:GLY:C | 1:30:A:HIS:N  | 1:30:A:HIS:CA | 1:30:A:HIS:C | 14       | 8.25          |
| (1,23)  | 1:28:A:ASN:C | 1:29:A:GLY:N  | 1:29:A:GLY:CA | 1:29:A:GLY:C | 8        | 8.25          |
| (1,24)  | 1:29:A:GLY:C | 1:30:A:HIS:N  | 1:30:A:HIS:CA | 1:30:A:HIS:C | 2        | 8.2           |
| (1,24)  | 1:29:A:GLY:C | 1:30:A:HIS:N  | 1:30:A:HIS:CA | 1:30:A:HIS:C | 4        | 8.13          |
| (1,24)  | 1:29:A:GLY:C | 1:30:A:HIS:N  | 1:30:A:HIS:CA | 1:30:A:HIS:C | 15       | 8.12          |
| (1,10)  | 1:14:A:VAL:C | 1:15:A:ASP:N  | 1:15:A:ASP:CA | 1:15:A:ASP:C | 8        | 8.09          |
| (1,23)  | 1:28:A:ASN:C | 1:29:A:GLY:N  | 1:29:A:GLY:CA | 1:29:A:GLY:C | 7        | 8.04          |
| (1,24)  | 1:29:A:GLY:C | 1:30:A:HIS:N  | 1:30:A:HIS:CA | 1:30:A:HIS:C | 10       | 7.89          |
| (1,24)  | 1:29:A:GLY:C | 1:30:A:HIS:N  | 1:30:A:HIS:CA | 1:30:A:HIS:C | 12       | 7.89          |
| (1,24)  | 1:29:A:GLY:C | 1:30:A:HIS:N  | 1:30:A:HIS:CA | 1:30:A:HIS:C | 3        | 7.88          |
| (1,23)  | 1:28:A:ASN:C | 1:29:A:GLY:N  | 1:29:A:GLY:CA | 1:29:A:GLY:C | 6        | 7.88          |
| (1,24)  | 1:29:A:GLY:C | 1:30:A:HIS:N  | 1:30:A:HIS:CA | 1:30:A:HIS:C | 6        | 7.84          |
| (1,24)  | 1:29:A:GLY:C | 1:30:A:HIS:N  | 1:30:A:HIS:CA | 1:30:A:HIS:C | 9        | 7.84          |
| (1,24)  | 1:29:A:GLY:C | 1:30:A:HIS:N  | 1:30:A:HIS:CA | 1:30:A:HIS:C | 13       | 7.8           |
| (1,23)  | 1:28:A:ASN:C | 1:29:A:GLY:N  | 1:29:A:GLY:CA | 1:29:A:GLY:C | 12       | 7.8           |
| (1,25)  | 1:30:A:HIS:C | 1:31:A:VAL:N  | 1:31:A:VAL:CA | 1:31:A:VAL:C | 5        | 7.74          |
| (1,24)  | 1:29:A:GLY:C | 1:30:A:HIS:N  | 1:30:A:HIS:CA | 1:30:A:HIS:C | 1        | 7.68          |
| (1,24)  | 1:29:A:GLY:C | 1:30:A:HIS:N  | 1:30:A:HIS:CA | 1:30:A:HIS:C | 11       | 7.66          |
| (1,24)  | 1:29:A:GLY:C | 1:30:A:HIS:N  | 1:30:A:HIS:CA | 1:30:A:HIS:C | 8        | 7.59          |
| (1,25)  | 1:30:A:HIS:C | 1:31:A:VAL:N  | 1:31:A:VAL:CA | 1:31:A:VAL:C | 14       | 7.55          |
| (1,23)  | 1:28:A:ASN:C | 1:29:A:GLY:N  | 1:29:A:GLY:CA | 1:29:A:GLY:C | 9        | 7.53          |
| (1,24)  | 1:29:A:GLY:C | 1:30:A:HIS:N  | 1:30:A:HIS:CA | 1:30:A:HIS:C | 5        | 7.52          |
| (1,24)  | 1:29:A:GLY:C | 1:30:A:HIS:N  | 1:30:A:HIS:CA | 1:30:A:HIS:C | 7        | 7.44          |
| (1,114) | 1:62:A:LEU:N | 1:62:A:LEU:CA | 1:62:A:LEU:C  | 1:63:A:SER:N | 7        | 7.4           |
| (1,23)  | 1:28:A:ASN:C | 1:29:A:GLY:N  | 1:29:A:GLY:CA | 1:29:A:GLY:C | 14       | 7.37          |

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| Key     | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Model ID | Violation (°) |
|---------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,25)  | 1:30:A:HIS:C | 1:31:A:VAL:N  | 1:31:A:VAL:CA | 1:31:A:VAL:C | 7        | 7.34          |
| (1,23)  | 1:28:A:ASN:C | 1:29:A:GLY:N  | 1:29:A:GLY:CA | 1:29:A:GLY:C | 11       | 7.29          |
| (1,25)  | 1:30:A:HIS:C | 1:31:A:VAL:N  | 1:31:A:VAL:CA | 1:31:A:VAL:C | 12       | 7.26          |
| (1,25)  | 1:30:A:HIS:C | 1:31:A:VAL:N  | 1:31:A:VAL:CA | 1:31:A:VAL:C | 2        | 7.23          |
| (1,23)  | 1:28:A:ASN:C | 1:29:A:GLY:N  | 1:29:A:GLY:CA | 1:29:A:GLY:C | 2        | 7.2           |
| (1,25)  | 1:30:A:HIS:C | 1:31:A:VAL:N  | 1:31:A:VAL:CA | 1:31:A:VAL:C | 13       | 7.18          |
| (1,23)  | 1:28:A:ASN:C | 1:29:A:GLY:N  | 1:29:A:GLY:CA | 1:29:A:GLY:C | 5        | 7.14          |
| (1,23)  | 1:28:A:ASN:C | 1:29:A:GLY:N  | 1:29:A:GLY:CA | 1:29:A:GLY:C | 4        | 7.08          |
| (1,25)  | 1:30:A:HIS:C | 1:31:A:VAL:N  | 1:31:A:VAL:CA | 1:31:A:VAL:C | 10       | 7.05          |
| (1,23)  | 1:28:A:ASN:C | 1:29:A:GLY:N  | 1:29:A:GLY:CA | 1:29:A:GLY:C | 3        | 6.96          |
| (1,23)  | 1:28:A:ASN:C | 1:29:A:GLY:N  | 1:29:A:GLY:CA | 1:29:A:GLY:C | 1        | 6.93          |
| (1,25)  | 1:30:A:HIS:C | 1:31:A:VAL:N  | 1:31:A:VAL:CA | 1:31:A:VAL:C | 8        | 6.89          |
| (1,23)  | 1:28:A:ASN:C | 1:29:A:GLY:N  | 1:29:A:GLY:CA | 1:29:A:GLY:C | 13       | 6.79          |
| (1,114) | 1:62:A:LEU:N | 1:62:A:LEU:CA | 1:62:A:LEU:C  | 1:63:A:SER:N | 14       | 6.76          |
| (1,23)  | 1:28:A:ASN:C | 1:29:A:GLY:N  | 1:29:A:GLY:CA | 1:29:A:GLY:C | 10       | 6.74          |
| (1,23)  | 1:28:A:ASN:C | 1:29:A:GLY:N  | 1:29:A:GLY:CA | 1:29:A:GLY:C | 15       | 6.72          |
| (1,25)  | 1:30:A:HIS:C | 1:31:A:VAL:N  | 1:31:A:VAL:CA | 1:31:A:VAL:C | 11       | 6.7           |
| (1,25)  | 1:30:A:HIS:C | 1:31:A:VAL:N  | 1:31:A:VAL:CA | 1:31:A:VAL:C | 9        | 6.65          |
| (1,114) | 1:62:A:LEU:N | 1:62:A:LEU:CA | 1:62:A:LEU:C  | 1:63:A:SER:N | 15       | 6.51          |
| (1,25)  | 1:30:A:HIS:C | 1:31:A:VAL:N  | 1:31:A:VAL:CA | 1:31:A:VAL:C | 6        | 6.51          |
| (1,25)  | 1:30:A:HIS:C | 1:31:A:VAL:N  | 1:31:A:VAL:CA | 1:31:A:VAL:C | 1        | 6.42          |
| (1,25)  | 1:30:A:HIS:C | 1:31:A:VAL:N  | 1:31:A:VAL:CA | 1:31:A:VAL:C | 3        | 6.25          |
| (1,117) | 1:65:A:GLY:N | 1:65:A:GLY:CA | 1:65:A:GLY:C  | 1:66:A:ARG:N | 8        | 6.17          |
| (1,25)  | 1:30:A:HIS:C | 1:31:A:VAL:N  | 1:31:A:VAL:CA | 1:31:A:VAL:C | 15       | 5.77          |
| (1,117) | 1:65:A:GLY:N | 1:65:A:GLY:CA | 1:65:A:GLY:C  | 1:66:A:ARG:N | 4        | 5.53          |
| (1,25)  | 1:30:A:HIS:C | 1:31:A:VAL:N  | 1:31:A:VAL:CA | 1:31:A:VAL:C | 4        | 5.52          |
| (1,117) | 1:65:A:GLY:N | 1:65:A:GLY:CA | 1:65:A:GLY:C  | 1:66:A:ARG:N | 9        | 5.33          |
| (1,117) | 1:65:A:GLY:N | 1:65:A:GLY:CA | 1:65:A:GLY:C  | 1:66:A:ARG:N | 6        | 5.2           |
| (1,117) | 1:65:A:GLY:N | 1:65:A:GLY:CA | 1:65:A:GLY:C  | 1:66:A:ARG:N | 1        | 5.19          |
| (1,117) | 1:65:A:GLY:N | 1:65:A:GLY:CA | 1:65:A:GLY:C  | 1:66:A:ARG:N | 2        | 5.11          |
| (1,117) | 1:65:A:GLY:N | 1:65:A:GLY:CA | 1:65:A:GLY:C  | 1:66:A:ARG:N | 13       | 4.97          |
| (1,59)  | 1:67:A:ILE:C | 1:68:A:THR:N  | 1:68:A:THR:CA | 1:68:A:THR:C | 10       | 4.94          |
| (1,117) | 1:65:A:GLY:N | 1:65:A:GLY:CA | 1:65:A:GLY:C  | 1:66:A:ARG:N | 5        | 4.75          |
| (1,37)  | 1:42:A:LYS:C | 1:43:A:ASN:N  | 1:43:A:ASN:CA | 1:43:A:ASN:C | 9        | 4.68          |
| (1,117) | 1:65:A:GLY:N | 1:65:A:GLY:CA | 1:65:A:GLY:C  | 1:66:A:ARG:N | 3        | 4.65          |
| (1,117) | 1:65:A:GLY:N | 1:65:A:GLY:CA | 1:65:A:GLY:C  | 1:66:A:ARG:N | 7        | 4.61          |
| (1,59)  | 1:67:A:ILE:C | 1:68:A:THR:N  | 1:68:A:THR:CA | 1:68:A:THR:C | 9        | 4.47          |
| (1,104) | 1:51:A:ASP:N | 1:51:A:ASP:CA | 1:51:A:ASP:C  | 1:52:A:LYS:N | 6        | 4.46          |
| (1,117) | 1:65:A:GLY:N | 1:65:A:GLY:CA | 1:65:A:GLY:C  | 1:66:A:ARG:N | 10       | 4.45          |
| (1,117) | 1:65:A:GLY:N | 1:65:A:GLY:CA | 1:65:A:GLY:C  | 1:66:A:ARG:N | 11       | 4.38          |
| (1,59)  | 1:67:A:ILE:C | 1:68:A:THR:N  | 1:68:A:THR:CA | 1:68:A:THR:C | 7        | 4.32          |
| (1,8)   | 1:12:A:THR:C | 1:13:A:VAL:N  | 1:13:A:VAL:CA | 1:13:A:VAL:C | 2        | 4.3           |
| (1,117) | 1:65:A:GLY:N | 1:65:A:GLY:CA | 1:65:A:GLY:C  | 1:66:A:ARG:N | 15       | 4.12          |
| (1,97)  | 1:42:A:LYS:N | 1:42:A:LYS:CA | 1:42:A:LYS:C  | 1:43:A:ASN:N | 9        | 4.01          |
| (1,105) | 1:52:A:LYS:N | 1:52:A:LYS:CA | 1:52:A:LYS:C  | 1:53:A:VAL:N | 15       | 3.96          |
| (1,8)   | 1:12:A:THR:C | 1:13:A:VAL:N  | 1:13:A:VAL:CA | 1:13:A:VAL:C | 11       | 3.96          |
| (1,8)   | 1:12:A:THR:C | 1:13:A:VAL:N  | 1:13:A:VAL:CA | 1:13:A:VAL:C | 3        | 3.92          |
| (1,59)  | 1:67:A:ILE:C | 1:68:A:THR:N  | 1:68:A:THR:CA | 1:68:A:THR:C | 3        | 3.89          |
| (1,117) | 1:65:A:GLY:N | 1:65:A:GLY:CA | 1:65:A:GLY:C  | 1:66:A:ARG:N | 14       | 3.88          |
| (1,49)  | 1:56:A:GLU:C | 1:57:A:LEU:N  | 1:57:A:LEU:CA | 1:57:A:LEU:C | 12       | 3.88          |
| (1,104) | 1:51:A:ASP:N | 1:51:A:ASP:CA | 1:51:A:ASP:C  | 1:52:A:LYS:N | 1        | 3.86          |

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| Key     | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Model ID | Violation (°) |
|---------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,49)  | 1:56:A:GLU:C | 1:57:A:LEU:N  | 1:57:A:LEU:CA | 1:57:A:LEU:C | 15       | 3.77          |
| (1,58)  | 1:66:A:ARG:C | 1:67:A:ILE:N  | 1:67:A:ILE:CA | 1:67:A:ILE:C | 5        | 3.76          |
| (1,17)  | 1:22:A:PHE:C | 1:23:A:ARG:N  | 1:23:A:ARG:CA | 1:23:A:ARG:C | 1        | 3.73          |
| (1,105) | 1:52:A:LYS:N | 1:52:A:LYS:CA | 1:52:A:LYS:C  | 1:53:A:VAL:N | 2        | 3.72          |
| (1,49)  | 1:56:A:GLU:C | 1:57:A:LEU:N  | 1:57:A:LEU:CA | 1:57:A:LEU:C | 11       | 3.72          |
| (1,8)   | 1:12:A:THR:C | 1:13:A:VAL:N  | 1:13:A:VAL:CA | 1:13:A:VAL:C | 6        | 3.72          |
| (1,49)  | 1:56:A:GLU:C | 1:57:A:LEU:N  | 1:57:A:LEU:CA | 1:57:A:LEU:C | 7        | 3.71          |
| (1,59)  | 1:67:A:ILE:C | 1:68:A:THR:N  | 1:68:A:THR:CA | 1:68:A:THR:C | 4        | 3.7           |
| (1,49)  | 1:56:A:GLU:C | 1:57:A:LEU:N  | 1:57:A:LEU:CA | 1:57:A:LEU:C | 14       | 3.7           |
| (1,104) | 1:51:A:ASP:N | 1:51:A:ASP:CA | 1:51:A:ASP:C  | 1:52:A:LYS:N | 14       | 3.66          |
| (1,8)   | 1:12:A:THR:C | 1:13:A:VAL:N  | 1:13:A:VAL:CA | 1:13:A:VAL:C | 15       | 3.65          |
| (1,49)  | 1:56:A:GLU:C | 1:57:A:LEU:N  | 1:57:A:LEU:CA | 1:57:A:LEU:C | 5        | 3.63          |
| (1,104) | 1:51:A:ASP:N | 1:51:A:ASP:CA | 1:51:A:ASP:C  | 1:52:A:LYS:N | 15       | 3.62          |
| (1,59)  | 1:67:A:ILE:C | 1:68:A:THR:N  | 1:68:A:THR:CA | 1:68:A:THR:C | 14       | 3.61          |
| (1,8)   | 1:12:A:THR:C | 1:13:A:VAL:N  | 1:13:A:VAL:CA | 1:13:A:VAL:C | 12       | 3.6           |
| (1,74)  | 1:18:A:PRO:N | 1:18:A:PRO:CA | 1:18:A:PRO:C  | 1:19:A:ASN:N | 11       | 3.58          |
| (1,17)  | 1:22:A:PHE:C | 1:23:A:ARG:N  | 1:23:A:ARG:CA | 1:23:A:ARG:C | 12       | 3.58          |
| (1,105) | 1:52:A:LYS:N | 1:52:A:LYS:CA | 1:52:A:LYS:C  | 1:53:A:VAL:N | 8        | 3.57          |
| (1,8)   | 1:12:A:THR:C | 1:13:A:VAL:N  | 1:13:A:VAL:CA | 1:13:A:VAL:C | 7        | 3.54          |
| (1,49)  | 1:56:A:GLU:C | 1:57:A:LEU:N  | 1:57:A:LEU:CA | 1:57:A:LEU:C | 8        | 3.52          |
| (1,104) | 1:51:A:ASP:N | 1:51:A:ASP:CA | 1:51:A:ASP:C  | 1:52:A:LYS:N | 7        | 3.48          |
| (1,8)   | 1:12:A:THR:C | 1:13:A:VAL:N  | 1:13:A:VAL:CA | 1:13:A:VAL:C | 8        | 3.38          |
| (1,105) | 1:52:A:LYS:N | 1:52:A:LYS:CA | 1:52:A:LYS:C  | 1:53:A:VAL:N | 3        | 3.37          |
| (1,8)   | 1:12:A:THR:C | 1:13:A:VAL:N  | 1:13:A:VAL:CA | 1:13:A:VAL:C | 14       | 3.35          |
| (1,59)  | 1:67:A:ILE:C | 1:68:A:THR:N  | 1:68:A:THR:CA | 1:68:A:THR:C | 11       | 3.34          |
| (1,105) | 1:52:A:LYS:N | 1:52:A:LYS:CA | 1:52:A:LYS:C  | 1:53:A:VAL:N | 6        | 3.33          |
| (1,8)   | 1:12:A:THR:C | 1:13:A:VAL:N  | 1:13:A:VAL:CA | 1:13:A:VAL:C | 5        | 3.33          |
| (1,49)  | 1:56:A:GLU:C | 1:57:A:LEU:N  | 1:57:A:LEU:CA | 1:57:A:LEU:C | 2        | 3.32          |
| (1,104) | 1:51:A:ASP:N | 1:51:A:ASP:CA | 1:51:A:ASP:C  | 1:52:A:LYS:N | 8        | 3.16          |
| (1,59)  | 1:67:A:ILE:C | 1:68:A:THR:N  | 1:68:A:THR:CA | 1:68:A:THR:C | 2        | 3.16          |
| (1,105) | 1:52:A:LYS:N | 1:52:A:LYS:CA | 1:52:A:LYS:C  | 1:53:A:VAL:N | 4        | 3.15          |
| (1,83)  | 1:28:A:ASN:N | 1:28:A:ASN:CA | 1:28:A:ASN:C  | 1:29:A:GLY:N | 8        | 3.15          |
| (1,59)  | 1:67:A:ILE:C | 1:68:A:THR:N  | 1:68:A:THR:CA | 1:68:A:THR:C | 12       | 3.15          |
| (1,117) | 1:65:A:GLY:N | 1:65:A:GLY:CA | 1:65:A:GLY:C  | 1:66:A:ARG:N | 12       | 3.14          |
| (1,49)  | 1:56:A:GLU:C | 1:57:A:LEU:N  | 1:57:A:LEU:CA | 1:57:A:LEU:C | 6        | 3.08          |
| (1,44)  | 1:51:A:ASP:C | 1:52:A:LYS:N  | 1:52:A:LYS:CA | 1:52:A:LYS:C | 11       | 3.06          |
| (1,83)  | 1:28:A:ASN:N | 1:28:A:ASN:CA | 1:28:A:ASN:C  | 1:29:A:GLY:N | 12       | 3.04          |
| (1,58)  | 1:66:A:ARG:C | 1:67:A:ILE:N  | 1:67:A:ILE:CA | 1:67:A:ILE:C | 14       | 3.03          |
| (1,8)   | 1:12:A:THR:C | 1:13:A:VAL:N  | 1:13:A:VAL:CA | 1:13:A:VAL:C | 10       | 2.98          |
| (1,44)  | 1:51:A:ASP:C | 1:52:A:LYS:N  | 1:52:A:LYS:CA | 1:52:A:LYS:C | 4        | 2.96          |
| (1,83)  | 1:28:A:ASN:N | 1:28:A:ASN:CA | 1:28:A:ASN:C  | 1:29:A:GLY:N | 6        | 2.95          |
| (1,83)  | 1:28:A:ASN:N | 1:28:A:ASN:CA | 1:28:A:ASN:C  | 1:29:A:GLY:N | 7        | 2.95          |
| (1,83)  | 1:28:A:ASN:N | 1:28:A:ASN:CA | 1:28:A:ASN:C  | 1:29:A:GLY:N | 9        | 2.91          |
| (1,83)  | 1:28:A:ASN:N | 1:28:A:ASN:CA | 1:28:A:ASN:C  | 1:29:A:GLY:N | 14       | 2.91          |
| (1,49)  | 1:56:A:GLU:C | 1:57:A:LEU:N  | 1:57:A:LEU:CA | 1:57:A:LEU:C | 4        | 2.88          |
| (1,83)  | 1:28:A:ASN:N | 1:28:A:ASN:CA | 1:28:A:ASN:C  | 1:29:A:GLY:N | 5        | 2.87          |
| (1,59)  | 1:67:A:ILE:C | 1:68:A:THR:N  | 1:68:A:THR:CA | 1:68:A:THR:C | 13       | 2.87          |
| (1,83)  | 1:28:A:ASN:N | 1:28:A:ASN:CA | 1:28:A:ASN:C  | 1:29:A:GLY:N | 1        | 2.77          |
| (1,8)   | 1:12:A:THR:C | 1:13:A:VAL:N  | 1:13:A:VAL:CA | 1:13:A:VAL:C | 4        | 2.76          |
| (1,83)  | 1:28:A:ASN:N | 1:28:A:ASN:CA | 1:28:A:ASN:C  | 1:29:A:GLY:N | 2        | 2.7           |
| (1,105) | 1:52:A:LYS:N | 1:52:A:LYS:CA | 1:52:A:LYS:C  | 1:53:A:VAL:N | 11       | 2.69          |

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| Key     | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Model ID | Violation (°) |
|---------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,83)  | 1:28:A:ASN:N | 1:28:A:ASN:CA | 1:28:A:ASN:C  | 1:29:A:GLY:N | 11       | 2.69          |
| (1,49)  | 1:56:A:GLU:C | 1:57:A:LEU:N  | 1:57:A:LEU:CA | 1:57:A:LEU:C | 10       | 2.66          |
| (1,8)   | 1:12:A:THR:C | 1:13:A:VAL:N  | 1:13:A:VAL:CA | 1:13:A:VAL:C | 13       | 2.65          |
| (1,83)  | 1:28:A:ASN:N | 1:28:A:ASN:CA | 1:28:A:ASN:C  | 1:29:A:GLY:N | 3        | 2.64          |
| (1,8)   | 1:12:A:THR:C | 1:13:A:VAL:N  | 1:13:A:VAL:CA | 1:13:A:VAL:C | 9        | 2.58          |
| (1,33)  | 1:38:A:GLY:C | 1:39:A:LYS:N  | 1:39:A:LYS:CA | 1:39:A:LYS:C | 8        | 2.57          |
| (1,83)  | 1:28:A:ASN:N | 1:28:A:ASN:CA | 1:28:A:ASN:C  | 1:29:A:GLY:N | 10       | 2.56          |
| (1,49)  | 1:56:A:GLU:C | 1:57:A:LEU:N  | 1:57:A:LEU:CA | 1:57:A:LEU:C | 3        | 2.55          |
| (1,47)  | 1:54:A:ARG:C | 1:55:A:VAL:N  | 1:55:A:VAL:CA | 1:55:A:VAL:C | 11       | 2.51          |
| (1,49)  | 1:56:A:GLU:C | 1:57:A:LEU:N  | 1:57:A:LEU:CA | 1:57:A:LEU:C | 13       | 2.49          |
| (1,44)  | 1:51:A:ASP:C | 1:52:A:LYS:N  | 1:52:A:LYS:CA | 1:52:A:LYS:C | 3        | 2.48          |
| (1,59)  | 1:67:A:ILE:C | 1:68:A:THR:N  | 1:68:A:THR:CA | 1:68:A:THR:C | 8        | 2.47          |
| (1,83)  | 1:28:A:ASN:N | 1:28:A:ASN:CA | 1:28:A:ASN:C  | 1:29:A:GLY:N | 13       | 2.43          |
| (1,49)  | 1:56:A:GLU:C | 1:57:A:LEU:N  | 1:57:A:LEU:CA | 1:57:A:LEU:C | 1        | 2.43          |
| (1,44)  | 1:51:A:ASP:C | 1:52:A:LYS:N  | 1:52:A:LYS:CA | 1:52:A:LYS:C | 2        | 2.42          |
| (1,93)  | 1:38:A:GLY:N | 1:38:A:GLY:CA | 1:38:A:GLY:C  | 1:39:A:LYS:N | 8        | 2.41          |
| (1,59)  | 1:67:A:ILE:C | 1:68:A:THR:N  | 1:68:A:THR:CA | 1:68:A:THR:C | 5        | 2.41          |
| (1,58)  | 1:66:A:ARG:C | 1:67:A:ILE:N  | 1:67:A:ILE:CA | 1:67:A:ILE:C | 13       | 2.41          |
| (1,105) | 1:52:A:LYS:N | 1:52:A:LYS:CA | 1:52:A:LYS:C  | 1:53:A:VAL:N | 14       | 2.4           |
| (1,58)  | 1:66:A:ARG:C | 1:67:A:ILE:N  | 1:67:A:ILE:CA | 1:67:A:ILE:C | 11       | 2.4           |
| (1,47)  | 1:54:A:ARG:C | 1:55:A:VAL:N  | 1:55:A:VAL:CA | 1:55:A:VAL:C | 5        | 2.4           |
| (1,105) | 1:52:A:LYS:N | 1:52:A:LYS:CA | 1:52:A:LYS:C  | 1:53:A:VAL:N | 5        | 2.38          |
| (1,83)  | 1:28:A:ASN:N | 1:28:A:ASN:CA | 1:28:A:ASN:C  | 1:29:A:GLY:N | 4        | 2.32          |
| (1,83)  | 1:28:A:ASN:N | 1:28:A:ASN:CA | 1:28:A:ASN:C  | 1:29:A:GLY:N | 15       | 2.32          |
| (1,47)  | 1:54:A:ARG:C | 1:55:A:VAL:N  | 1:55:A:VAL:CA | 1:55:A:VAL:C | 3        | 2.32          |
| (1,105) | 1:52:A:LYS:N | 1:52:A:LYS:CA | 1:52:A:LYS:C  | 1:53:A:VAL:N | 10       | 2.3           |
| (1,105) | 1:52:A:LYS:N | 1:52:A:LYS:CA | 1:52:A:LYS:C  | 1:53:A:VAL:N | 7        | 2.29          |
| (1,58)  | 1:66:A:ARG:C | 1:67:A:ILE:N  | 1:67:A:ILE:CA | 1:67:A:ILE:C | 7        | 2.27          |
| (1,49)  | 1:56:A:GLU:C | 1:57:A:LEU:N  | 1:57:A:LEU:CA | 1:57:A:LEU:C | 9        | 2.22          |
| (1,47)  | 1:54:A:ARG:C | 1:55:A:VAL:N  | 1:55:A:VAL:CA | 1:55:A:VAL:C | 13       | 2.21          |
| (1,47)  | 1:54:A:ARG:C | 1:55:A:VAL:N  | 1:55:A:VAL:CA | 1:55:A:VAL:C | 7        | 2.2           |
| (1,100) | 1:47:A:ILE:N | 1:47:A:ILE:CA | 1:47:A:ILE:C  | 1:48:A:LEU:N | 9        | 2.17          |
| (1,100) | 1:47:A:ILE:N | 1:47:A:ILE:CA | 1:47:A:ILE:C  | 1:48:A:LEU:N | 1        | 2.14          |
| (1,58)  | 1:66:A:ARG:C | 1:67:A:ILE:N  | 1:67:A:ILE:CA | 1:67:A:ILE:C | 8        | 2.13          |
| (1,8)   | 1:12:A:THR:C | 1:13:A:VAL:N  | 1:13:A:VAL:CA | 1:13:A:VAL:C | 1        | 2.13          |
| (1,47)  | 1:54:A:ARG:C | 1:55:A:VAL:N  | 1:55:A:VAL:CA | 1:55:A:VAL:C | 2        | 2.12          |
| (1,58)  | 1:66:A:ARG:C | 1:67:A:ILE:N  | 1:67:A:ILE:CA | 1:67:A:ILE:C | 4        | 2.11          |
| (1,59)  | 1:67:A:ILE:C | 1:68:A:THR:N  | 1:68:A:THR:CA | 1:68:A:THR:C | 6        | 2.09          |
| (1,17)  | 1:22:A:PHE:C | 1:23:A:ARG:N  | 1:23:A:ARG:CA | 1:23:A:ARG:C | 5        | 2.09          |
| (1,59)  | 1:67:A:ILE:C | 1:68:A:THR:N  | 1:68:A:THR:CA | 1:68:A:THR:C | 15       | 2.08          |
| (1,58)  | 1:66:A:ARG:C | 1:67:A:ILE:N  | 1:67:A:ILE:CA | 1:67:A:ILE:C | 15       | 2.08          |
| (1,58)  | 1:66:A:ARG:C | 1:67:A:ILE:N  | 1:67:A:ILE:CA | 1:67:A:ILE:C | 9        | 2.06          |
| (1,119) | 1:67:A:ILE:N | 1:67:A:ILE:CA | 1:67:A:ILE:C  | 1:68:A:THR:N | 1        | 2.03          |
| (1,105) | 1:52:A:LYS:N | 1:52:A:LYS:CA | 1:52:A:LYS:C  | 1:53:A:VAL:N | 1        | 2.02          |
| (1,74)  | 1:18:A:PRO:N | 1:18:A:PRO:CA | 1:18:A:PRO:C  | 1:19:A:ASN:N | 6        | 2.02          |
| (1,44)  | 1:51:A:ASP:C | 1:52:A:LYS:N  | 1:52:A:LYS:CA | 1:52:A:LYS:C | 10       | 2.02          |
| (1,61)  | 1:70:A:ARG:C | 1:71:A:ALA:N  | 1:71:A:ALA:CA | 1:71:A:ALA:C | 8        | 1.98          |
| (1,99)  | 1:46:A:ARG:N | 1:46:A:ARG:CA | 1:46:A:ARG:C  | 1:47:A:ILE:N | 8        | 1.94          |
| (1,54)  | 1:62:A:LEU:C | 1:63:A:SER:N  | 1:63:A:SER:CA | 1:63:A:SER:C | 8        | 1.9           |
| (1,104) | 1:51:A:ASP:N | 1:51:A:ASP:CA | 1:51:A:ASP:C  | 1:52:A:LYS:N | 12       | 1.89          |
| (1,74)  | 1:18:A:PRO:N | 1:18:A:PRO:CA | 1:18:A:PRO:C  | 1:19:A:ASN:N | 10       | 1.89          |

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| Key     | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Model ID | Violation (°) |
|---------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,102) | 1:49:A:THR:N | 1:49:A:THR:CA | 1:49:A:THR:C  | 1:50:A:GLY:N | 12       | 1.88          |
| (1,47)  | 1:54:A:ARG:C | 1:55:A:VAL:N  | 1:55:A:VAL:CA | 1:55:A:VAL:C | 14       | 1.86          |
| (1,42)  | 1:49:A:THR:C | 1:50:A:GLY:N  | 1:50:A:GLY:CA | 1:50:A:GLY:C | 5        | 1.84          |
| (1,42)  | 1:49:A:THR:C | 1:50:A:GLY:N  | 1:50:A:GLY:CA | 1:50:A:GLY:C | 8        | 1.84          |
| (1,74)  | 1:18:A:PRO:N | 1:18:A:PRO:CA | 1:18:A:PRO:C  | 1:19:A:ASN:N | 9        | 1.83          |
| (1,19)  | 1:24:A:VAL:C | 1:25:A:GLU:N  | 1:25:A:GLU:CA | 1:25:A:GLU:C | 8        | 1.83          |
| (1,100) | 1:47:A:ILE:N | 1:47:A:ILE:CA | 1:47:A:ILE:C  | 1:48:A:LEU:N | 10       | 1.8           |
| (1,74)  | 1:18:A:PRO:N | 1:18:A:PRO:CA | 1:18:A:PRO:C  | 1:19:A:ASN:N | 7        | 1.78          |
| (1,104) | 1:51:A:ASP:N | 1:51:A:ASP:CA | 1:51:A:ASP:C  | 1:52:A:LYS:N | 5        | 1.77          |
| (1,40)  | 1:47:A:ILE:C | 1:48:A:LEU:N  | 1:48:A:LEU:CA | 1:48:A:LEU:C | 9        | 1.77          |
| (1,2)   | 1:6:A:SER:C  | 1:7:A:PHE:N   | 1:7:A:PHE:CA  | 1:7:A:PHE:C  | 14       | 1.75          |
| (1,121) | 1:70:A:ARG:N | 1:70:A:ARG:CA | 1:70:A:ARG:C  | 1:71:A:ALA:N | 4        | 1.74          |
| (1,121) | 1:70:A:ARG:N | 1:70:A:ARG:CA | 1:70:A:ARG:C  | 1:71:A:ALA:N | 12       | 1.73          |
| (1,58)  | 1:66:A:ARG:C | 1:67:A:ILE:N  | 1:67:A:ILE:CA | 1:67:A:ILE:C | 3        | 1.73          |
| (1,58)  | 1:66:A:ARG:C | 1:67:A:ILE:N  | 1:67:A:ILE:CA | 1:67:A:ILE:C | 6        | 1.73          |
| (1,93)  | 1:38:A:GLY:N | 1:38:A:GLY:CA | 1:38:A:GLY:C  | 1:39:A:LYS:N | 4        | 1.72          |
| (1,47)  | 1:54:A:ARG:C | 1:55:A:VAL:N  | 1:55:A:VAL:CA | 1:55:A:VAL:C | 4        | 1.71          |
| (1,38)  | 1:45:A:ILE:C | 1:46:A:ARG:N  | 1:46:A:ARG:CA | 1:46:A:ARG:C | 9        | 1.71          |
| (1,42)  | 1:49:A:THR:C | 1:50:A:GLY:N  | 1:50:A:GLY:CA | 1:50:A:GLY:C | 2        | 1.7           |
| (1,58)  | 1:66:A:ARG:C | 1:67:A:ILE:N  | 1:67:A:ILE:CA | 1:67:A:ILE:C | 12       | 1.69          |
| (1,40)  | 1:47:A:ILE:C | 1:48:A:LEU:N  | 1:48:A:LEU:CA | 1:48:A:LEU:C | 1        | 1.69          |
| (1,58)  | 1:66:A:ARG:C | 1:67:A:ILE:N  | 1:67:A:ILE:CA | 1:67:A:ILE:C | 10       | 1.67          |
| (1,44)  | 1:51:A:ASP:C | 1:52:A:LYS:N  | 1:52:A:LYS:CA | 1:52:A:LYS:C | 13       | 1.67          |
| (1,42)  | 1:49:A:THR:C | 1:50:A:GLY:N  | 1:50:A:GLY:CA | 1:50:A:GLY:C | 11       | 1.67          |
| (1,47)  | 1:54:A:ARG:C | 1:55:A:VAL:N  | 1:55:A:VAL:CA | 1:55:A:VAL:C | 6        | 1.66          |
| (1,44)  | 1:51:A:ASP:C | 1:52:A:LYS:N  | 1:52:A:LYS:CA | 1:52:A:LYS:C | 12       | 1.66          |
| (1,121) | 1:70:A:ARG:N | 1:70:A:ARG:CA | 1:70:A:ARG:C  | 1:71:A:ALA:N | 13       | 1.63          |
| (1,119) | 1:67:A:ILE:N | 1:67:A:ILE:CA | 1:67:A:ILE:C  | 1:68:A:THR:N | 8        | 1.63          |
| (1,58)  | 1:66:A:ARG:C | 1:67:A:ILE:N  | 1:67:A:ILE:CA | 1:67:A:ILE:C | 1        | 1.63          |
| (1,33)  | 1:38:A:GLY:C | 1:39:A:LYS:N  | 1:39:A:LYS:CA | 1:39:A:LYS:C | 4        | 1.61          |
| (1,42)  | 1:49:A:THR:C | 1:50:A:GLY:N  | 1:50:A:GLY:CA | 1:50:A:GLY:C | 3        | 1.6           |
| (1,47)  | 1:54:A:ARG:C | 1:55:A:VAL:N  | 1:55:A:VAL:CA | 1:55:A:VAL:C | 12       | 1.53          |
| (1,14)  | 1:19:A:ASN:C | 1:20:A:THR:N  | 1:20:A:THR:CA | 1:20:A:THR:C | 13       | 1.53          |
| (1,119) | 1:67:A:ILE:N | 1:67:A:ILE:CA | 1:67:A:ILE:C  | 1:68:A:THR:N | 6        | 1.5           |
| (1,39)  | 1:46:A:ARG:C | 1:47:A:ILE:N  | 1:47:A:ILE:CA | 1:47:A:ILE:C | 8        | 1.5           |
| (1,100) | 1:47:A:ILE:N | 1:47:A:ILE:CA | 1:47:A:ILE:C  | 1:48:A:LEU:N | 11       | 1.45          |
| (1,42)  | 1:49:A:THR:C | 1:50:A:GLY:N  | 1:50:A:GLY:CA | 1:50:A:GLY:C | 6        | 1.45          |
| (1,40)  | 1:47:A:ILE:C | 1:48:A:LEU:N  | 1:48:A:LEU:CA | 1:48:A:LEU:C | 10       | 1.45          |
| (1,118) | 1:66:A:ARG:N | 1:66:A:ARG:CA | 1:66:A:ARG:C  | 1:67:A:ILE:N | 5        | 1.42          |
| (1,92)  | 1:37:A:SER:N | 1:37:A:SER:CA | 1:37:A:SER:C  | 1:38:A:GLY:N | 9        | 1.42          |
| (1,42)  | 1:49:A:THR:C | 1:50:A:GLY:N  | 1:50:A:GLY:CA | 1:50:A:GLY:C | 10       | 1.4           |
| (1,69)  | 1:13:A:VAL:N | 1:13:A:VAL:CA | 1:13:A:VAL:C  | 1:14:A:VAL:N | 5        | 1.39          |
| (1,121) | 1:70:A:ARG:N | 1:70:A:ARG:CA | 1:70:A:ARG:C  | 1:71:A:ALA:N | 3        | 1.36          |
| (1,100) | 1:47:A:ILE:N | 1:47:A:ILE:CA | 1:47:A:ILE:C  | 1:48:A:LEU:N | 14       | 1.36          |
| (1,47)  | 1:54:A:ARG:C | 1:55:A:VAL:N  | 1:55:A:VAL:CA | 1:55:A:VAL:C | 1        | 1.36          |
| (1,101) | 1:48:A:LEU:N | 1:48:A:LEU:CA | 1:48:A:LEU:C  | 1:49:A:THR:N | 13       | 1.32          |
| (1,42)  | 1:49:A:THR:C | 1:50:A:GLY:N  | 1:50:A:GLY:CA | 1:50:A:GLY:C | 4        | 1.32          |
| (1,2)   | 1:6:A:SER:C  | 1:7:A:PHE:N   | 1:7:A:PHE:CA  | 1:7:A:PHE:C  | 10       | 1.28          |
| (1,102) | 1:49:A:THR:N | 1:49:A:THR:CA | 1:49:A:THR:C  | 1:50:A:GLY:N | 1        | 1.27          |
| (1,59)  | 1:67:A:ILE:C | 1:68:A:THR:N  | 1:68:A:THR:CA | 1:68:A:THR:C | 1        | 1.27          |
| (1,105) | 1:52:A:LYS:N | 1:52:A:LYS:CA | 1:52:A:LYS:C  | 1:53:A:VAL:N | 13       | 1.24          |

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*Continued from previous page...*

| Key     | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Model ID | Violation (°) |
|---------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,87)  | 1:32:A:VAL:N | 1:32:A:VAL:CA | 1:32:A:VAL:C  | 1:33:A:THR:N | 12       | 1.22          |
| (1,61)  | 1:70:A:ARG:C | 1:71:A:ALA:N  | 1:71:A:ALA:CA | 1:71:A:ALA:C | 7        | 1.22          |
| (1,58)  | 1:66:A:ARG:C | 1:67:A:ILE:N  | 1:67:A:ILE:CA | 1:67:A:ILE:C | 2        | 1.2           |
| (1,47)  | 1:54:A:ARG:C | 1:55:A:VAL:N  | 1:55:A:VAL:CA | 1:55:A:VAL:C | 9        | 1.18          |
| (1,121) | 1:70:A:ARG:N | 1:70:A:ARG:CA | 1:70:A:ARG:C  | 1:71:A:ALA:N | 11       | 1.16          |
| (1,122) | 1:71:A:ALA:N | 1:71:A:ALA:CA | 1:71:A:ALA:C  | 1:72:A:ARG:N | 11       | 1.14          |
| (1,47)  | 1:54:A:ARG:C | 1:55:A:VAL:N  | 1:55:A:VAL:CA | 1:55:A:VAL:C | 10       | 1.13          |
| (1,42)  | 1:49:A:THR:C | 1:50:A:GLY:N  | 1:50:A:GLY:CA | 1:50:A:GLY:C | 15       | 1.09          |
| (1,47)  | 1:54:A:ARG:C | 1:55:A:VAL:N  | 1:55:A:VAL:CA | 1:55:A:VAL:C | 15       | 1.08          |
| (1,100) | 1:47:A:ILE:N | 1:47:A:ILE:CA | 1:47:A:ILE:C  | 1:48:A:LEU:N | 7        | 1.06          |
| (1,36)  | 1:41:A:ARG:C | 1:42:A:LYS:N  | 1:42:A:LYS:CA | 1:42:A:LYS:C | 9        | 1.06          |
| (1,69)  | 1:13:A:VAL:N | 1:13:A:VAL:CA | 1:13:A:VAL:C  | 1:14:A:VAL:N | 12       | 1.05          |
| (1,74)  | 1:18:A:PRO:N | 1:18:A:PRO:CA | 1:18:A:PRO:C  | 1:19:A:ASN:N | 13       | 1.04          |
| (1,54)  | 1:62:A:LEU:C | 1:63:A:SER:N  | 1:63:A:SER:CA | 1:63:A:SER:C | 5        | 1.03          |
| (1,116) | 1:64:A:LYS:N | 1:64:A:LYS:CA | 1:64:A:LYS:C  | 1:65:A:GLY:N | 1        | 1.02          |
| (1,38)  | 1:45:A:ILE:C | 1:46:A:ARG:N  | 1:46:A:ARG:CA | 1:46:A:ARG:C | 13       | 1.02          |
| (1,19)  | 1:24:A:VAL:C | 1:25:A:GLU:N  | 1:25:A:GLU:CA | 1:25:A:GLU:C | 14       | 1.02          |
| (1,40)  | 1:47:A:ILE:C | 1:48:A:LEU:N  | 1:48:A:LEU:CA | 1:48:A:LEU:C | 11       | 1.01          |