



# Full wwPDB NMR Structure Validation Report ⓘ

Mar 10, 2026 – 06:12 AM UTC

PDB ID : 2OFN / pdb\_00002ofn  
BMRB ID : 15038  
Title : Solution structure of FK506-binding domain (FKBD) of FKBP35 from Plasmodium falciparum  
Authors : Kang, C.B.; Ye, H.; Yoon, H.R.; Yoon, H.S.  
Deposited on : 2007-01-04

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

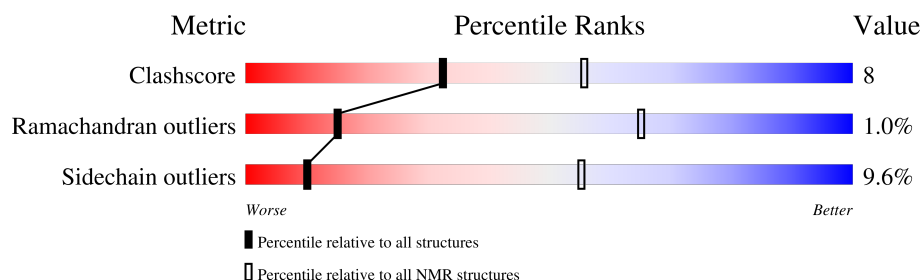
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 90%.

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     | 135    |                  |

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 12 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:7-A:101, A:109-A:127<br>(114) | 0.76              | 12           |

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 6 clusters and 4 single-model clusters were found.

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

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2130 atoms, of which 1052 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called 70 kDa peptidylprolyl isomerase, putative.

| Mol | Chain | Residues | Atoms |     |      |     |     |   | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|-------|
| 1   | A     | 135      | Total | C   | H    | N   | O   | S | 0     |
|     |       |          | 2130  | 678 | 1052 | 183 | 211 | 6 |       |

There are 8 discrepancies between the modelled and reference sequences:

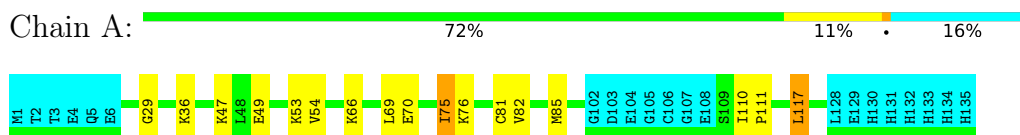
| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | 128     | LEU      | -      | expression tag | UNP Q8I4V8 |
| A     | 129     | GLU      | -      | expression tag | UNP Q8I4V8 |
| A     | 130     | HIS      | -      | expression tag | UNP Q8I4V8 |
| A     | 131     | HIS      | -      | expression tag | UNP Q8I4V8 |
| A     | 132     | HIS      | -      | expression tag | UNP Q8I4V8 |
| A     | 133     | HIS      | -      | expression tag | UNP Q8I4V8 |
| A     | 134     | HIS      | -      | expression tag | UNP Q8I4V8 |
| A     | 135     | HIS      | -      | expression tag | UNP Q8I4V8 |

## 4 Residue-property plots

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

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

- Molecule 1: 70 kDa peptidylprolyl isomerase, putative

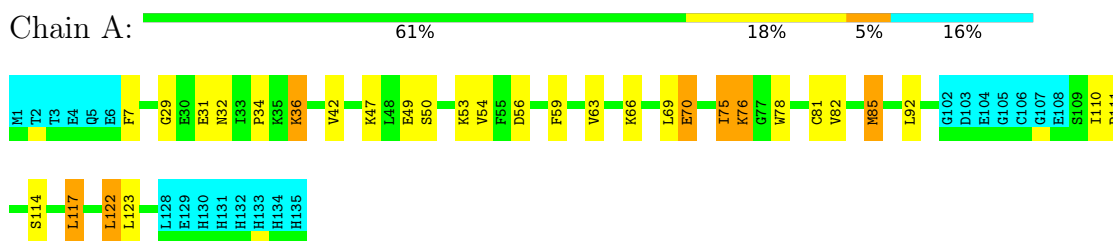


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

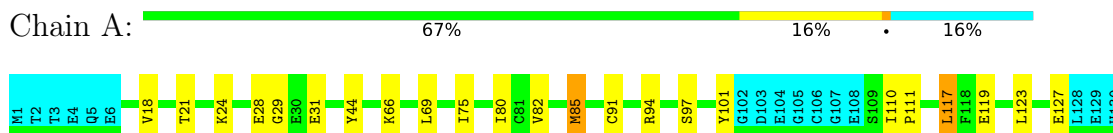
#### 4.2.1 Score per residue for model 1

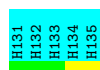
- Molecule 1: 70 kDa peptidylprolyl isomerase, putative



#### 4.2.2 Score per residue for model 2

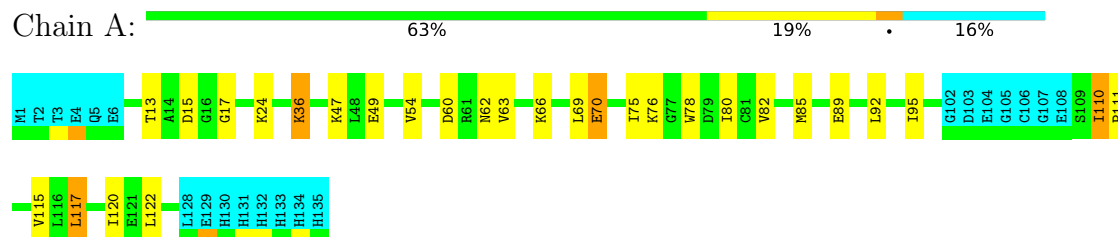
- Molecule 1: 70 kDa peptidylprolyl isomerase, putative





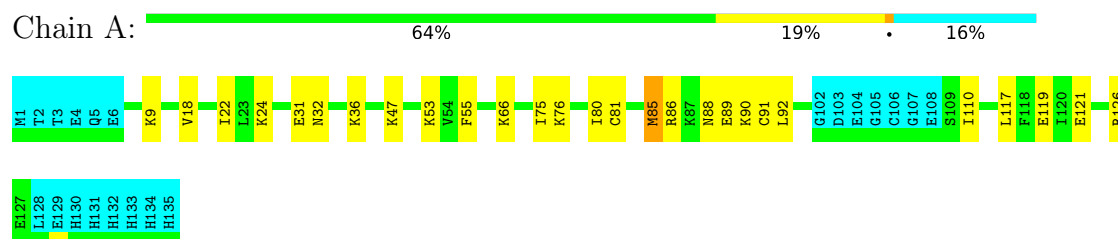
### 4.2.3 Score per residue for model 3

- Molecule 1: 70 kDa peptidylprolyl isomerase, putative



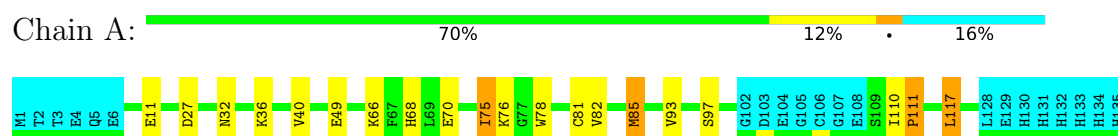
### 4.2.4 Score per residue for model 4

- Molecule 1: 70 kDa peptidylprolyl isomerase, putative



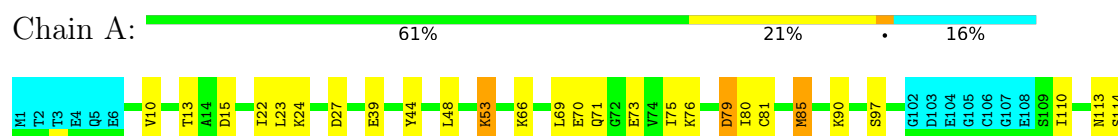
### 4.2.5 Score per residue for model 5

- Molecule 1: 70 kDa peptidylprolyl isomerase, putative



### 4.2.6 Score per residue for model 6

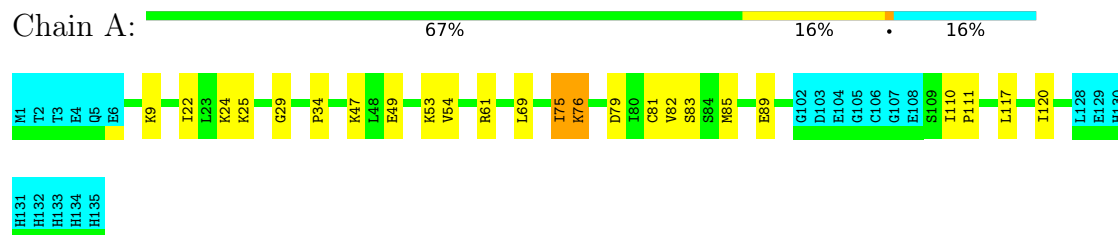
- Molecule 1: 70 kDa peptidylprolyl isomerase, putative





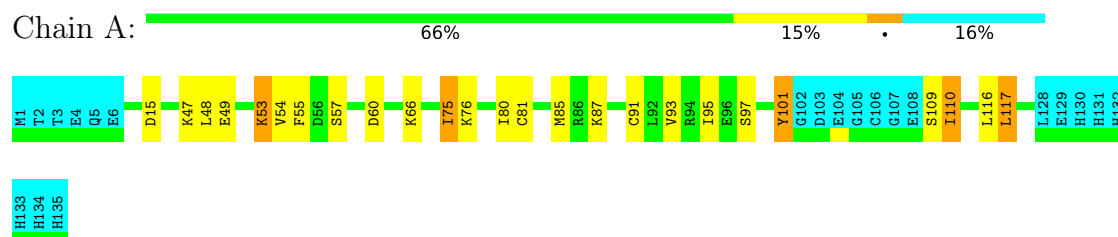
#### 4.2.7 Score per residue for model 7

- Molecule 1: 70 kDa peptidylprolyl isomerase, putative



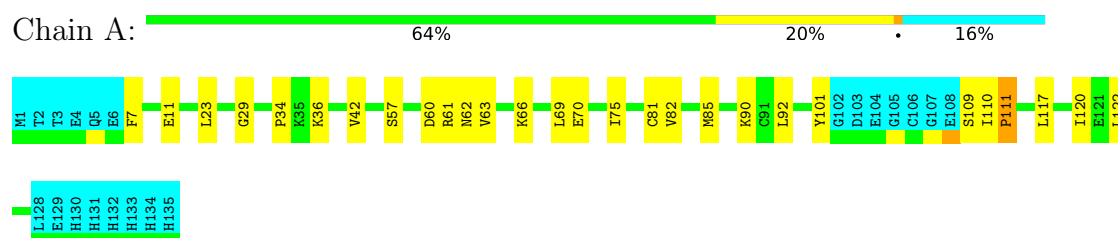
#### 4.2.8 Score per residue for model 8

- Molecule 1: 70 kDa peptidylprolyl isomerase, putative



#### 4.2.9 Score per residue for model 9

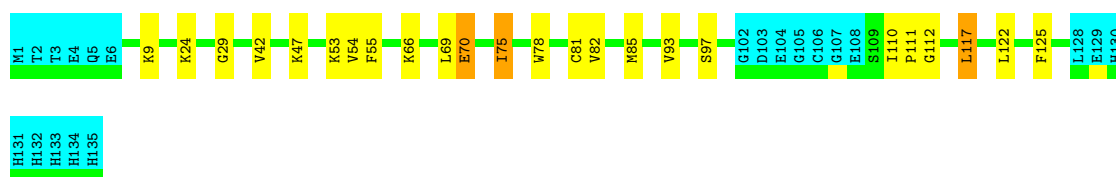
- Molecule 1: 70 kDa peptidylprolyl isomerase, putative



#### 4.2.10 Score per residue for model 10

- Molecule 1: 70 kDa peptidylprolyl isomerase, putative

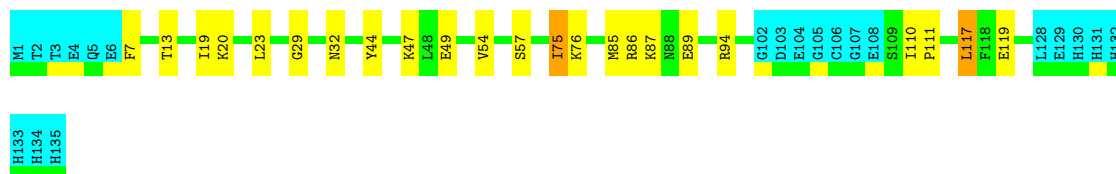




#### 4.2.11 Score per residue for model 11

- Molecule 1: 70 kDa peptidylprolyl isomerase, putative

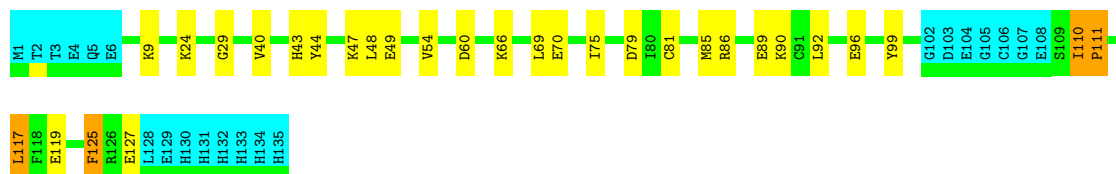
Chain A: 67% 16% 16%



#### 4.2.12 Score per residue for model 12 (medoid)

- Molecule 1: 70 kDa peptidylprolyl isomerase, putative

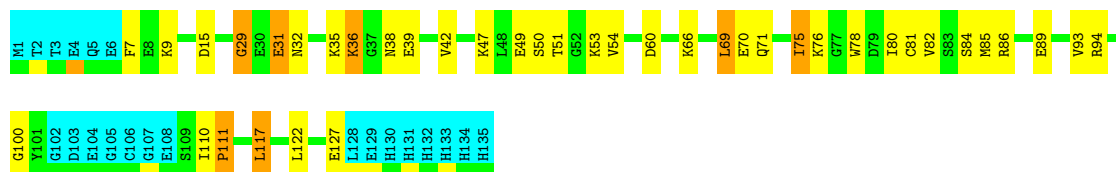
Chain A: 62% 19% 16%



#### 4.2.13 Score per residue for model 13

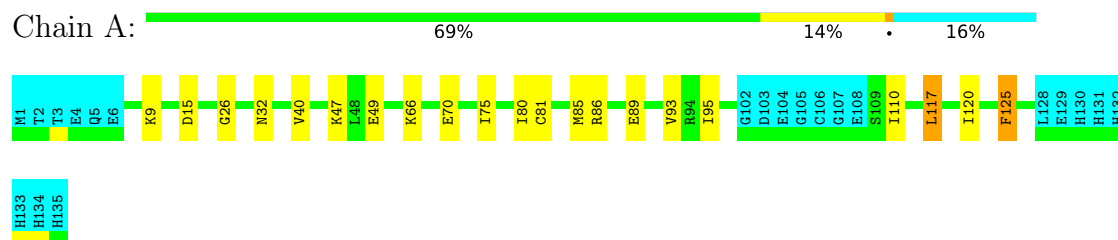
- Molecule 1: 70 kDa peptidylprolyl isomerase, putative

Chain A: 55% 24% 5% 16%



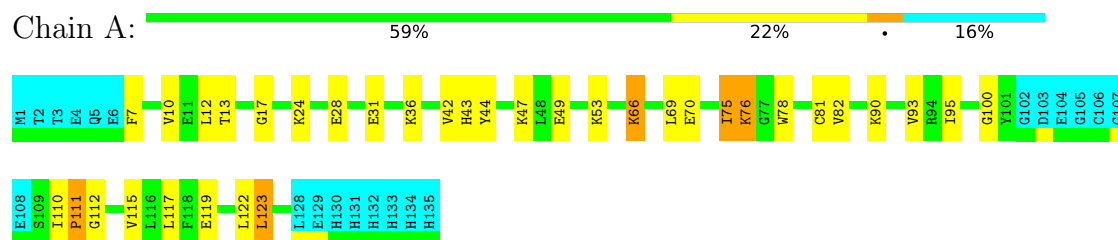
#### 4.2.14 Score per residue for model 14

- Molecule 1: 70 kDa peptidylprolyl isomerase, putative



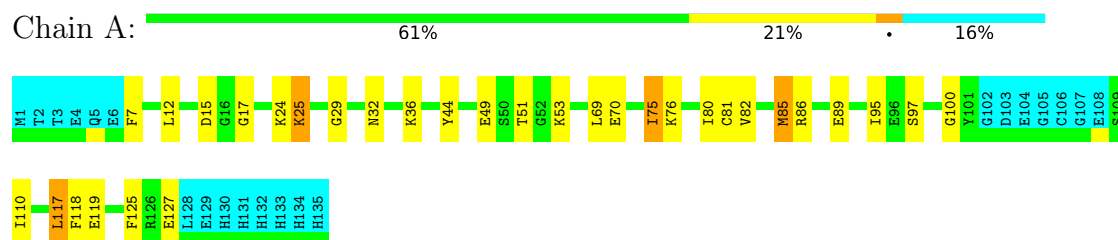
#### 4.2.15 Score per residue for model 15

- Molecule 1: 70 kDa peptidylprolyl isomerase, putative



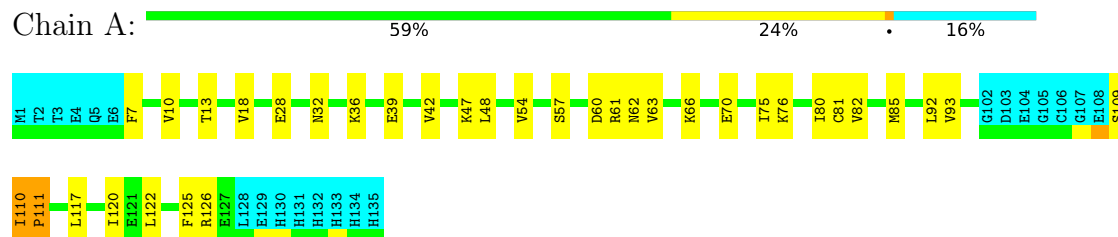
#### 4.2.16 Score per residue for model 16

- Molecule 1: 70 kDa peptidylprolyl isomerase, putative



#### 4.2.17 Score per residue for model 17

- Molecule 1: 70 kDa peptidylprolyl isomerase, putative



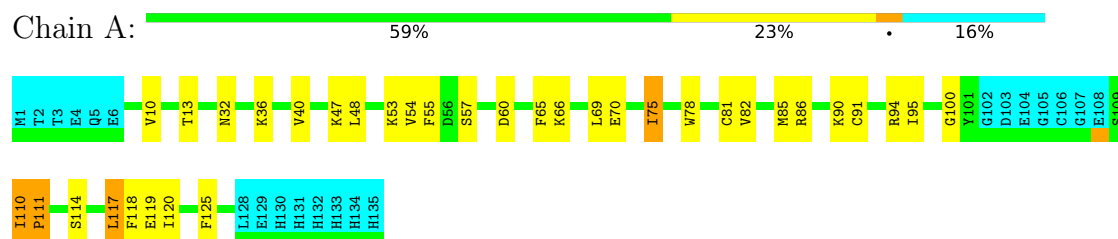
### 4.2.18 Score per residue for model 18

- Molecule 1: 70 kDa peptidylprolyl isomerase, putative



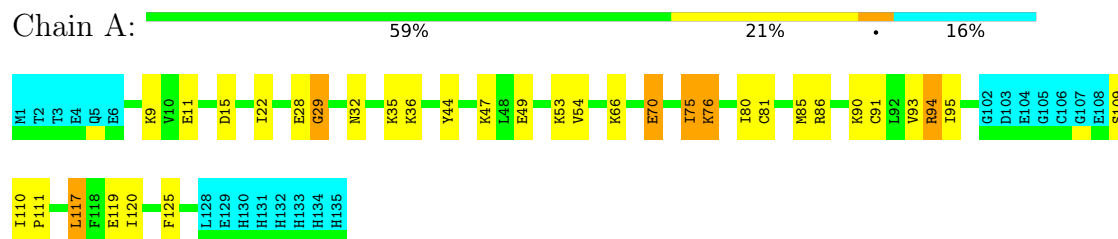
### 4.2.19 Score per residue for model 19

- Molecule 1: 70 kDa peptidylprolyl isomerase, putative



### 4.2.20 Score per residue for model 20

- Molecule 1: 70 kDa peptidylprolyl isomerase, putative



## 5 Refinement protocol and experimental data overview

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

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

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

| Software name | Classification | Version |
|---------------|----------------|---------|
| CYANA         | refinement     | 2.1     |
| ARIA          | refinement     | 1.2     |
| CNS           | refinement     | 1.1     |

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                       | 1526           |
| Number of shifts mapped to atoms             | 1526           |
| Number of unparsed shifts                    | 0              |
| Number of shifts with mapping errors         | 0              |
| Number of shifts with mapping warnings       | 0              |
| Assignment completeness (well-defined parts) | 90%            |

## 6 Model quality [i](#)

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

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes |
|-----|-------|-------|----------|----------|---------|
| 1   | A     | 907   | 912      | 910      | 15±5    |
| All | All   | 18140 | 18240    | 18200    | 309     |

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 9.

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

| Atom-1          | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|-----------------|------------------|----------|-------------|--------|-------|
|                 |                  |          |             | Worst  | Total |
| 1:A:36:LYS:HE3  | 1:A:70:GLU:HG3   | 0.91     | 1.42        | 1      | 1     |
| 1:A:36:LYS:HD3  | 1:A:70:GLU:HG3   | 0.88     | 1.45        | 18     | 2     |
| 1:A:82:VAL:HA   | 1:A:85:MET:HE2   | 0.78     | 1.55        | 13     | 4     |
| 1:A:86:ARG:HD3  | 1:A:88:ASN:H     | 0.76     | 1.40        | 4      | 1     |
| 1:A:92:LEU:HD21 | 1:A:117:LEU:HB3  | 0.76     | 1.58        | 17     | 1     |
| 1:A:85:MET:HA   | 1:A:85:MET:HE2   | 0.74     | 1.59        | 6      | 8     |
| 1:A:85:MET:HE1  | 1:A:90:LYS:HA    | 0.74     | 1.56        | 12     | 2     |
| 1:A:85:MET:HE2  | 1:A:85:MET:HA    | 0.73     | 1.58        | 20     | 2     |
| 1:A:82:VAL:HG12 | 1:A:120:ILE:HG21 | 0.70     | 1.62        | 18     | 5     |
| 1:A:12:LEU:HA   | 1:A:17:GLY:HA2   | 0.70     | 1.62        | 15     | 2     |
| 1:A:49:GLU:HB2  | 1:A:117:LEU:HD11 | 0.67     | 1.65        | 14     | 7     |
| 1:A:48:LEU:HA   | 1:A:116:LEU:HD23 | 0.66     | 1.67        | 8      | 1     |
| 1:A:42:VAL:HG12 | 1:A:122:LEU:HA   | 0.63     | 1.69        | 1      | 6     |
| 1:A:47:LYS:HG3  | 1:A:117:LEU:HD13 | 0.63     | 1.68        | 18     | 4     |

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| Atom-1          | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|-----------------|------------------|----------|-------------|--------|-------|
|                 |                  |          |             | Worst  | Total |
| 1:A:62:ASN:HD22 | 1:A:63:VAL:HG23  | 0.62     | 1.53        | 3      | 1     |
| 1:A:48:LEU:HD22 | 1:A:110:ILE:HG13 | 0.61     | 1.72        | 18     | 4     |
| 1:A:47:LYS:CB   | 1:A:54:VAL:HA    | 0.60     | 2.27        | 20     | 11    |
| 1:A:81:CYS:HB2  | 1:A:93:VAL:HG21  | 0.60     | 1.73        | 13     | 1     |
| 1:A:44:TYR:HA   | 1:A:119:GLU:O    | 0.60     | 1.96        | 11     | 8     |
| 1:A:48:LEU:HD11 | 1:A:114:SER:HB2  | 0.60     | 1.74        | 19     | 1     |
| 1:A:15:ASP:OD2  | 1:A:80:ILE:HA    | 0.59     | 1.97        | 13     | 1     |
| 1:A:24:LYS:HB3  | 1:A:90:LYS:HB3   | 0.59     | 1.73        | 6      | 1     |
| 1:A:47:LYS:HB2  | 1:A:54:VAL:HA    | 0.59     | 1.74        | 8      | 6     |
| 1:A:69:LEU:HD13 | 1:A:82:VAL:HG23  | 0.59     | 1.73        | 15     | 1     |
| 1:A:81:CYS:SG   | 1:A:93:VAL:HB    | 0.58     | 2.38        | 5      | 5     |
| 1:A:94:ARG:HE   | 1:A:117:LEU:HD23 | 0.58     | 1.59        | 19     | 1     |
| 1:A:57:SER:HB2  | 1:A:60:ASP:OD1   | 0.58     | 1.98        | 18     | 4     |
| 1:A:69:LEU:HD11 | 1:A:79:ASP:HA    | 0.58     | 1.75        | 12     | 1     |
| 1:A:75:ILE:HD13 | 1:A:75:ILE:H     | 0.57     | 1.60        | 8      | 5     |
| 1:A:32:ASN:HB2  | 1:A:86:ARG:HH21  | 0.57     | 1.60        | 13     | 2     |
| 1:A:93:VAL:HG13 | 1:A:95:ILE:HD11  | 0.56     | 1.77        | 8      | 2     |
| 1:A:75:ILE:HG12 | 1:A:76:LYS:H     | 0.56     | 1.61        | 15     | 4     |
| 1:A:19:ILE:HB   | 1:A:94:ARG:HB2   | 0.56     | 1.77        | 11     | 1     |
| 1:A:81:CYS:O    | 1:A:85:MET:HG2   | 0.55     | 2.01        | 16     | 9     |
| 1:A:10:VAL:CG1  | 1:A:13:THR:HB    | 0.55     | 2.32        | 18     | 3     |
| 1:A:47:LYS:O    | 1:A:117:LEU:HD12 | 0.55     | 2.02        | 1      | 2     |
| 1:A:69:LEU:HD13 | 1:A:82:VAL:CG2   | 0.55     | 2.32        | 15     | 8     |
| 1:A:36:LYS:CD   | 1:A:70:GLU:HG3   | 0.53     | 2.27        | 18     | 1     |
| 1:A:31:GLU:H    | 1:A:31:GLU:CD    | 0.52     | 2.12        | 1      | 2     |
| 1:A:76:LYS:HA   | 1:A:79:ASP:OD2   | 0.51     | 2.06        | 6      | 1     |
| 1:A:78:TRP:O    | 1:A:82:VAL:HG22  | 0.51     | 2.06        | 15     | 7     |
| 1:A:85:MET:HA   | 1:A:89:GLU:OE1   | 0.51     | 2.06        | 18     | 2     |
| 1:A:57:SER:O    | 1:A:61:ARG:HG3   | 0.51     | 2.05        | 18     | 1     |
| 1:A:29:GLY:HA3  | 1:A:86:ARG:HD3   | 0.51     | 1.83        | 18     | 1     |
| 1:A:85:MET:O    | 1:A:122:LEU:HD22 | 0.51     | 2.06        | 9      | 1     |
| 1:A:76:LYS:HE2  | 1:A:76:LYS:HA    | 0.50     | 1.83        | 4      | 2     |
| 1:A:47:LYS:HB3  | 1:A:54:VAL:HA    | 0.49     | 1.82        | 18     | 6     |
| 1:A:40:VAL:O    | 1:A:68:HIS:HA    | 0.49     | 2.08        | 5      | 1     |
| 1:A:85:MET:HE1  | 1:A:91:CYS:SG    | 0.49     | 2.48        | 19     | 1     |
| 1:A:69:LEU:HD11 | 1:A:79:ASP:OD1   | 0.49     | 2.07        | 7      | 1     |
| 1:A:85:MET:SD   | 1:A:120:ILE:HG22 | 0.49     | 2.47        | 7      | 2     |
| 1:A:95:ILE:O    | 1:A:115:VAL:HA   | 0.49     | 2.07        | 15     | 2     |
| 1:A:51:THR:HG23 | 1:A:53:LYS:HD3   | 0.49     | 1.84        | 16     | 2     |
| 1:A:36:LYS:HA   | 1:A:69:LEU:HD12  | 0.49     | 1.84        | 13     | 1     |
| 1:A:15:ASP:O    | 1:A:80:ILE:HG13  | 0.49     | 2.07        | 14     | 5     |

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| Atom-1          | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|-----------------|------------------|----------|-------------|--------|-------|
|                 |                  |          |             | Worst  | Total |
| 1:A:85:MET:HA   | 1:A:85:MET:CE    | 0.49     | 2.38        | 1      | 8     |
| 1:A:21:THR:O    | 1:A:91:CYS:HB2   | 0.49     | 2.08        | 2      | 1     |
| 1:A:22:ILE:HD12 | 1:A:91:CYS:SG    | 0.49     | 2.47        | 20     | 1     |
| 1:A:36:LYS:HB3  | 1:A:69:LEU:HG    | 0.49     | 1.83        | 18     | 1     |
| 1:A:69:LEU:HD13 | 1:A:82:VAL:HG21  | 0.48     | 1.84        | 3      | 4     |
| 1:A:81:CYS:O    | 1:A:85:MET:HG3   | 0.48     | 2.08        | 13     | 2     |
| 1:A:23:LEU:CD2  | 1:A:92:LEU:HG    | 0.48     | 2.39        | 9      | 1     |
| 1:A:85:MET:HE3  | 1:A:122:LEU:HB2  | 0.48     | 1.85        | 3      | 4     |
| 1:A:12:LEU:HA   | 1:A:17:GLY:CA    | 0.47     | 2.35        | 15     | 1     |
| 1:A:81:CYS:SG   | 1:A:120:ILE:HD12 | 0.47     | 2.49        | 7      | 2     |
| 1:A:24:LYS:O    | 1:A:89:GLU:HG3   | 0.47     | 2.09        | 4      | 3     |
| 1:A:49:GLU:HB2  | 1:A:117:LEU:HG   | 0.47     | 1.86        | 7      | 6     |
| 1:A:69:LEU:CD1  | 1:A:79:ASP:HA    | 0.47     | 2.39        | 7      | 2     |
| 1:A:48:LEU:HD11 | 1:A:114:SER:HB3  | 0.47     | 1.86        | 6      | 1     |
| 1:A:13:THR:HG21 | 1:A:20:LYS:HD3   | 0.47     | 1.87        | 11     | 1     |
| 1:A:86:ARG:HB2  | 1:A:89:GLU:CB    | 0.47     | 2.40        | 12     | 1     |
| 1:A:75:ILE:HD11 | 1:A:100:GLY:HA2  | 0.47     | 1.84        | 13     | 4     |
| 1:A:10:VAL:HG11 | 1:A:13:THR:HB    | 0.47     | 1.87        | 18     | 1     |
| 1:A:75:ILE:HG12 | 1:A:76:LYS:N     | 0.46     | 2.24        | 5      | 3     |
| 1:A:86:ARG:HB3  | 1:A:89:GLU:HB2   | 0.46     | 1.87        | 11     | 1     |
| 1:A:40:VAL:HG12 | 1:A:125:PHE:HB2  | 0.46     | 1.86        | 14     | 3     |
| 1:A:44:TYR:HB2  | 1:A:118:PHE:HB3  | 0.46     | 1.86        | 18     | 1     |
| 1:A:123:LEU:H   | 1:A:123:LEU:HD23 | 0.46     | 1.70        | 1      | 4     |
| 1:A:92:LEU:HD23 | 1:A:93:VAL:N     | 0.46     | 2.26        | 17     | 1     |
| 1:A:59:PHE:O    | 1:A:63:VAL:HG12  | 0.46     | 2.11        | 1      | 1     |
| 1:A:36:LYS:HE3  | 1:A:70:GLU:HB3   | 0.46     | 1.87        | 9      | 1     |
| 1:A:51:THR:HG23 | 1:A:53:LYS:HG2   | 0.46     | 1.87        | 18     | 1     |
| 1:A:90:LYS:HE3  | 1:A:119:GLU:HB3  | 0.45     | 1.88        | 19     | 3     |
| 1:A:10:VAL:HG12 | 1:A:13:THR:HB    | 0.45     | 1.89        | 15     | 3     |
| 1:A:29:GLY:HA3  | 1:A:86:ARG:NH2   | 0.45     | 2.26        | 16     | 2     |
| 1:A:22:ILE:C    | 1:A:23:LEU:HD22  | 0.45     | 2.36        | 6      | 1     |
| 1:A:57:SER:O    | 1:A:61:ARG:HG2   | 0.45     | 2.11        | 17     | 1     |
| 1:A:36:LYS:HA   | 1:A:69:LEU:HG    | 0.45     | 1.89        | 1      | 3     |
| 1:A:9:LYS:N     | 1:A:9:LYS:HD3    | 0.45     | 2.27        | 10     | 1     |
| 1:A:29:GLY:HA3  | 1:A:32:ASN:HB2   | 0.45     | 1.86        | 1      | 1     |
| 1:A:15:ASP:HB3  | 1:A:80:ILE:HG13  | 0.45     | 1.89        | 13     | 1     |
| 1:A:39:GLU:HB2  | 1:A:126:ARG:HD2  | 0.44     | 1.88        | 6      | 1     |
| 1:A:90:LYS:CE   | 1:A:119:GLU:HB3  | 0.44     | 2.42        | 20     | 1     |
| 1:A:53:LYS:HA   | 1:A:53:LYS:HE3   | 0.44     | 1.88        | 6      | 1     |
| 1:A:80:ILE:O    | 1:A:84:SER:HB3   | 0.44     | 2.12        | 13     | 1     |
| 1:A:13:THR:HG21 | 1:A:80:ILE:HG21  | 0.44     | 1.90        | 3      | 1     |

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| Atom-1          | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|-----------------|------------------|----------|-------------|--------|-------|
|                 |                  |          |             | Worst  | Total |
| 1:A:47:LYS:HA   | 1:A:55:PHE:CD1   | 0.44     | 2.46        | 10     | 1     |
| 1:A:36:LYS:HB2  | 1:A:70:GLU:HG3   | 0.44     | 1.90        | 3      | 1     |
| 1:A:47:LYS:HB2  | 1:A:53:LYS:O     | 0.44     | 2.12        | 20     | 5     |
| 1:A:69:LEU:HD22 | 1:A:82:VAL:HG23  | 0.44     | 1.88        | 16     | 1     |
| 1:A:55:PHE:HB3  | 1:A:60:ASP:OD2   | 0.44     | 2.13        | 19     | 1     |
| 1:A:71:GLN:NE2  | 1:A:73:GLU:HB2   | 0.43     | 2.28        | 6      | 1     |
| 1:A:55:PHE:CE1  | 1:A:110:ILE:HD11 | 0.43     | 2.47        | 8      | 1     |
| 1:A:36:LYS:CB   | 1:A:69:LEU:HG    | 0.43     | 2.42        | 18     | 1     |
| 1:A:95:ILE:HD13 | 1:A:118:PHE:HD2  | 0.43     | 1.73        | 19     | 2     |
| 1:A:94:ARG:HD2  | 1:A:117:LEU:HB3  | 0.43     | 1.90        | 20     | 2     |
| 1:A:110:ILE:N   | 1:A:111:PRO:HD3  | 0.43     | 2.29        | 12     | 2     |
| 1:A:85:MET:HE1  | 1:A:91:CYS:H     | 0.43     | 1.74        | 8      | 1     |
| 1:A:36:LYS:HA   | 1:A:69:LEU:CD1   | 0.43     | 2.43        | 13     | 1     |
| 1:A:9:LYS:HD2   | 1:A:9:LYS:N      | 0.43     | 2.28        | 20     | 1     |
| 1:A:66:LYS:HD2  | 1:A:66:LYS:C     | 0.43     | 2.38        | 14     | 1     |
| 1:A:18:VAL:HB   | 1:A:80:ILE:CB    | 0.43     | 2.44        | 17     | 1     |
| 1:A:25:LYS:HD3  | 1:A:25:LYS:H     | 0.43     | 1.73        | 16     | 1     |
| 1:A:18:VAL:CG2  | 1:A:80:ILE:HB    | 0.42     | 2.43        | 4      | 1     |
| 1:A:62:ASN:HD22 | 1:A:63:VAL:HG12  | 0.42     | 1.74        | 9      | 1     |
| 1:A:29:GLY:HA3  | 1:A:86:ARG:CZ    | 0.42     | 2.44        | 13     | 1     |
| 1:A:86:ARG:HB2  | 1:A:89:GLU:HB2   | 0.42     | 1.92        | 16     | 1     |
| 1:A:31:GLU:C    | 1:A:32:ASN:HD22  | 0.42     | 2.22        | 4      | 1     |
| 1:A:12:LEU:CA   | 1:A:17:GLY:HA2   | 0.42     | 2.40        | 15     | 1     |
| 1:A:18:VAL:HG21 | 1:A:80:ILE:HB    | 0.42     | 1.92        | 2      | 2     |
| 1:A:35:LYS:HB2  | 1:A:38:ASN:ND2   | 0.42     | 2.30        | 13     | 1     |
| 1:A:47:LYS:HA   | 1:A:55:PHE:CE1   | 0.42     | 2.49        | 4      | 1     |
| 1:A:26:GLY:HA3  | 1:A:86:ARG:NH1   | 0.42     | 2.30        | 14     | 1     |
| 1:A:36:LYS:HD2  | 1:A:36:LYS:C     | 0.42     | 2.39        | 17     | 1     |
| 1:A:47:LYS:HG3  | 1:A:117:LEU:CD1  | 0.41     | 2.45        | 13     | 2     |
| 1:A:90:LYS:HD2  | 1:A:121:GLU:CD   | 0.41     | 2.40        | 4      | 1     |
| 1:A:43:HIS:CD2  | 1:A:66:LYS:HB3   | 0.41     | 2.50        | 15     | 1     |
| 1:A:95:ILE:HD13 | 1:A:118:PHE:CD2  | 0.41     | 2.50        | 16     | 1     |
| 1:A:22:ILE:HG12 | 1:A:25:LYS:HG3   | 0.41     | 1.92        | 7      | 1     |
| 1:A:96:GLU:H    | 1:A:99:TYR:HD2   | 0.41     | 1.58        | 12     | 1     |
| 1:A:49:GLU:OE1  | 1:A:49:GLU:HA    | 0.41     | 2.14        | 13     | 1     |
| 1:A:62:ASN:ND2  | 1:A:63:VAL:HG23  | 0.41     | 2.30        | 17     | 1     |
| 1:A:11:GLU:HG3  | 1:A:11:GLU:O     | 0.41     | 2.14        | 5      | 1     |
| 1:A:34:PRO:HG3  | 1:A:85:MET:O     | 0.41     | 2.16        | 9      | 1     |
| 1:A:47:LYS:HG3  | 1:A:117:LEU:HD12 | 0.41     | 1.92        | 15     | 1     |
| 1:A:34:PRO:O    | 1:A:83:SER:HA    | 0.41     | 2.16        | 7      | 1     |
| 1:A:81:CYS:HB3  | 1:A:120:ILE:HD12 | 0.41     | 1.93        | 20     | 2     |

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| Atom-1         | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|----------------|------------------|----------|-------------|--------|-------|
|                |                  |          |             | Worst  | Total |
| 1:A:22:ILE:HA  | 1:A:91:CYS:SG    | 0.41     | 2.56        | 4      | 1     |
| 1:A:49:GLU:HB2 | 1:A:117:LEU:CD1  | 0.41     | 2.46        | 12     | 1     |
| 1:A:34:PRO:HG3 | 1:A:122:LEU:HD22 | 0.41     | 1.91        | 1      | 1     |
| 1:A:97:SER:HB3 | 1:A:113:ASN:HA   | 0.41     | 1.93        | 6      | 1     |
| 1:A:39:GLU:HB3 | 1:A:126:ARG:CG   | 0.41     | 2.45        | 17     | 1     |
| 1:A:24:LYS:HE2 | 1:A:90:LYS:CB    | 0.40     | 2.47        | 15     | 1     |
| 1:A:110:ILE:O  | 1:A:110:ILE:HG12 | 0.40     | 2.16        | 3      | 1     |
| 1:A:95:ILE:N   | 1:A:95:ILE:HD12  | 0.40     | 2.32        | 20     | 1     |
| 1:A:50:SER:CB  | 1:A:114:SER:HB3  | 0.40     | 2.47        | 1      | 1     |
| 1:A:32:ASN:OD1 | 1:A:87:LYS:HE3   | 0.40     | 2.17        | 11     | 1     |

## 6.3 Torsion angles ⓘ

### 6.3.1 Protein backbone ⓘ

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

| Mol | Chain | Analysed        | Favoured      | Allowed      | Outliers   | Percentiles |    |
|-----|-------|-----------------|---------------|--------------|------------|-------------|----|
| 1   | A     | 114/135 (84%)   | 100±2 (88±2%) | 13±2 (11±2%) | 1±1 (1±1%) | 15          | 65 |
| All | All   | 2280/2700 (84%) | 2005 (88%)    | 253 (11%)    | 22 (1%)    | 15          | 65 |

All 5 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     | 111 | PRO  | 10             |
| 1   | A     | 29  | GLY  | 8              |
| 1   | A     | 70  | GLU  | 2              |
| 1   | A     | 17  | GLY  | 1              |
| 1   | A     | 112 | GLY  | 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     | 102/120 (85%)   | 92±3 (90±3%) | 10±3 (10±3%) | 10          | 55 |
| All | All   | 2040/2400 (85%) | 1844 (90%)   | 196 (10%)    | 10          | 55 |

All 45 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     | 75  | ILE  | 20             |
| 1   | A     | 110 | ILE  | 20             |
| 1   | A     | 117 | LEU  | 17             |
| 1   | A     | 66  | LYS  | 16             |
| 1   | A     | 70  | GLU  | 12             |
| 1   | A     | 36  | LYS  | 8              |
| 1   | A     | 76  | LYS  | 7              |
| 1   | A     | 125 | PHE  | 7              |
| 1   | A     | 7   | PHE  | 6              |
| 1   | A     | 85  | MET  | 6              |
| 1   | A     | 127 | GLU  | 6              |
| 1   | A     | 53  | LYS  | 5              |
| 1   | A     | 9   | LYS  | 5              |
| 1   | A     | 32  | ASN  | 5              |
| 1   | A     | 92  | LEU  | 4              |
| 1   | A     | 24  | LYS  | 4              |
| 1   | A     | 28  | GLU  | 4              |
| 1   | A     | 97  | SER  | 4              |
| 1   | A     | 60  | ASP  | 4              |
| 1   | A     | 31  | GLU  | 3              |
| 1   | A     | 69  | LEU  | 3              |
| 1   | A     | 101 | TYR  | 2              |
| 1   | A     | 27  | ASP  | 2              |
| 1   | A     | 61  | ARG  | 2              |
| 1   | A     | 109 | SER  | 2              |
| 1   | A     | 11  | GLU  | 2              |
| 1   | A     | 94  | ARG  | 2              |
| 1   | A     | 56  | ASP  | 1              |
| 1   | A     | 122 | LEU  | 1              |
| 1   | A     | 15  | ASP  | 1              |
| 1   | A     | 126 | ARG  | 1              |
| 1   | A     | 79  | ASP  | 1              |
| 1   | A     | 87  | LYS  | 1              |
| 1   | A     | 23  | LEU  | 1              |
| 1   | A     | 57  | SER  | 1              |
| 1   | A     | 43  | HIS  | 1              |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 39  | GLU  | 1              |
| 1   | A     | 50  | SER  | 1              |
| 1   | A     | 71  | GLN  | 1              |
| 1   | A     | 89  | GLU  | 1              |
| 1   | A     | 123 | LEU  | 1              |
| 1   | A     | 25  | LYS  | 1              |
| 1   | A     | 65  | PHE  | 1              |
| 1   | A     | 86  | ARG  | 1              |
| 1   | A     | 35  | LYS  | 1              |

### 6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 6.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 6.7 Other polymers [i](#)

There are no such molecules in this entry.

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

There are no chain breaks in this entry.

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

The completeness of assignment taking into account all chemical shift lists is 90% for the well-defined parts and 83% 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 [i](#)

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

|                                         |      |
|-----------------------------------------|------|
| Total number of shifts                  | 1526 |
| Number of shifts mapped to atoms        | 1526 |
| Number of unparsed shifts               | 0    |
| Number of shifts with mapping errors    | 0    |
| Number of shifts with mapping warnings  | 0    |
| Number of shift outliers (ShiftChecker) | 0    |

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

The following table shows the suggested chemical shift referencing corrections.

| Nucleus                | # values | Correction $\pm$ precision, ppm | Suggested action           |
|------------------------|----------|---------------------------------|----------------------------|
| $^{13}\text{C}_\alpha$ | 126      | $-0.13 \pm 0.20$                | None needed ( $< 0.5$ ppm) |
| $^{13}\text{C}_\beta$  | 112      | $-0.21 \pm 0.14$                | None needed ( $< 0.5$ ppm) |
| $^{13}\text{C}'$       | 121      | $0.21 \pm 0.22$                 | None needed ( $< 0.5$ ppm) |
| $^{15}\text{N}$        | 122      | $0.07 \pm 0.42$                 | None needed ( $< 0.5$ ppm) |

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

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 90%, i.e. 1413 atoms were assigned a chemical shift out of a possible 1569. 0 out of 20 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total         | $^1\text{H}$   | $^{13}\text{C}$ | $^{15}\text{N}$ |
|-----------|---------------|----------------|-----------------|-----------------|
| Backbone  | 570/575 (99%) | 236/236 (100%) | 223/228 (98%)   | 111/111 (100%)  |
| Sidechain | 791/869 (91%) | 535/561 (95%)  | 250/278 (90%)   | 6/30 (20%)      |

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|          | Total           | <sup>1</sup> H | <sup>13</sup> C | <sup>15</sup> N |
|----------|-----------------|----------------|-----------------|-----------------|
| Aromatic | 52/125 (42%)    | 52/61 (85%)    | 0/59 (0%)       | 0/5 (0%)        |
| Overall  | 1413/1569 (90%) | 823/858 (96%)  | 473/565 (84%)   | 117/146 (80%)   |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 83%, i.e. 1526 atoms were assigned a chemical shift out of a possible 1830. 0 out of 21 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total           | <sup>1</sup> H | <sup>13</sup> C | <sup>15</sup> N |
|-----------|-----------------|----------------|-----------------|-----------------|
| Backbone  | 631/683 (92%)   | 262/281 (93%)  | 247/270 (91%)   | 122/132 (92%)   |
| Sidechain | 843/974 (87%)   | 569/627 (91%)  | 267/316 (84%)   | 7/31 (23%)      |
| Aromatic  | 52/173 (30%)    | 52/85 (61%)    | 0/71 (0%)       | 0/17 (0%)       |
| Overall   | 1526/1830 (83%) | 883/993 (89%)  | 514/657 (78%)   | 129/180 (72%)   |

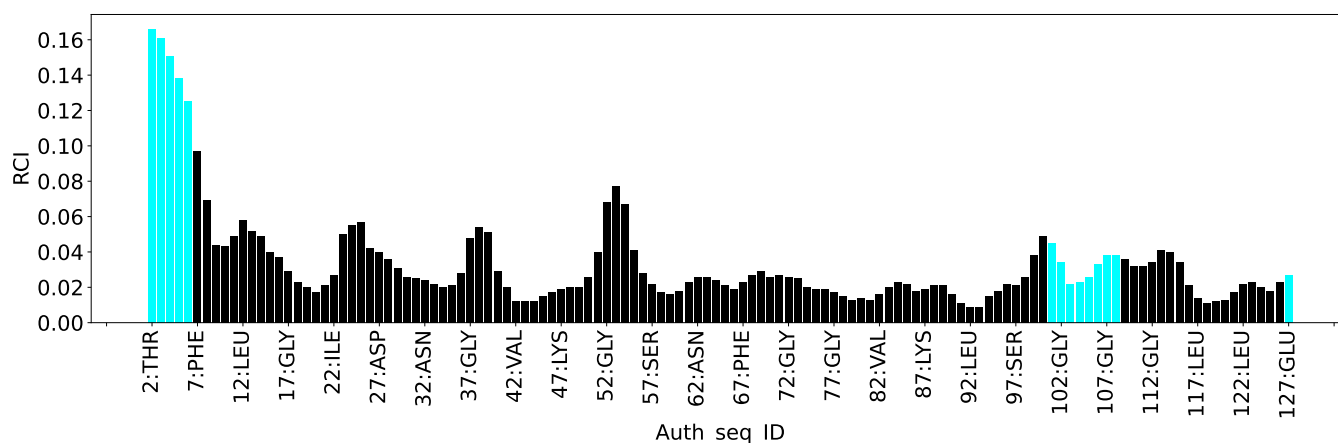
#### 7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

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

Random coil index (RCI) for chain A:



## 8 NMR restraints analysis

### 8.1 Conformationally restricting restraints

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

| Description                                              | Value |
|----------------------------------------------------------|-------|
| Total distance restraints                                | 2538  |
| Intra-residue ( $ i-j =0$ )                              | 567   |
| Sequential ( $ i-j =1$ )                                 | 701   |
| Medium range ( $ i-j >1$ and $ i-j <5$ )                 | 345   |
| Long range ( $ i-j \geq 5$ )                             | 925   |
| Inter-chain                                              | 0     |
| Hydrogen bond restraints                                 | 0     |
| Disulfide bond restraints                                | 0     |
| Total dihedral-angle restraints                          | 185   |
| Number of unmapped restraints                            | 0     |
| Number of restraints per residue                         | 20.2  |
| Number of long range restraints per residue <sup>1</sup> | 6.9   |

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

### 8.2 Residual restraint violations

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

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

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

| Bins (Å)         | Average number of violations per model | Max (Å) |
|------------------|----------------------------------------|---------|
| 0.1-0.2 (Small)  | 6.6                                    | 0.2     |
| 0.2-0.5 (Medium) | 4.2                                    | 0.5     |
| >0.5 (Large)     | 24.6                                   | 3.93    |

### 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)   | 14.1                                   | 4.85    |
| 10.0-20.0 (Medium) | None                                   | None    |
| >20.0 (Large)      | None                                   | None    |

## 9 Distance violation analysis ⓘ

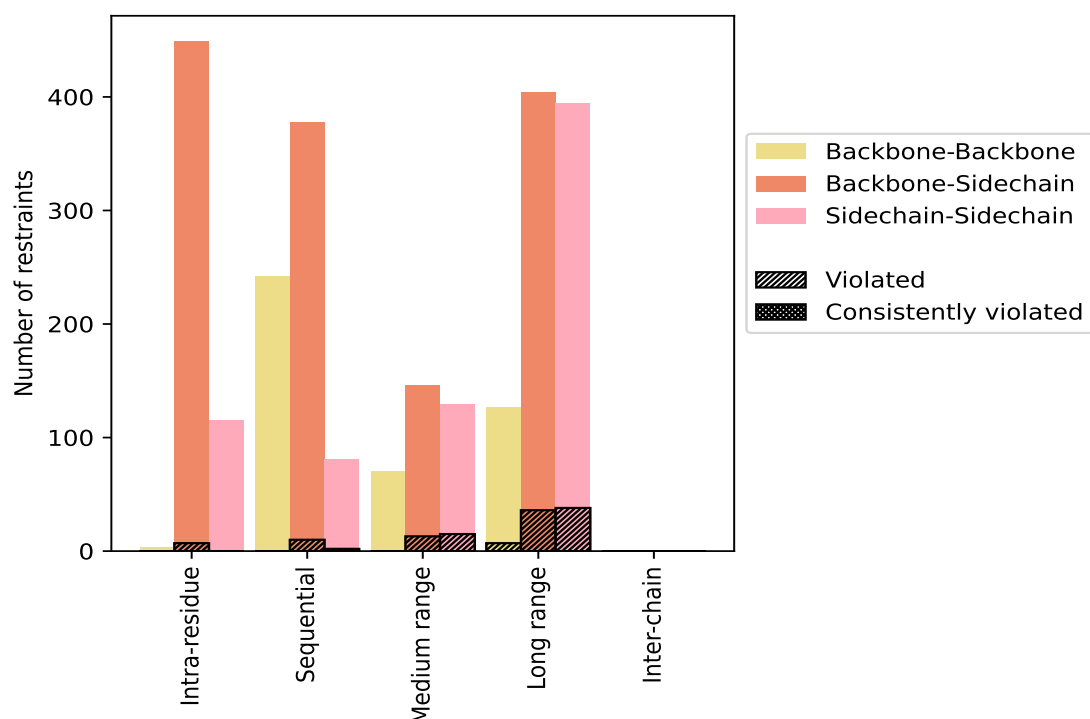
### 9.1 Summary of distance violations ⓘ

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

| Restrains type                                                              | Count       | % <sup>1</sup> | Violated <sup>3</sup> |                |                | Consistently Violated <sup>4</sup> |                |                |
|-----------------------------------------------------------------------------|-------------|----------------|-----------------------|----------------|----------------|------------------------------------|----------------|----------------|
|                                                                             |             |                | Count                 | % <sup>2</sup> | % <sup>1</sup> | Count                              | % <sup>2</sup> | % <sup>1</sup> |
| <b>Intra-residue (<math> i-j =0</math>)</b>                                 | <b>567</b>  | <b>22.3</b>    | <b>7</b>              | <b>1.2</b>     | <b>0.3</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| Backbone-Backbone                                                           | 3           | 0.1            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 449         | 17.7           | 7                     | 1.6            | 0.3            | 0                                  | 0.0            | 0.0            |
| Sidechain-Sidechain                                                         | 115         | 4.5            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| <b>Sequential (<math> i-j =1</math>)</b>                                    | <b>701</b>  | <b>27.6</b>    | <b>12</b>             | <b>1.7</b>     | <b>0.5</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| Backbone-Backbone                                                           | 242         | 9.5            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 378         | 14.9           | 10                    | 2.6            | 0.4            | 0                                  | 0.0            | 0.0            |
| Sidechain-Sidechain                                                         | 81          | 3.2            | 2                     | 2.5            | 0.1            | 0                                  | 0.0            | 0.0            |
| <b>Medium range (<math> i-j &gt;1</math> &amp; <math> i-j &lt;5</math>)</b> | <b>345</b>  | <b>13.6</b>    | <b>28</b>             | <b>8.1</b>     | <b>1.1</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| Backbone-Backbone                                                           | 70          | 2.8            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 146         | 5.8            | 13                    | 8.9            | 0.5            | 0                                  | 0.0            | 0.0            |
| Sidechain-Sidechain                                                         | 129         | 5.1            | 15                    | 11.6           | 0.6            | 0                                  | 0.0            | 0.0            |
| <b>Long range (<math> i-j \geq 5</math>)</b>                                | <b>925</b>  | <b>36.4</b>    | <b>81</b>             | <b>8.8</b>     | <b>3.2</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| Backbone-Backbone                                                           | 127         | 5.0            | 7                     | 5.5            | 0.3            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 404         | 15.9           | 36                    | 8.9            | 1.4            | 0                                  | 0.0            | 0.0            |
| Sidechain-Sidechain                                                         | 394         | 15.5           | 38                    | 9.6            | 1.5            | 0                                  | 0.0            | 0.0            |
| <b>Inter-chain</b>                                                          | <b>0</b>    | <b>0.0</b>     | <b>0</b>              | <b>0.0</b>     | <b>0.0</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| Backbone-Backbone                                                           | 0           | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 0           | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Sidechain-Sidechain                                                         | 0           | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| <b>Hydrogen bond</b>                                                        | <b>0</b>    | <b>0.0</b>     | <b>0</b>              | <b>0.0</b>     | <b>0.0</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| <b>Disulfide bond</b>                                                       | <b>0</b>    | <b>0.0</b>     | <b>0</b>              | <b>0.0</b>     | <b>0.0</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| <b>Total</b>                                                                | <b>2538</b> | <b>100.0</b>   | <b>128</b>            | <b>5.0</b>     | <b>5.0</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| Backbone-Backbone                                                           | 442         | 17.4           | 7                     | 1.6            | 0.3            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 1377        | 54.3           | 66                    | 4.8            | 2.6            | 0                                  | 0.0            | 0.0            |
| Sidechain-Sidechain                                                         | 719         | 28.3           | 55                    | 7.6            | 2.2            | 0                                  | 0.0            | 0.0            |

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

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



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

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

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

| Model ID | Number of violations |                 |                 |                 |                 |       | Mean (Å) | Max (Å) | SD <sup>6</sup> (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
|          | IR <sup>1</sup>      | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total |          |         |                     |            |
| 1        | 1                    | 3               | 3               | 19              | 0               | 26    | 1.35     | 3.22    | 1.1                 | 1.18       |
| 2        | 2                    | 0               | 9               | 17              | 0               | 28    | 0.8      | 2.08    | 0.68                | 0.62       |
| 3        | 1                    | 1               | 4               | 24              | 0               | 30    | 1.02     | 2.84    | 0.81                | 0.93       |
| 4        | 2                    | 5               | 10              | 27              | 0               | 44    | 0.88     | 3.13    | 0.82                | 0.56       |
| 5        | 2                    | 1               | 14              | 27              | 0               | 44    | 1.03     | 3.48    | 0.85                | 0.82       |
| 6        | 2                    | 3               | 4               | 17              | 0               | 26    | 1.12     | 3.05    | 0.67                | 1.17       |
| 7        | 1                    | 3               | 14              | 30              | 0               | 48    | 1.11     | 3.31    | 0.84                | 1.02       |
| 8        | 4                    | 2               | 13              | 30              | 0               | 49    | 0.92     | 3.16    | 0.8                 | 0.82       |
| 9        | 0                    | 3               | 2               | 8               | 0               | 13    | 0.59     | 1.34    | 0.51                | 0.35       |
| 10       | 2                    | 1               | 8               | 15              | 0               | 26    | 1.0      | 3.38    | 0.88                | 0.76       |

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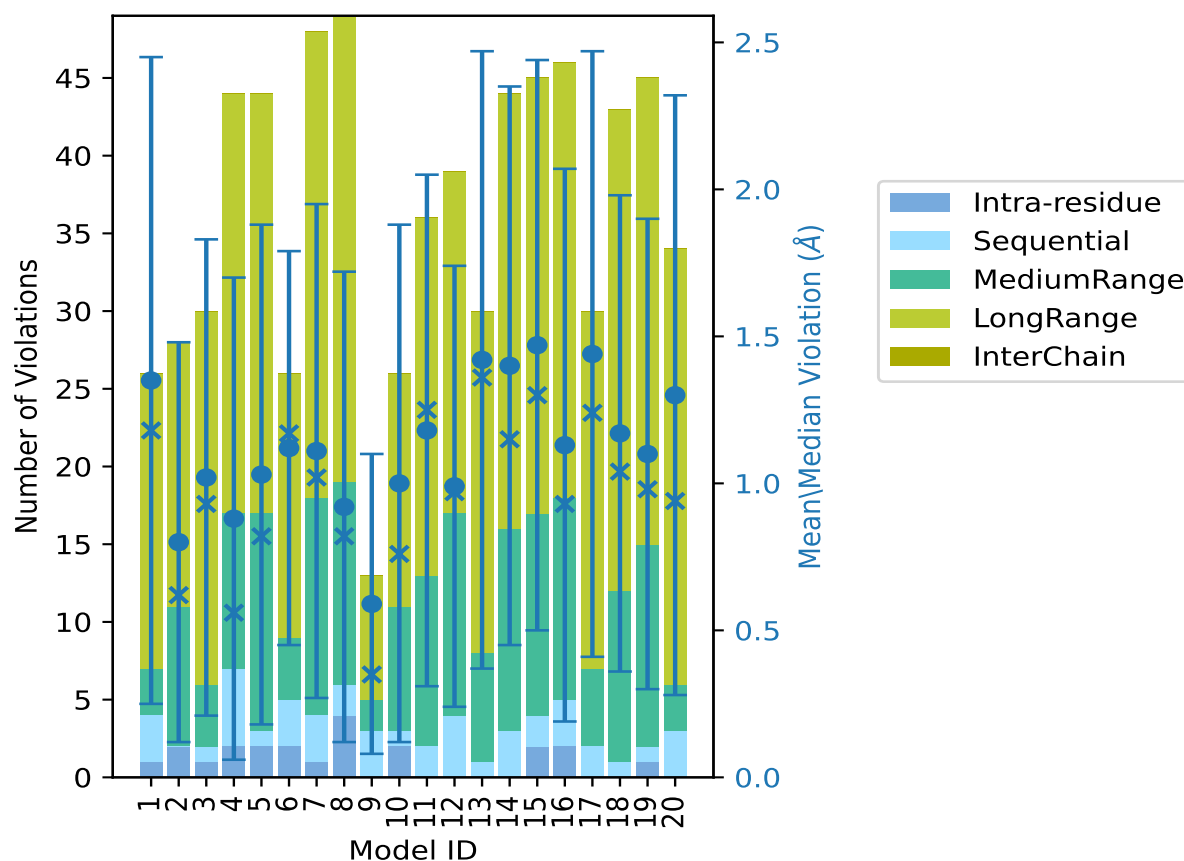
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| Model ID | Number of violations |                 |                 |                 |                 |       | Mean (Å) | Max (Å) | SD <sup>6</sup> (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
|          | IR <sup>1</sup>      | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total |          |         |                     |            |
| 11       | 0                    | 2               | 11              | 23              | 0               | 36    | 1.18     | 3.38    | 0.87                | 1.25       |
| 12       | 0                    | 4               | 13              | 22              | 0               | 39    | 0.99     | 2.52    | 0.75                | 0.97       |
| 13       | 0                    | 1               | 7               | 22              | 0               | 30    | 1.42     | 3.57    | 1.05                | 1.36       |
| 14       | 0                    | 3               | 13              | 28              | 0               | 44    | 1.4      | 3.49    | 0.95                | 1.15       |
| 15       | 2                    | 2               | 13              | 28              | 0               | 45    | 1.47     | 3.63    | 0.97                | 1.3        |
| 16       | 2                    | 3               | 13              | 28              | 0               | 46    | 1.13     | 3.35    | 0.94                | 0.93       |
| 17       | 0                    | 2               | 5               | 23              | 0               | 30    | 1.44     | 3.93    | 1.03                | 1.24       |
| 18       | 0                    | 1               | 11              | 31              | 0               | 43    | 1.17     | 3.18    | 0.81                | 1.04       |
| 19       | 1                    | 1               | 13              | 30              | 0               | 45    | 1.1      | 3.29    | 0.8                 | 0.98       |
| 20       | 0                    | 3               | 3               | 28              | 0               | 34    | 1.3      | 3.66    | 1.02                | 0.94       |

<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

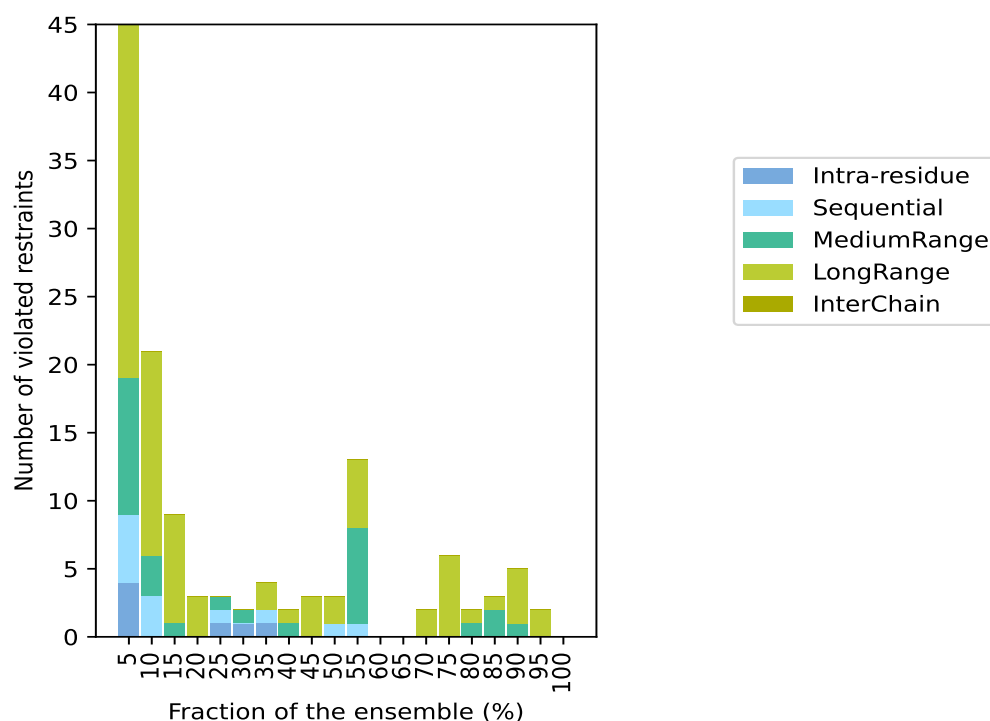
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 2410(IR:560, SQ:689, MR:317, LR:844, IC:0) restraints are not violated in the ensemble.

| Number of violated restraints |                 |                 |                 |                 |       | Fraction of the ensemble |       |
|-------------------------------|-----------------|-----------------|-----------------|-----------------|-------|--------------------------|-------|
| IR <sup>1</sup>               | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total | Count <sup>6</sup>       | %     |
| 4                             | 5               | 10              | 26              | 0               | 45    | 1                        | 5.0   |
| 0                             | 3               | 3               | 15              | 0               | 21    | 2                        | 10.0  |
| 0                             | 0               | 1               | 8               | 0               | 9     | 3                        | 15.0  |
| 0                             | 0               | 0               | 3               | 0               | 3     | 4                        | 20.0  |
| 1                             | 1               | 1               | 0               | 0               | 3     | 5                        | 25.0  |
| 1                             | 0               | 1               | 0               | 0               | 2     | 6                        | 30.0  |
| 1                             | 1               | 0               | 2               | 0               | 4     | 7                        | 35.0  |
| 0                             | 0               | 1               | 1               | 0               | 2     | 8                        | 40.0  |
| 0                             | 0               | 0               | 3               | 0               | 3     | 9                        | 45.0  |
| 0                             | 1               | 0               | 2               | 0               | 3     | 10                       | 50.0  |
| 0                             | 1               | 7               | 5               | 0               | 13    | 11                       | 55.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 12                       | 60.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 13                       | 65.0  |
| 0                             | 0               | 0               | 2               | 0               | 2     | 14                       | 70.0  |
| 0                             | 0               | 0               | 6               | 0               | 6     | 15                       | 75.0  |
| 0                             | 0               | 1               | 1               | 0               | 2     | 16                       | 80.0  |
| 0                             | 0               | 2               | 1               | 0               | 3     | 17                       | 85.0  |
| 0                             | 0               | 1               | 4               | 0               | 5     | 18                       | 90.0  |
| 0                             | 0               | 0               | 2               | 0               | 2     | 19                       | 95.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 20                       | 100.0 |

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

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

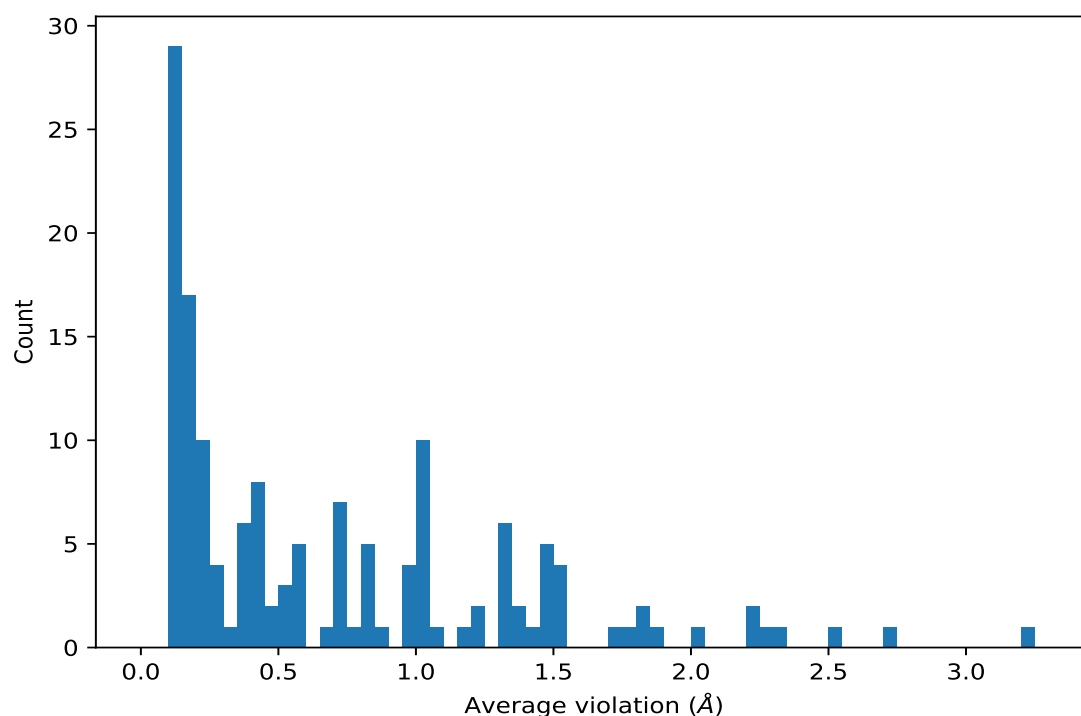
### 9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

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

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



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

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

| Key      | Atom-1         | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,651)  | 1:7:A:PHE:HE1  | 1:23:A:LEU:HB2  | 19                  | 2.02     | 0.65                | 1.96       |
| (1,650)  | 1:7:A:PHE:HD1  | 1:23:A:LEU:HB2  | 19                  | 1.88     | 0.58                | 1.91       |
| (1,660)  | 1:7:A:PHE:HD1  | 1:23:A:LEU:HB3  | 18                  | 1.84     | 0.79                | 1.6        |
| (1,903)  | 1:44:A:TYR:HD1 | 1:65:A:PHE:HD1  | 18                  | 1.5      | 0.41                | 1.5        |
| (1,921)  | 1:44:A:TYR:HE1 | 1:65:A:PHE:HD1  | 18                  | 1.2      | 0.24                | 1.19       |
| (1,1855) | 1:5:A:GLN:HG2  | 1:7:A:PHE:HD1   | 18                  | 1.0      | 0.56                | 0.97       |
| (1,1855) | 1:5:A:GLN:HG3  | 1:7:A:PHE:HD1   | 18                  | 1.0      | 0.56                | 0.97       |
| (1,927)  | 1:44:A:TYR:HE1 | 1:65:A:PHE:HE1  | 18                  | 0.8      | 0.25                | 0.72       |
| (1,1728) | 1:5:A:GLN:HG2  | 1:7:A:PHE:HE1   | 17                  | 2.31     | 0.77                | 2.37       |
| (1,1729) | 1:5:A:GLN:HG3  | 1:7:A:PHE:HE1   | 17                  | 2.24     | 0.83                | 2.4        |
| (1,1464) | 1:7:A:PHE:HE1  | 1:23:A:LEU:HB3  | 17                  | 1.81     | 0.92                | 1.51       |
| (1,879)  | 1:65:A:PHE:HD1 | 1:67:A:PHE:H    | 16                  | 1.79     | 0.48                | 1.68       |
| (1,1365) | 1:7:A:PHE:HD1  | 1:23:A:LEU:HA   | 16                  | 1.23     | 0.8                 | 1.12       |
| (1,944)  | 1:78:A:TRP:HE3 | 1:101:A:TYR:HE1 | 15                  | 3.23     | 0.35                | 3.16       |
| (1,858)  | 1:78:A:TRP:HH2 | 1:101:A:TYR:HE1 | 15                  | 2.51     | 0.41                | 2.54       |
| (1,902)  | 1:75:A:ILE:H   | 1:101:A:TYR:HD1 | 15                  | 1.47     | 0.38                | 1.36       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1356) | 1:74:A:VAL:HA   | 1:101:A:TYR:HE1 | 15                  | 1.38     | 0.45                | 1.3        |
| (1,869)  | 1:78:A:TRP:HZ3  | 1:101:A:TYR:HD1 | 15                  | 1.19     | 0.46                | 1.1        |
| (1,926)  | 1:75:A:ILE:H    | 1:101:A:TYR:HE1 | 15                  | 1.01     | 0.54                | 0.87       |
| (1,862)  | 1:78:A:TRP:HH2  | 1:101:A:TYR:HD1 | 14                  | 1.72     | 0.51                | 1.66       |
| (1,1382) | 1:75:A:ILE:HA   | 1:101:A:TYR:HE1 | 14                  | 1.0      | 0.72                | 0.88       |
| (1,777)  | 1:67:A:PHE:HE1  | 1:70:A:GLU:H    | 11                  | 2.72     | 0.41                | 2.63       |
| (1,908)  | 1:67:A:PHE:HD1  | 1:74:A:VAL:H    | 11                  | 2.26     | 0.33                | 2.3        |
| (1,827)  | 1:67:A:PHE:HE1  | 1:69:A:LEU:H    | 11                  | 2.2      | 0.21                | 2.27       |
| (1,643)  | 1:67:A:PHE:HE1  | 1:74:A:VAL:HG21 | 11                  | 1.54     | 0.37                | 1.56       |
| (1,643)  | 1:67:A:PHE:HE1  | 1:74:A:VAL:HG22 | 11                  | 1.54     | 0.37                | 1.56       |
| (1,643)  | 1:67:A:PHE:HE1  | 1:74:A:VAL:HG23 | 11                  | 1.54     | 0.37                | 1.56       |
| (1,1370) | 1:67:A:PHE:HD1  | 1:69:A:LEU:HA   | 11                  | 1.47     | 0.16                | 1.5        |
| (1,1686) | 1:67:A:PHE:HE1  | 1:69:A:LEU:HA   | 11                  | 1.4      | 0.2                 | 1.46       |
| (1,2224) | 1:67:A:PHE:HD1  | 1:69:A:LEU:HD11 | 11                  | 1.3      | 0.23                | 1.32       |
| (1,2224) | 1:67:A:PHE:HD1  | 1:69:A:LEU:HD12 | 11                  | 1.3      | 0.23                | 1.32       |
| (1,2224) | 1:67:A:PHE:HD1  | 1:69:A:LEU:HD13 | 11                  | 1.3      | 0.23                | 1.32       |
| (1,2224) | 1:67:A:PHE:HD1  | 1:69:A:LEU:HD21 | 11                  | 1.3      | 0.23                | 1.32       |
| (1,2224) | 1:67:A:PHE:HD1  | 1:69:A:LEU:HD22 | 11                  | 1.3      | 0.23                | 1.32       |
| (1,2224) | 1:67:A:PHE:HD1  | 1:69:A:LEU:HD23 | 11                  | 1.3      | 0.23                | 1.32       |
| (1,644)  | 1:67:A:PHE:HE1  | 1:82:A:VAL:HB   | 11                  | 1.08     | 0.46                | 0.92       |
| (1,2228) | 1:67:A:PHE:HE1  | 1:71:A:GLN:HE21 | 11                  | 0.81     | 0.22                | 0.88       |
| (1,2228) | 1:67:A:PHE:HE1  | 1:71:A:GLN:HE22 | 11                  | 0.81     | 0.22                | 0.88       |
| (1,2227) | 1:67:A:PHE:HE1  | 1:69:A:LEU:HD11 | 11                  | 0.74     | 0.28                | 0.77       |
| (1,2227) | 1:67:A:PHE:HE1  | 1:69:A:LEU:HD12 | 11                  | 0.74     | 0.28                | 0.77       |
| (1,2227) | 1:67:A:PHE:HE1  | 1:69:A:LEU:HD13 | 11                  | 0.74     | 0.28                | 0.77       |
| (1,2227) | 1:67:A:PHE:HE1  | 1:69:A:LEU:HD21 | 11                  | 0.74     | 0.28                | 0.77       |
| (1,2227) | 1:67:A:PHE:HE1  | 1:69:A:LEU:HD22 | 11                  | 0.74     | 0.28                | 0.77       |
| (1,2227) | 1:67:A:PHE:HE1  | 1:69:A:LEU:HD23 | 11                  | 0.74     | 0.28                | 0.77       |
| (1,1870) | 1:7:A:PHE:HD1   | 1:23:A:LEU:HD11 | 11                  | 0.38     | 0.32                | 0.19       |
| (1,1870) | 1:7:A:PHE:HD1   | 1:23:A:LEU:HD12 | 11                  | 0.38     | 0.32                | 0.19       |
| (1,1870) | 1:7:A:PHE:HD1   | 1:23:A:LEU:HD13 | 11                  | 0.38     | 0.32                | 0.19       |
| (1,1870) | 1:7:A:PHE:HD1   | 1:23:A:LEU:HD21 | 11                  | 0.38     | 0.32                | 0.19       |
| (1,1870) | 1:7:A:PHE:HD1   | 1:23:A:LEU:HD22 | 11                  | 0.38     | 0.32                | 0.19       |
| (1,1870) | 1:7:A:PHE:HD1   | 1:23:A:LEU:HD23 | 11                  | 0.38     | 0.32                | 0.19       |
| (1,521)  | 1:75:A:ILE:HG12 | 1:76:A:LYS:H    | 11                  | 0.22     | 0.1                 | 0.23       |
| (1,1200) | 1:34:A:PRO:HA   | 1:122:A:LEU:HG  | 11                  | 0.16     | 0.04                | 0.16       |
| (1,1518) | 1:40:A:VAL:HG21 | 1:67:A:PHE:HE1  | 10                  | 0.98     | 0.21                | 0.96       |
| (1,1518) | 1:40:A:VAL:HG22 | 1:67:A:PHE:HE1  | 10                  | 0.98     | 0.21                | 0.96       |
| (1,1518) | 1:40:A:VAL:HG23 | 1:67:A:PHE:HE1  | 10                  | 0.98     | 0.21                | 0.96       |
| (1,1177) | 1:95:A:ILE:HB   | 1:100:A:GLY:HA2 | 10                  | 0.78     | 0.22                | 0.76       |
| (1,2527) | 1:125:A:PHE:HD1 | 1:126:A:ARG:HG2 | 10                  | 0.12     | 0.02                | 0.12       |
| (1,2527) | 1:125:A:PHE:HD1 | 1:126:A:ARG:HG3 | 10                  | 0.12     | 0.02                | 0.12       |

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| Key      | Atom-1          | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,687)  | 1:67:A:PHE:HD1  | 1:82:A:VAL:HG21  | 9                   | 1.0      | 0.28                | 0.96       |
| (1,687)  | 1:67:A:PHE:HD1  | 1:82:A:VAL:HG22  | 9                   | 1.0      | 0.28                | 0.96       |
| (1,687)  | 1:67:A:PHE:HD1  | 1:82:A:VAL:HG23  | 9                   | 1.0      | 0.28                | 0.96       |
| (1,2226) | 1:67:A:PHE:HD1  | 1:73:A:GLU:HB2   | 9                   | 0.41     | 0.25                | 0.38       |
| (1,2226) | 1:67:A:PHE:HD1  | 1:73:A:GLU:HB3   | 9                   | 0.41     | 0.25                | 0.38       |
| (1,1367) | 1:50:A:SER:HA   | 1:116:A:LEU:HA   | 9                   | 0.13     | 0.02                | 0.12       |
| (1,1852) | 1:5:A:GLN:HB2   | 1:7:A:PHE:HE1    | 8                   | 0.57     | 0.32                | 0.53       |
| (1,1852) | 1:5:A:GLN:HB3   | 1:7:A:PHE:HE1    | 8                   | 0.57     | 0.32                | 0.53       |
| (1,699)  | 1:75:A:ILE:HG13 | 1:101:A:TYR:HD1  | 8                   | 0.45     | 0.37                | 0.33       |
| (1,717)  | 1:58:A:SER:HA   | 1:59:A:PHE:HD1   | 7                   | 0.82     | 0.31                | 0.92       |
| (1,878)  | 1:7:A:PHE:H     | 1:7:A:PHE:HE1    | 7                   | 0.45     | 0.23                | 0.37       |
| (1,1219) | 1:46:A:GLY:HA3  | 1:117:A:LEU:HB3  | 7                   | 0.31     | 0.13                | 0.29       |
| (1,1503) | 1:42:A:VAL:HG11 | 1:67:A:PHE:HD1   | 7                   | 0.23     | 0.06                | 0.23       |
| (1,1503) | 1:42:A:VAL:HG12 | 1:67:A:PHE:HD1   | 7                   | 0.23     | 0.06                | 0.23       |
| (1,1503) | 1:42:A:VAL:HG13 | 1:67:A:PHE:HD1   | 7                   | 0.23     | 0.06                | 0.23       |
| (1,1509) | 1:123:A:LEU:H   | 1:123:A:LEU:HD21 | 6                   | 0.21     | 0.04                | 0.22       |
| (1,1509) | 1:123:A:LEU:H   | 1:123:A:LEU:HD22 | 6                   | 0.21     | 0.04                | 0.22       |
| (1,1509) | 1:123:A:LEU:H   | 1:123:A:LEU:HD23 | 6                   | 0.21     | 0.04                | 0.22       |
| (1,2241) | 1:69:A:LEU:HA   | 1:71:A:GLN:HE21  | 6                   | 0.13     | 0.02                | 0.12       |
| (1,2241) | 1:69:A:LEU:HA   | 1:71:A:GLN:HE22  | 6                   | 0.13     | 0.02                | 0.12       |
| (1,1)    | 1:92:A:LEU:HB3  | 1:93:A:VAL:H     | 5                   | 0.16     | 0.03                | 0.17       |
| (1,1085) | 1:78:A:TRP:HB3  | 1:82:A:VAL:HA    | 5                   | 0.13     | 0.01                | 0.13       |
| (1,1523) | 1:75:A:ILE:H    | 1:75:A:ILE:HD11  | 5                   | 0.12     | 0.02                | 0.11       |
| (1,1523) | 1:75:A:ILE:H    | 1:75:A:ILE:HD12  | 5                   | 0.12     | 0.02                | 0.11       |
| (1,1523) | 1:75:A:ILE:H    | 1:75:A:ILE:HD13  | 5                   | 0.12     | 0.02                | 0.11       |
| (1,1531) | 1:67:A:PHE:HD1  | 1:74:A:VAL:HG21  | 4                   | 0.41     | 0.13                | 0.42       |
| (1,1531) | 1:67:A:PHE:HD1  | 1:74:A:VAL:HG22  | 4                   | 0.41     | 0.13                | 0.42       |
| (1,1531) | 1:67:A:PHE:HD1  | 1:74:A:VAL:HG23  | 4                   | 0.41     | 0.13                | 0.42       |
| (1,642)  | 1:67:A:PHE:HE1  | 1:74:A:VAL:HG11  | 4                   | 0.21     | 0.04                | 0.22       |
| (1,642)  | 1:67:A:PHE:HE1  | 1:74:A:VAL:HG12  | 4                   | 0.21     | 0.04                | 0.22       |
| (1,642)  | 1:67:A:PHE:HE1  | 1:74:A:VAL:HG13  | 4                   | 0.21     | 0.04                | 0.22       |
| (1,256)  | 1:27:A:ASP:H    | 1:86:A:ARG:HB2   | 4                   | 0.13     | 0.02                | 0.13       |
| (1,1156) | 1:26:A:GLY:HA2  | 1:89:A:GLU:HB3   | 3                   | 0.67     | 0.34                | 0.51       |
| (1,1467) | 1:9:A:LYS:HG3   | 1:21:A:THR:H     | 3                   | 0.58     | 0.29                | 0.39       |
| (1,259)  | 1:27:A:ASP:H    | 1:88:A:ASN:HB3   | 3                   | 0.56     | 0.4                 | 0.31       |
| (1,645)  | 1:7:A:PHE:HD1   | 1:23:A:LEU:HD21  | 3                   | 0.29     | 0.24                | 0.13       |
| (1,645)  | 1:7:A:PHE:HD1   | 1:23:A:LEU:HD22  | 3                   | 0.29     | 0.24                | 0.13       |
| (1,645)  | 1:7:A:PHE:HD1   | 1:23:A:LEU:HD23  | 3                   | 0.29     | 0.24                | 0.13       |
| (1,991)  | 1:85:A:MET:HA   | 1:120:A:ILE:HG21 | 3                   | 0.18     | 0.06                | 0.17       |
| (1,991)  | 1:85:A:MET:HA   | 1:120:A:ILE:HG22 | 3                   | 0.18     | 0.06                | 0.17       |
| (1,991)  | 1:85:A:MET:HA   | 1:120:A:ILE:HG23 | 3                   | 0.18     | 0.06                | 0.17       |
| (1,162)  | 1:36:A:LYS:HD2  | 1:38:A:ASN:H     | 3                   | 0.17     | 0.04                | 0.15       |

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| Key      | Atom-1          | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,84)   | 1:50:A:SER:H    | 1:117:A:LEU:HD21 | 3                   | 0.15     | 0.03                | 0.13       |
| (1,84)   | 1:50:A:SER:H    | 1:117:A:LEU:HD22 | 3                   | 0.15     | 0.03                | 0.13       |
| (1,84)   | 1:50:A:SER:H    | 1:117:A:LEU:HD23 | 3                   | 0.15     | 0.03                | 0.13       |
| (1,799)  | 1:68:A:HIS:H    | 1:73:A:GLU:H     | 3                   | 0.12     | 0.03                | 0.11       |
| (1,1334) | 1:74:A:VAL:HB   | 1:120:A:ILE:HD11 | 3                   | 0.11     | 0.01                | 0.1        |
| (1,1334) | 1:74:A:VAL:HB   | 1:120:A:ILE:HD12 | 3                   | 0.11     | 0.01                | 0.1        |
| (1,1334) | 1:74:A:VAL:HB   | 1:120:A:ILE:HD13 | 3                   | 0.11     | 0.01                | 0.1        |
| (1,1528) | 1:44:A:TYR:HD1  | 1:120:A:ILE:HG21 | 2                   | 1.46     | 0.26                | 1.46       |
| (1,1528) | 1:44:A:TYR:HD1  | 1:120:A:ILE:HG22 | 2                   | 1.46     | 0.26                | 1.46       |
| (1,1528) | 1:44:A:TYR:HD1  | 1:120:A:ILE:HG23 | 2                   | 1.46     | 0.26                | 1.46       |
| (1,867)  | 1:44:A:TYR:HE1  | 1:66:A:LYS:H     | 2                   | 1.37     | 0.6                 | 1.37       |
| (1,688)  | 1:67:A:PHE:HD1  | 1:82:A:VAL:HG11  | 2                   | 1.04     | 0.27                | 1.04       |
| (1,688)  | 1:67:A:PHE:HD1  | 1:82:A:VAL:HG12  | 2                   | 1.04     | 0.27                | 1.04       |
| (1,688)  | 1:67:A:PHE:HD1  | 1:82:A:VAL:HG13  | 2                   | 1.04     | 0.27                | 1.04       |
| (1,1205) | 1:26:A:GLY:HA2  | 1:86:A:ARG:HB2   | 2                   | 0.96     | 0.27                | 0.96       |
| (1,1575) | 1:44:A:TYR:HD1  | 1:66:A:LYS:HA    | 2                   | 0.87     | 0.19                | 0.87       |
| (1,923)  | 1:44:A:TYR:HE1  | 1:66:A:LYS:HA    | 2                   | 0.83     | 0.37                | 0.83       |
| (1,608)  | 1:78:A:TRP:HH2  | 1:95:A:ILE:HG13  | 2                   | 0.72     | 0.25                | 0.72       |
| (1,1574) | 1:43:A:HIS:HA   | 1:44:A:TYR:HD1   | 2                   | 0.55     | 0.03                | 0.55       |
| (1,1537) | 1:75:A:ILE:HG21 | 1:101:A:TYR:HE1  | 2                   | 0.54     | 0.05                | 0.54       |
| (1,1537) | 1:75:A:ILE:HG22 | 1:101:A:TYR:HE1  | 2                   | 0.54     | 0.05                | 0.54       |
| (1,1537) | 1:75:A:ILE:HG23 | 1:101:A:TYR:HE1  | 2                   | 0.54     | 0.05                | 0.54       |
| (1,1851) | 1:5:A:GLN:HB2   | 1:7:A:PHE:HD1    | 2                   | 0.44     | 0.3                 | 0.44       |
| (1,1851) | 1:5:A:GLN:HB3   | 1:7:A:PHE:HD1    | 2                   | 0.44     | 0.3                 | 0.44       |
| (1,254)  | 1:27:A:ASP:H    | 1:28:A:GLU:HB3   | 2                   | 0.42     | 0.08                | 0.42       |
| (1,1390) | 1:26:A:GLY:HA2  | 1:89:A:GLU:H     | 2                   | 0.28     | 0.18                | 0.28       |
| (1,1944) | 1:20:A:LYS:HD2  | 1:120:A:ILE:HD11 | 2                   | 0.16     | 0.0                 | 0.16       |
| (1,1944) | 1:20:A:LYS:HD2  | 1:120:A:ILE:HD12 | 2                   | 0.16     | 0.0                 | 0.16       |
| (1,1944) | 1:20:A:LYS:HD2  | 1:120:A:ILE:HD13 | 2                   | 0.16     | 0.0                 | 0.16       |
| (1,1944) | 1:20:A:LYS:HD3  | 1:120:A:ILE:HD11 | 2                   | 0.16     | 0.0                 | 0.16       |
| (1,1944) | 1:20:A:LYS:HD3  | 1:120:A:ILE:HD12 | 2                   | 0.16     | 0.0                 | 0.16       |
| (1,1944) | 1:20:A:LYS:HD3  | 1:120:A:ILE:HD13 | 2                   | 0.16     | 0.0                 | 0.16       |
| (1,1875) | 1:8:A:GLU:HA    | 1:9:A:LYS:HD2    | 2                   | 0.15     | 0.01                | 0.15       |
| (1,1875) | 1:8:A:GLU:HA    | 1:9:A:LYS:HD3    | 2                   | 0.15     | 0.01                | 0.15       |
| (1,843)  | 1:57:A:SER:H    | 1:62:A:ASN:H     | 2                   | 0.14     | 0.04                | 0.14       |
| (1,2105) | 1:42:A:VAL:HA   | 1:66:A:LYS:HD2   | 2                   | 0.14     | 0.02                | 0.14       |
| (1,2105) | 1:42:A:VAL:HA   | 1:66:A:LYS:HD3   | 2                   | 0.14     | 0.02                | 0.14       |
| (1,1437) | 1:9:A:LYS:HA    | 1:22:A:ILE:HB    | 2                   | 0.13     | 0.02                | 0.13       |
| (1,400)  | 1:28:A:GLU:HG2  | 1:30:A:GLU:H     | 2                   | 0.12     | 0.01                | 0.12       |
| (1,2404) | 1:94:A:ARG:HD2  | 1:116:A:LEU:HA   | 2                   | 0.12     | 0.02                | 0.12       |
| (1,2404) | 1:94:A:ARG:HD3  | 1:116:A:LEU:HA   | 2                   | 0.12     | 0.02                | 0.12       |
| (1,2146) | 1:49:A:GLU:HB2  | 1:117:A:LEU:HG   | 2                   | 0.11     | 0.01                | 0.11       |

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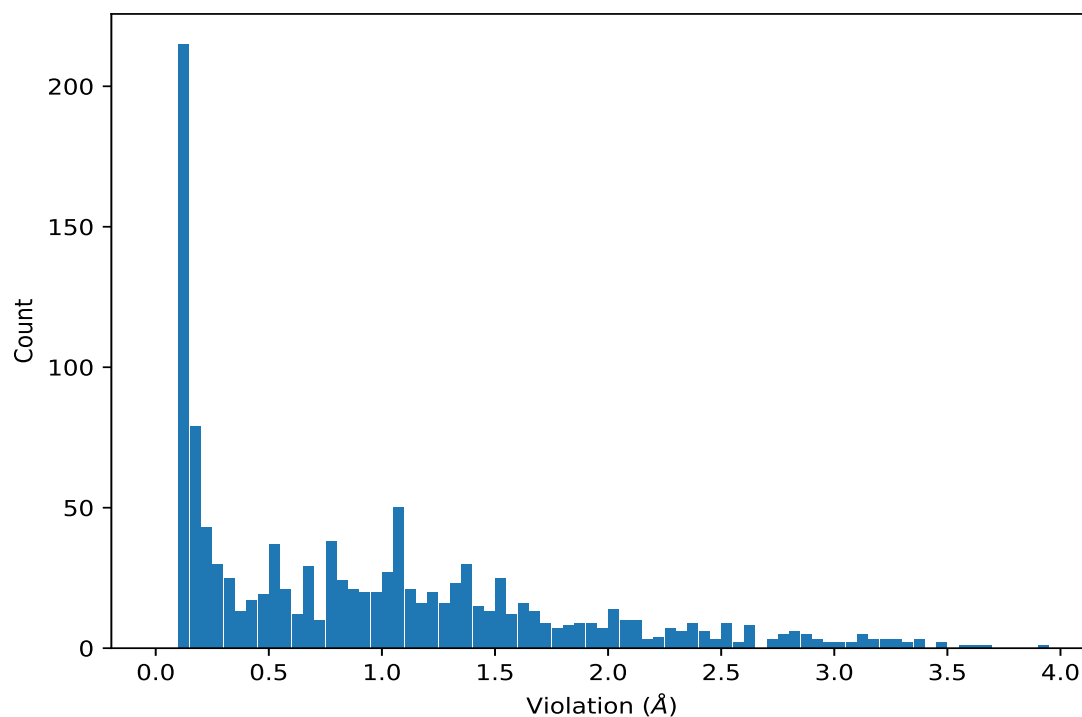
| Key      | Atom-1          | Atom-2         | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|----------------|---------------------|----------|---------------------|------------|
| (1,2146) | 1:49:A:GLU:HB3  | 1:117:A:LEU:HG | 2                   | 0.11     | 0.01                | 0.11       |
| (1,1910) | 1:12:A:LEU:HD11 | 1:16:A:GLY:HA2 | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1910) | 1:12:A:LEU:HD12 | 1:16:A:GLY:HA2 | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1910) | 1:12:A:LEU:HD13 | 1:16:A:GLY:HA2 | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1910) | 1:12:A:LEU:HD21 | 1:16:A:GLY:HA2 | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1910) | 1:12:A:LEU:HD22 | 1:16:A:GLY:HA2 | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1910) | 1:12:A:LEU:HD23 | 1:16:A:GLY:HA2 | 2                   | 0.11     | 0.0                 | 0.11       |

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

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

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

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



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

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

| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,944)  | 1:78:A:TRP:HE3 | 1:101:A:TYR:HE1 | 17       | 3.93          |
| (1,944)  | 1:78:A:TRP:HE3 | 1:101:A:TYR:HE1 | 20       | 3.66          |
| (1,944)  | 1:78:A:TRP:HE3 | 1:101:A:TYR:HE1 | 15       | 3.63          |
| (1,944)  | 1:78:A:TRP:HE3 | 1:101:A:TYR:HE1 | 13       | 3.57          |
| (1,1729) | 1:5:A:GLN:HG3  | 1:7:A:PHE:HE1   | 14       | 3.49          |
| (1,944)  | 1:78:A:TRP:HE3 | 1:101:A:TYR:HE1 | 5        | 3.48          |
| (1,1729) | 1:5:A:GLN:HG3  | 1:7:A:PHE:HE1   | 10       | 3.38          |
| (1,1728) | 1:5:A:GLN:HG2  | 1:7:A:PHE:HE1   | 11       | 3.38          |
| (1,651)  | 1:7:A:PHE:HE1  | 1:23:A:LEU:HB2  | 16       | 3.35          |
| (1,944)  | 1:78:A:TRP:HE3 | 1:101:A:TYR:HE1 | 7        | 3.31          |
| (1,777)  | 1:67:A:PHE:HE1 | 1:70:A:GLU:H    | 14       | 3.31          |
| (1,944)  | 1:78:A:TRP:HE3 | 1:101:A:TYR:HE1 | 19       | 3.29          |
| (1,1728) | 1:5:A:GLN:HG2  | 1:7:A:PHE:HE1   | 14       | 3.27          |
| (1,1729) | 1:5:A:GLN:HG3  | 1:7:A:PHE:HE1   | 13       | 3.25          |
| (1,1464) | 1:7:A:PHE:HE1  | 1:23:A:LEU:HB3  | 1        | 3.22          |
| (1,858)  | 1:78:A:TRP:HH2 | 1:101:A:TYR:HE1 | 13       | 3.22          |
| (1,1728) | 1:5:A:GLN:HG2  | 1:7:A:PHE:HE1   | 13       | 3.21          |
| (1,879)  | 1:65:A:PHE:HD1 | 1:67:A:PHE:H    | 19       | 3.19          |
| (1,777)  | 1:67:A:PHE:HE1 | 1:70:A:GLU:H    | 18       | 3.18          |
| (1,944)  | 1:78:A:TRP:HE3 | 1:101:A:TYR:HE1 | 8        | 3.16          |
| (1,944)  | 1:78:A:TRP:HE3 | 1:101:A:TYR:HE1 | 4        | 3.13          |
| (1,858)  | 1:78:A:TRP:HH2 | 1:101:A:TYR:HE1 | 20       | 3.12          |
| (1,777)  | 1:67:A:PHE:HE1 | 1:70:A:GLU:H    | 4        | 3.11          |
| (1,777)  | 1:67:A:PHE:HE1 | 1:70:A:GLU:H    | 8        | 3.11          |
| (1,858)  | 1:78:A:TRP:HH2 | 1:101:A:TYR:HE1 | 15       | 3.1           |
| (1,650)  | 1:7:A:PHE:HD1  | 1:23:A:LEU:HB2  | 16       | 3.07          |
| (1,1464) | 1:7:A:PHE:HE1  | 1:23:A:LEU:HB3  | 15       | 3.06          |
| (1,944)  | 1:78:A:TRP:HE3 | 1:101:A:TYR:HE1 | 6        | 3.05          |
| (1,651)  | 1:7:A:PHE:HE1  | 1:23:A:LEU:HB2  | 15       | 3.01          |
| (1,651)  | 1:7:A:PHE:HE1  | 1:23:A:LEU:HB2  | 1        | 2.98          |
| (1,660)  | 1:7:A:PHE:HD1  | 1:23:A:LEU:HB3  | 15       | 2.97          |
| (1,660)  | 1:7:A:PHE:HD1  | 1:23:A:LEU:HB3  | 1        | 2.94          |
| (1,1464) | 1:7:A:PHE:HE1  | 1:23:A:LEU:HB3  | 20       | 2.93          |
| (1,944)  | 1:78:A:TRP:HE3 | 1:101:A:TYR:HE1 | 1        | 2.91          |
| (1,1728) | 1:5:A:GLN:HG2  | 1:7:A:PHE:HE1   | 17       | 2.89          |
| (1,944)  | 1:78:A:TRP:HE3 | 1:101:A:TYR:HE1 | 14       | 2.89          |
| (1,1464) | 1:7:A:PHE:HE1  | 1:23:A:LEU:HB3  | 16       | 2.88          |
| (1,1382) | 1:75:A:ILE:HA  | 1:101:A:TYR:HE1 | 5        | 2.85          |
| (1,777)  | 1:67:A:PHE:HE1 | 1:70:A:GLU:H    | 11       | 2.85          |
| (1,1728) | 1:5:A:GLN:HG2  | 1:7:A:PHE:HE1   | 7        | 2.84          |
| (1,944)  | 1:78:A:TRP:HE3 | 1:101:A:TYR:HE1 | 3        | 2.84          |
| (1,660)  | 1:7:A:PHE:HD1  | 1:23:A:LEU:HB3  | 20       | 2.84          |
| (1,660)  | 1:7:A:PHE:HD1  | 1:23:A:LEU:HB3  | 16       | 2.82          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,650)  | 1:7:A:PHE:HD1  | 1:23:A:LEU:HB2  | 15       | 2.82          |
| (1,944)  | 1:78:A:TRP:HE3 | 1:101:A:TYR:HE1 | 10       | 2.81          |
| (1,1729) | 1:5:A:GLN:HG3  | 1:7:A:PHE:HE1   | 1        | 2.79          |
| (1,1729) | 1:5:A:GLN:HG3  | 1:7:A:PHE:HE1   | 11       | 2.79          |
| (1,1728) | 1:5:A:GLN:HG2  | 1:7:A:PHE:HE1   | 15       | 2.77          |
| (1,944)  | 1:78:A:TRP:HE3 | 1:101:A:TYR:HE1 | 18       | 2.77          |
| (1,1729) | 1:5:A:GLN:HG3  | 1:7:A:PHE:HE1   | 18       | 2.76          |
| (1,908)  | 1:67:A:PHE:HD1 | 1:74:A:VAL:H    | 14       | 2.71          |
| (1,1464) | 1:7:A:PHE:HE1  | 1:23:A:LEU:HB3  | 17       | 2.7           |
| (1,858)  | 1:78:A:TRP:HH2 | 1:101:A:TYR:HE1 | 18       | 2.7           |
| (1,1464) | 1:7:A:PHE:HE1  | 1:23:A:LEU:HB3  | 14       | 2.65          |
| (1,908)  | 1:67:A:PHE:HD1 | 1:74:A:VAL:H    | 5        | 2.64          |
| (1,777)  | 1:67:A:PHE:HE1 | 1:70:A:GLU:H    | 7        | 2.63          |
| (1,908)  | 1:67:A:PHE:HD1 | 1:74:A:VAL:H    | 18       | 2.62          |
| (1,660)  | 1:7:A:PHE:HD1  | 1:23:A:LEU:HB3  | 17       | 2.62          |
| (1,650)  | 1:7:A:PHE:HD1  | 1:23:A:LEU:HB2  | 1        | 2.61          |
| (1,858)  | 1:78:A:TRP:HH2 | 1:101:A:TYR:HE1 | 19       | 2.6           |
| (1,777)  | 1:67:A:PHE:HE1 | 1:70:A:GLU:H    | 15       | 2.6           |
| (1,858)  | 1:78:A:TRP:HH2 | 1:101:A:TYR:HE1 | 10       | 2.58          |
| (1,660)  | 1:7:A:PHE:HD1  | 1:23:A:LEU:HB3  | 14       | 2.57          |
| (1,862)  | 1:78:A:TRP:HH2 | 1:101:A:TYR:HD1 | 20       | 2.55          |
| (1,858)  | 1:78:A:TRP:HH2 | 1:101:A:TYR:HE1 | 7        | 2.55          |
| (1,858)  | 1:78:A:TRP:HH2 | 1:101:A:TYR:HE1 | 3        | 2.54          |
| (1,862)  | 1:78:A:TRP:HH2 | 1:101:A:TYR:HD1 | 15       | 2.53          |
| (1,651)  | 1:7:A:PHE:HE1  | 1:23:A:LEU:HB2  | 17       | 2.53          |
| (1,1729) | 1:5:A:GLN:HG3  | 1:7:A:PHE:HE1   | 12       | 2.52          |
| (1,1365) | 1:7:A:PHE:HD1  | 1:23:A:LEU:HA   | 16       | 2.52          |
| (1,879)  | 1:65:A:PHE:HD1 | 1:67:A:PHE:H    | 14       | 2.52          |
| (1,777)  | 1:67:A:PHE:HE1 | 1:70:A:GLU:H    | 5        | 2.5           |
| (1,908)  | 1:67:A:PHE:HD1 | 1:74:A:VAL:H    | 4        | 2.48          |
| (1,862)  | 1:78:A:TRP:HH2 | 1:101:A:TYR:HD1 | 13       | 2.47          |
| (1,827)  | 1:67:A:PHE:HE1 | 1:69:A:LEU:H    | 11       | 2.46          |
| (1,1728) | 1:5:A:GLN:HG2  | 1:7:A:PHE:HE1   | 3        | 2.44          |
| (1,1729) | 1:5:A:GLN:HG3  | 1:7:A:PHE:HE1   | 17       | 2.43          |
| (1,777)  | 1:67:A:PHE:HE1 | 1:70:A:GLU:H    | 16       | 2.43          |
| (1,651)  | 1:7:A:PHE:HE1  | 1:23:A:LEU:HB2  | 20       | 2.43          |
| (1,1365) | 1:7:A:PHE:HD1  | 1:23:A:LEU:HA   | 15       | 2.42          |
| (1,827)  | 1:67:A:PHE:HE1 | 1:69:A:LEU:H    | 15       | 2.42          |
| (1,1729) | 1:5:A:GLN:HG3  | 1:7:A:PHE:HE1   | 19       | 2.4           |
| (1,1728) | 1:5:A:GLN:HG2  | 1:7:A:PHE:HE1   | 1        | 2.4           |
| (1,827)  | 1:67:A:PHE:HE1 | 1:69:A:LEU:H    | 8        | 2.38          |
| (1,827)  | 1:67:A:PHE:HE1 | 1:69:A:LEU:H    | 16       | 2.38          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,1728) | 1:5:A:GLN:HG2  | 1:7:A:PHE:HE1   | 12       | 2.37          |
| (1,1728) | 1:5:A:GLN:HG2  | 1:7:A:PHE:HE1   | 20       | 2.37          |
| (1,908)  | 1:67:A:PHE:HD1 | 1:74:A:VAL:H    | 8        | 2.37          |
| (1,858)  | 1:78:A:TRP:HH2 | 1:101:A:TYR:HE1 | 8        | 2.35          |
| (1,827)  | 1:67:A:PHE:HE1 | 1:69:A:LEU:H    | 12       | 2.35          |
| (1,858)  | 1:78:A:TRP:HH2 | 1:101:A:TYR:HE1 | 17       | 2.34          |
| (1,651)  | 1:7:A:PHE:HE1  | 1:23:A:LEU:HB2  | 13       | 2.34          |
| (1,858)  | 1:78:A:TRP:HH2 | 1:101:A:TYR:HE1 | 4        | 2.33          |
| (1,858)  | 1:78:A:TRP:HH2 | 1:101:A:TYR:HE1 | 14       | 2.33          |
| (1,1382) | 1:75:A:ILE:HA  | 1:101:A:TYR:HE1 | 17       | 2.31          |
| (1,650)  | 1:7:A:PHE:HD1  | 1:23:A:LEU:HB2  | 17       | 2.31          |
| (1,1728) | 1:5:A:GLN:HG2  | 1:7:A:PHE:HE1   | 16       | 2.3           |
| (1,908)  | 1:67:A:PHE:HD1 | 1:74:A:VAL:H    | 19       | 2.3           |
| (1,777)  | 1:67:A:PHE:HE1 | 1:70:A:GLU:H    | 12       | 2.3           |
| (1,908)  | 1:67:A:PHE:HD1 | 1:74:A:VAL:H    | 16       | 2.29          |
| (1,1365) | 1:7:A:PHE:HD1  | 1:23:A:LEU:HA   | 1        | 2.28          |
| (1,827)  | 1:67:A:PHE:HE1 | 1:69:A:LEU:H    | 7        | 2.27          |
| (1,1356) | 1:74:A:VAL:HA  | 1:101:A:TYR:HE1 | 17       | 2.25          |
| (1,651)  | 1:7:A:PHE:HE1  | 1:23:A:LEU:HB2  | 14       | 2.24          |
| (1,858)  | 1:78:A:TRP:HH2 | 1:101:A:TYR:HE1 | 1        | 2.22          |
| (1,858)  | 1:78:A:TRP:HH2 | 1:101:A:TYR:HE1 | 6        | 2.2           |
| (1,650)  | 1:7:A:PHE:HD1  | 1:23:A:LEU:HB2  | 20       | 2.2           |
| (1,1729) | 1:5:A:GLN:HG3  | 1:7:A:PHE:HE1   | 15       | 2.19          |
| (1,1729) | 1:5:A:GLN:HG3  | 1:7:A:PHE:HE1   | 16       | 2.15          |
| (1,660)  | 1:7:A:PHE:HD1  | 1:23:A:LEU:HB3  | 7        | 2.15          |
| (1,1728) | 1:5:A:GLN:HG2  | 1:7:A:PHE:HE1   | 5        | 2.14          |
| (1,1464) | 1:7:A:PHE:HE1  | 1:23:A:LEU:HB3  | 11       | 2.14          |
| (1,926)  | 1:75:A:ILE:H   | 1:101:A:TYR:HE1 | 17       | 2.14          |
| (1,651)  | 1:7:A:PHE:HE1  | 1:23:A:LEU:HB2  | 7        | 2.14          |
| (1,1855) | 1:5:A:GLN:HG2  | 1:7:A:PHE:HD1   | 13       | 2.13          |
| (1,1855) | 1:5:A:GLN:HG3  | 1:7:A:PHE:HD1   | 13       | 2.13          |
| (1,1728) | 1:5:A:GLN:HG2  | 1:7:A:PHE:HE1   | 10       | 2.13          |
| (1,903)  | 1:44:A:TYR:HD1 | 1:65:A:PHE:HD1  | 3        | 2.13          |
| (1,650)  | 1:7:A:PHE:HD1  | 1:23:A:LEU:HB2  | 13       | 2.11          |
| (1,926)  | 1:75:A:ILE:H   | 1:101:A:TYR:HE1 | 5        | 2.1           |
| (1,1356) | 1:74:A:VAL:HA  | 1:101:A:TYR:HE1 | 5        | 2.09          |
| (1,903)  | 1:44:A:TYR:HD1 | 1:65:A:PHE:HD1  | 2        | 2.08          |
| (1,902)  | 1:75:A:ILE:H   | 1:101:A:TYR:HD1 | 13       | 2.08          |
| (1,902)  | 1:75:A:ILE:H   | 1:101:A:TYR:HD1 | 20       | 2.08          |
| (1,827)  | 1:67:A:PHE:HE1 | 1:69:A:LEU:H    | 18       | 2.08          |
| (1,827)  | 1:67:A:PHE:HE1 | 1:69:A:LEU:H    | 19       | 2.07          |
| (1,660)  | 1:7:A:PHE:HD1  | 1:23:A:LEU:HB3  | 11       | 2.07          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,1729) | 1:5:A:GLN:HG3  | 1:7:A:PHE:HE1   | 20       | 2.06          |
| (1,1365) | 1:7:A:PHE:HD1  | 1:23:A:LEU:HA   | 20       | 2.06          |
| (1,879)  | 1:65:A:PHE:HD1 | 1:67:A:PHE:H    | 13       | 2.06          |
| (1,908)  | 1:67:A:PHE:HD1 | 1:74:A:VAL:H    | 11       | 2.05          |
| (1,879)  | 1:65:A:PHE:HD1 | 1:67:A:PHE:H    | 3        | 2.05          |
| (1,650)  | 1:7:A:PHE:HD1  | 1:23:A:LEU:HB2  | 7        | 2.05          |
| (1,650)  | 1:7:A:PHE:HD1  | 1:23:A:LEU:HB2  | 14       | 2.05          |
| (1,643)  | 1:67:A:PHE:HE1 | 1:74:A:VAL:HG21 | 18       | 2.05          |
| (1,643)  | 1:67:A:PHE:HE1 | 1:74:A:VAL:HG22 | 18       | 2.05          |
| (1,643)  | 1:67:A:PHE:HE1 | 1:74:A:VAL:HG23 | 18       | 2.05          |
| (1,643)  | 1:67:A:PHE:HE1 | 1:74:A:VAL:HG21 | 5        | 2.04          |
| (1,643)  | 1:67:A:PHE:HE1 | 1:74:A:VAL:HG22 | 5        | 2.04          |
| (1,643)  | 1:67:A:PHE:HE1 | 1:74:A:VAL:HG23 | 5        | 2.04          |
| (1,1855) | 1:5:A:GLN:HG2  | 1:7:A:PHE:HD1   | 14       | 2.03          |
| (1,1855) | 1:5:A:GLN:HG3  | 1:7:A:PHE:HD1   | 14       | 2.03          |
| (1,1728) | 1:5:A:GLN:HG2  | 1:7:A:PHE:HE1   | 2        | 2.03          |
| (1,827)  | 1:67:A:PHE:HE1 | 1:69:A:LEU:H    | 4        | 2.0           |
| (1,879)  | 1:65:A:PHE:HD1 | 1:67:A:PHE:H    | 7        | 1.99          |
| (1,827)  | 1:67:A:PHE:HE1 | 1:69:A:LEU:H    | 14       | 1.99          |
| (1,651)  | 1:7:A:PHE:HE1  | 1:23:A:LEU:HB2  | 12       | 1.99          |
| (1,903)  | 1:44:A:TYR:HD1 | 1:65:A:PHE:HD1  | 14       | 1.97          |
| (1,867)  | 1:44:A:TYR:HE1 | 1:66:A:LYS:H    | 16       | 1.97          |
| (1,862)  | 1:78:A:TRP:HH2 | 1:101:A:TYR:HD1 | 18       | 1.97          |
| (1,651)  | 1:7:A:PHE:HE1  | 1:23:A:LEU:HB2  | 2        | 1.96          |
| (1,1365) | 1:7:A:PHE:HD1  | 1:23:A:LEU:HA   | 14       | 1.95          |
| (1,908)  | 1:67:A:PHE:HD1 | 1:74:A:VAL:H    | 15       | 1.94          |
| (1,862)  | 1:78:A:TRP:HH2 | 1:101:A:TYR:HD1 | 4        | 1.94          |
| (1,902)  | 1:75:A:ILE:H   | 1:101:A:TYR:HD1 | 15       | 1.93          |
| (1,777)  | 1:67:A:PHE:HE1 | 1:70:A:GLU:H    | 19       | 1.93          |
| (1,869)  | 1:78:A:TRP:HZ3 | 1:101:A:TYR:HD1 | 20       | 1.92          |
| (1,651)  | 1:7:A:PHE:HE1  | 1:23:A:LEU:HB2  | 19       | 1.92          |
| (1,650)  | 1:7:A:PHE:HD1  | 1:23:A:LEU:HB2  | 2        | 1.92          |
| (1,650)  | 1:7:A:PHE:HD1  | 1:23:A:LEU:HB2  | 19       | 1.91          |
| (1,1356) | 1:74:A:VAL:HA  | 1:101:A:TYR:HE1 | 20       | 1.9           |
| (1,902)  | 1:75:A:ILE:H   | 1:101:A:TYR:HD1 | 17       | 1.89          |
| (1,651)  | 1:7:A:PHE:HE1  | 1:23:A:LEU:HB2  | 6        | 1.89          |
| (1,869)  | 1:78:A:TRP:HZ3 | 1:101:A:TYR:HD1 | 15       | 1.88          |
| (1,908)  | 1:67:A:PHE:HD1 | 1:74:A:VAL:H    | 7        | 1.87          |
| (1,643)  | 1:67:A:PHE:HE1 | 1:74:A:VAL:HG21 | 14       | 1.87          |
| (1,643)  | 1:67:A:PHE:HE1 | 1:74:A:VAL:HG22 | 14       | 1.87          |
| (1,643)  | 1:67:A:PHE:HE1 | 1:74:A:VAL:HG23 | 14       | 1.87          |
| (1,650)  | 1:7:A:PHE:HD1  | 1:23:A:LEU:HB2  | 12       | 1.86          |

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| Key      | Atom-1         | Atom-2           | Model ID | Violation (Å) |
|----------|----------------|------------------|----------|---------------|
| (1,1464) | 1:7:A:PHE:HE1  | 1:23:A:LEU:HB3   | 7        | 1.83          |
| (1,1356) | 1:74:A:VAL:HA  | 1:101:A:TYR:HE1  | 13       | 1.83          |
| (1,862)  | 1:78:A:TRP:HH2 | 1:101:A:TYR:HD1  | 19       | 1.81          |
| (1,879)  | 1:65:A:PHE:HD1 | 1:67:A:PHE:H     | 15       | 1.8           |
| (1,827)  | 1:67:A:PHE:HE1 | 1:69:A:LEU:H     | 5        | 1.8           |
| (1,643)  | 1:67:A:PHE:HE1 | 1:74:A:VAL:HG21  | 11       | 1.8           |
| (1,643)  | 1:67:A:PHE:HE1 | 1:74:A:VAL:HG22  | 11       | 1.8           |
| (1,643)  | 1:67:A:PHE:HE1 | 1:74:A:VAL:HG23  | 11       | 1.8           |
| (1,1365) | 1:7:A:PHE:HD1  | 1:23:A:LEU:HA    | 17       | 1.77          |
| (1,903)  | 1:44:A:TYR:HD1 | 1:65:A:PHE:HD1   | 18       | 1.77          |
| (1,869)  | 1:78:A:TRP:HZ3 | 1:101:A:TYR:HD1  | 13       | 1.77          |
| (1,651)  | 1:7:A:PHE:HE1  | 1:23:A:LEU:HB2   | 3        | 1.77          |
| (1,862)  | 1:78:A:TRP:HH2 | 1:101:A:TYR:HD1  | 3        | 1.75          |
| (1,650)  | 1:7:A:PHE:HD1  | 1:23:A:LEU:HB2   | 3        | 1.75          |
| (1,650)  | 1:7:A:PHE:HD1  | 1:23:A:LEU:HB2   | 6        | 1.75          |
| (1,903)  | 1:44:A:TYR:HD1 | 1:65:A:PHE:HD1   | 8        | 1.74          |
| (1,902)  | 1:75:A:ILE:H   | 1:101:A:TYR:HD1  | 5        | 1.73          |
| (1,879)  | 1:65:A:PHE:HD1 | 1:67:A:PHE:H     | 5        | 1.73          |
| (1,879)  | 1:65:A:PHE:HD1 | 1:67:A:PHE:H     | 8        | 1.73          |
| (1,1855) | 1:5:A:GLN:HG2  | 1:7:A:PHE:HD1    | 11       | 1.71          |
| (1,1855) | 1:5:A:GLN:HG3  | 1:7:A:PHE:HD1    | 11       | 1.71          |
| (1,1528) | 1:44:A:TYR:HD1 | 1:120:A:ILE:HG21 | 16       | 1.71          |
| (1,1528) | 1:44:A:TYR:HD1 | 1:120:A:ILE:HG22 | 16       | 1.71          |
| (1,1528) | 1:44:A:TYR:HD1 | 1:120:A:ILE:HG23 | 16       | 1.71          |
| (1,2224) | 1:67:A:PHE:HD1 | 1:69:A:LEU:HD11  | 8        | 1.7           |
| (1,2224) | 1:67:A:PHE:HD1 | 1:69:A:LEU:HD12  | 8        | 1.7           |
| (1,2224) | 1:67:A:PHE:HD1 | 1:69:A:LEU:HD13  | 8        | 1.7           |
| (1,2224) | 1:67:A:PHE:HD1 | 1:69:A:LEU:HD21  | 8        | 1.7           |
| (1,2224) | 1:67:A:PHE:HD1 | 1:69:A:LEU:HD22  | 8        | 1.7           |
| (1,2224) | 1:67:A:PHE:HD1 | 1:69:A:LEU:HD23  | 8        | 1.7           |
| (1,1370) | 1:67:A:PHE:HD1 | 1:69:A:LEU:HA    | 8        | 1.7           |
| (1,902)  | 1:75:A:ILE:H   | 1:101:A:TYR:HD1  | 1        | 1.7           |
| (1,660)  | 1:7:A:PHE:HD1  | 1:23:A:LEU:HB3   | 12       | 1.7           |
| (1,1729) | 1:5:A:GLN:HG3  | 1:7:A:PHE:HE1    | 7        | 1.69          |
| (1,644)  | 1:67:A:PHE:HE1 | 1:82:A:VAL:HB    | 16       | 1.68          |
| (1,869)  | 1:78:A:TRP:HZ3 | 1:101:A:TYR:HD1  | 4        | 1.67          |
| (1,650)  | 1:7:A:PHE:HD1  | 1:23:A:LEU:HB2   | 18       | 1.66          |
| (1,1686) | 1:67:A:PHE:HE1 | 1:69:A:LEU:HA    | 8        | 1.65          |
| (1,921)  | 1:44:A:TYR:HE1 | 1:65:A:PHE:HD1   | 2        | 1.65          |
| (1,908)  | 1:67:A:PHE:HD1 | 1:74:A:VAL:H     | 12       | 1.64          |
| (1,651)  | 1:7:A:PHE:HE1  | 1:23:A:LEU:HB2   | 18       | 1.64          |
| (1,644)  | 1:67:A:PHE:HE1 | 1:82:A:VAL:HB    | 12       | 1.64          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,1729) | 1:5:A:GLN:HG3  | 1:7:A:PHE:HE1   | 2        | 1.63          |
| (1,879)  | 1:65:A:PHE:HD1 | 1:67:A:PHE:H    | 12       | 1.63          |
| (1,2224) | 1:67:A:PHE:HD1 | 1:69:A:LEU:HD11 | 15       | 1.6           |
| (1,2224) | 1:67:A:PHE:HD1 | 1:69:A:LEU:HD12 | 15       | 1.6           |
| (1,2224) | 1:67:A:PHE:HD1 | 1:69:A:LEU:HD13 | 15       | 1.6           |
| (1,2224) | 1:67:A:PHE:HD1 | 1:69:A:LEU:HD21 | 15       | 1.6           |
| (1,2224) | 1:67:A:PHE:HD1 | 1:69:A:LEU:HD22 | 15       | 1.6           |
| (1,2224) | 1:67:A:PHE:HD1 | 1:69:A:LEU:HD23 | 15       | 1.6           |
| (1,1370) | 1:67:A:PHE:HD1 | 1:69:A:LEU:HA   | 18       | 1.6           |
| (1,903)  | 1:44:A:TYR:HD1 | 1:65:A:PHE:HD1  | 12       | 1.6           |
| (1,651)  | 1:7:A:PHE:HE1  | 1:23:A:LEU:HB2  | 11       | 1.6           |
| (1,1686) | 1:67:A:PHE:HE1 | 1:69:A:LEU:HA   | 14       | 1.59          |
| (1,1370) | 1:67:A:PHE:HD1 | 1:69:A:LEU:HA   | 14       | 1.59          |
| (1,903)  | 1:44:A:TYR:HD1 | 1:65:A:PHE:HD1  | 6        | 1.59          |
| (1,903)  | 1:44:A:TYR:HD1 | 1:65:A:PHE:HD1  | 7        | 1.59          |
| (1,644)  | 1:67:A:PHE:HE1 | 1:82:A:VAL:HB   | 15       | 1.59          |
| (1,643)  | 1:67:A:PHE:HE1 | 1:74:A:VAL:HG21 | 15       | 1.59          |
| (1,643)  | 1:67:A:PHE:HE1 | 1:74:A:VAL:HG22 | 15       | 1.59          |
| (1,643)  | 1:67:A:PHE:HE1 | 1:74:A:VAL:HG23 | 15       | 1.59          |
| (1,862)  | 1:78:A:TRP:HH2 | 1:101:A:TYR:HD1 | 1        | 1.56          |
| (1,643)  | 1:67:A:PHE:HE1 | 1:74:A:VAL:HG21 | 8        | 1.56          |
| (1,643)  | 1:67:A:PHE:HE1 | 1:74:A:VAL:HG22 | 8        | 1.56          |
| (1,643)  | 1:67:A:PHE:HE1 | 1:74:A:VAL:HG23 | 8        | 1.56          |
| (1,1370) | 1:67:A:PHE:HD1 | 1:69:A:LEU:HA   | 15       | 1.54          |
| (1,1686) | 1:67:A:PHE:HE1 | 1:69:A:LEU:HA   | 11       | 1.53          |
| (1,903)  | 1:44:A:TYR:HD1 | 1:65:A:PHE:HD1  | 15       | 1.53          |
| (1,879)  | 1:65:A:PHE:HD1 | 1:67:A:PHE:H    | 10       | 1.53          |
| (1,858)  | 1:78:A:TRP:HH2 | 1:101:A:TYR:HE1 | 5        | 1.53          |
| (1,650)  | 1:7:A:PHE:HD1  | 1:23:A:LEU:HB2  | 4        | 1.53          |
| (1,1686) | 1:67:A:PHE:HE1 | 1:69:A:LEU:HA   | 18       | 1.52          |
| (1,1370) | 1:67:A:PHE:HD1 | 1:69:A:LEU:HA   | 4        | 1.52          |
| (1,879)  | 1:65:A:PHE:HD1 | 1:67:A:PHE:H    | 6        | 1.52          |
| (1,862)  | 1:78:A:TRP:HH2 | 1:101:A:TYR:HD1 | 7        | 1.52          |
| (1,1464) | 1:7:A:PHE:HE1  | 1:23:A:LEU:HB3  | 12       | 1.51          |
| (1,687)  | 1:67:A:PHE:HD1 | 1:82:A:VAL:HG21 | 16       | 1.51          |
| (1,687)  | 1:67:A:PHE:HD1 | 1:82:A:VAL:HG22 | 16       | 1.51          |
| (1,687)  | 1:67:A:PHE:HD1 | 1:82:A:VAL:HG23 | 16       | 1.51          |
| (1,2224) | 1:67:A:PHE:HD1 | 1:69:A:LEU:HD11 | 16       | 1.5           |
| (1,2224) | 1:67:A:PHE:HD1 | 1:69:A:LEU:HD12 | 16       | 1.5           |
| (1,2224) | 1:67:A:PHE:HD1 | 1:69:A:LEU:HD13 | 16       | 1.5           |
| (1,2224) | 1:67:A:PHE:HD1 | 1:69:A:LEU:HD21 | 16       | 1.5           |
| (1,2224) | 1:67:A:PHE:HD1 | 1:69:A:LEU:HD22 | 16       | 1.5           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2224) | 1:67:A:PHE:HD1  | 1:69:A:LEU:HD23 | 16       | 1.5           |
| (1,1686) | 1:67:A:PHE:HE1  | 1:69:A:LEU:HA   | 15       | 1.5           |
| (1,1370) | 1:67:A:PHE:HD1  | 1:69:A:LEU:HA   | 11       | 1.5           |
| (1,879)  | 1:65:A:PHE:HD1  | 1:67:A:PHE:H    | 11       | 1.5           |
| (1,660)  | 1:7:A:PHE:HD1   | 1:23:A:LEU:HB3  | 6        | 1.5           |
| (1,660)  | 1:7:A:PHE:HD1   | 1:23:A:LEU:HB3  | 19       | 1.5           |
| (1,1370) | 1:67:A:PHE:HD1  | 1:69:A:LEU:HA   | 7        | 1.49          |
| (1,921)  | 1:44:A:TYR:HE1  | 1:65:A:PHE:HD1  | 18       | 1.49          |
| (1,879)  | 1:65:A:PHE:HD1  | 1:67:A:PHE:H    | 18       | 1.49          |
| (1,1518) | 1:40:A:VAL:HG21 | 1:67:A:PHE:HE1  | 11       | 1.48          |
| (1,1518) | 1:40:A:VAL:HG22 | 1:67:A:PHE:HE1  | 11       | 1.48          |
| (1,1518) | 1:40:A:VAL:HG23 | 1:67:A:PHE:HE1  | 11       | 1.48          |
| (1,643)  | 1:67:A:PHE:HE1  | 1:74:A:VAL:HG21 | 16       | 1.48          |
| (1,643)  | 1:67:A:PHE:HE1  | 1:74:A:VAL:HG22 | 16       | 1.48          |
| (1,643)  | 1:67:A:PHE:HE1  | 1:74:A:VAL:HG23 | 16       | 1.48          |
| (1,1686) | 1:67:A:PHE:HE1  | 1:69:A:LEU:HA   | 4        | 1.46          |
| (1,1370) | 1:67:A:PHE:HD1  | 1:69:A:LEU:HA   | 12       | 1.46          |
| (1,921)  | 1:44:A:TYR:HE1  | 1:65:A:PHE:HD1  | 19       | 1.46          |
| (1,903)  | 1:44:A:TYR:HD1  | 1:65:A:PHE:HD1  | 5        | 1.46          |
| (1,903)  | 1:44:A:TYR:HD1  | 1:65:A:PHE:HD1  | 13       | 1.45          |
| (1,903)  | 1:44:A:TYR:HD1  | 1:65:A:PHE:HD1  | 19       | 1.44          |
| (1,1370) | 1:67:A:PHE:HD1  | 1:69:A:LEU:HA   | 16       | 1.43          |
| (1,903)  | 1:44:A:TYR:HD1  | 1:65:A:PHE:HD1  | 10       | 1.43          |
| (1,1686) | 1:67:A:PHE:HE1  | 1:69:A:LEU:HA   | 7        | 1.42          |
| (1,921)  | 1:44:A:TYR:HE1  | 1:65:A:PHE:HD1  | 8        | 1.42          |
| (1,643)  | 1:67:A:PHE:HE1  | 1:74:A:VAL:HG21 | 4        | 1.42          |
| (1,643)  | 1:67:A:PHE:HE1  | 1:74:A:VAL:HG22 | 4        | 1.42          |
| (1,643)  | 1:67:A:PHE:HE1  | 1:74:A:VAL:HG23 | 4        | 1.42          |
| (1,1356) | 1:74:A:VAL:HA   | 1:101:A:TYR:HE1 | 1        | 1.41          |
| (1,926)  | 1:75:A:ILE:H    | 1:101:A:TYR:HE1 | 20       | 1.41          |
| (1,921)  | 1:44:A:TYR:HE1  | 1:65:A:PHE:HD1  | 3        | 1.41          |
| (1,869)  | 1:78:A:TRP:HZ3  | 1:101:A:TYR:HD1 | 19       | 1.41          |
| (1,660)  | 1:7:A:PHE:HD1   | 1:23:A:LEU:HB3  | 2        | 1.41          |
| (1,644)  | 1:67:A:PHE:HE1  | 1:82:A:VAL:HB   | 11       | 1.41          |
| (1,2224) | 1:67:A:PHE:HD1  | 1:69:A:LEU:HD11 | 7        | 1.4           |
| (1,2224) | 1:67:A:PHE:HD1  | 1:69:A:LEU:HD12 | 7        | 1.4           |
| (1,2224) | 1:67:A:PHE:HD1  | 1:69:A:LEU:HD13 | 7        | 1.4           |
| (1,2224) | 1:67:A:PHE:HD1  | 1:69:A:LEU:HD21 | 7        | 1.4           |
| (1,2224) | 1:67:A:PHE:HD1  | 1:69:A:LEU:HD22 | 7        | 1.4           |
| (1,2224) | 1:67:A:PHE:HD1  | 1:69:A:LEU:HD23 | 7        | 1.4           |
| (1,1356) | 1:74:A:VAL:HA   | 1:101:A:TYR:HE1 | 10       | 1.4           |
| (1,903)  | 1:44:A:TYR:HD1  | 1:65:A:PHE:HD1  | 17       | 1.4           |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,1686) | 1:67:A:PHE:HE1 | 1:69:A:LEU:HA   | 16       | 1.39          |
| (1,902)  | 1:75:A:ILE:H   | 1:101:A:TYR:HD1 | 6        | 1.39          |
| (1,1464) | 1:7:A:PHE:HE1  | 1:23:A:LEU:HB3  | 6        | 1.38          |
| (1,926)  | 1:75:A:ILE:H   | 1:101:A:TYR:HE1 | 13       | 1.37          |
| (1,2224) | 1:67:A:PHE:HD1 | 1:69:A:LEU:HD11 | 18       | 1.36          |
| (1,2224) | 1:67:A:PHE:HD1 | 1:69:A:LEU:HD12 | 18       | 1.36          |
| (1,2224) | 1:67:A:PHE:HD1 | 1:69:A:LEU:HD13 | 18       | 1.36          |
| (1,2224) | 1:67:A:PHE:HD1 | 1:69:A:LEU:HD21 | 18       | 1.36          |
| (1,2224) | 1:67:A:PHE:HD1 | 1:69:A:LEU:HD22 | 18       | 1.36          |
| (1,2224) | 1:67:A:PHE:HD1 | 1:69:A:LEU:HD23 | 18       | 1.36          |
| (1,1464) | 1:7:A:PHE:HE1  | 1:23:A:LEU:HB3  | 13       | 1.36          |
| (1,1356) | 1:74:A:VAL:HA  | 1:101:A:TYR:HE1 | 6        | 1.36          |
| (1,902)  | 1:75:A:ILE:H   | 1:101:A:TYR:HD1 | 4        | 1.36          |
| (1,921)  | 1:44:A:TYR:HE1 | 1:65:A:PHE:HD1  | 14       | 1.35          |
| (1,879)  | 1:65:A:PHE:HD1 | 1:67:A:PHE:H    | 17       | 1.35          |
| (1,862)  | 1:78:A:TRP:HH2 | 1:101:A:TYR:HD1 | 6        | 1.35          |
| (1,660)  | 1:7:A:PHE:HD1  | 1:23:A:LEU:HB3  | 3        | 1.35          |
| (1,660)  | 1:7:A:PHE:HD1  | 1:23:A:LEU:HB3  | 13       | 1.35          |
| (1,660)  | 1:7:A:PHE:HD1  | 1:23:A:LEU:HB3  | 18       | 1.35          |
| (1,651)  | 1:7:A:PHE:HE1  | 1:23:A:LEU:HB2  | 4        | 1.35          |
| (1,650)  | 1:7:A:PHE:HD1  | 1:23:A:LEU:HB2  | 11       | 1.35          |
| (1,644)  | 1:67:A:PHE:HE1 | 1:82:A:VAL:HB   | 8        | 1.35          |
| (1,903)  | 1:44:A:TYR:HD1 | 1:65:A:PHE:HD1  | 9        | 1.34          |
| (1,902)  | 1:75:A:ILE:H   | 1:101:A:TYR:HD1 | 7        | 1.34          |
| (1,879)  | 1:65:A:PHE:HD1 | 1:67:A:PHE:H    | 2        | 1.34          |
| (1,862)  | 1:78:A:TRP:HH2 | 1:101:A:TYR:HD1 | 14       | 1.34          |
| (1,1852) | 1:5:A:GLN:HB2  | 1:7:A:PHE:HE1   | 6        | 1.33          |
| (1,1852) | 1:5:A:GLN:HB3  | 1:7:A:PHE:HE1   | 6        | 1.33          |
| (1,862)  | 1:78:A:TRP:HH2 | 1:101:A:TYR:HD1 | 10       | 1.33          |
| (1,2224) | 1:67:A:PHE:HD1 | 1:69:A:LEU:HD11 | 14       | 1.32          |
| (1,2224) | 1:67:A:PHE:HD1 | 1:69:A:LEU:HD12 | 14       | 1.32          |
| (1,2224) | 1:67:A:PHE:HD1 | 1:69:A:LEU:HD13 | 14       | 1.32          |
| (1,2224) | 1:67:A:PHE:HD1 | 1:69:A:LEU:HD21 | 14       | 1.32          |
| (1,2224) | 1:67:A:PHE:HD1 | 1:69:A:LEU:HD22 | 14       | 1.32          |
| (1,2224) | 1:67:A:PHE:HD1 | 1:69:A:LEU:HD23 | 14       | 1.32          |
| (1,1686) | 1:67:A:PHE:HE1 | 1:69:A:LEU:HA   | 12       | 1.32          |
| (1,927)  | 1:44:A:TYR:HE1 | 1:65:A:PHE:HE1  | 19       | 1.32          |
| (1,903)  | 1:44:A:TYR:HD1 | 1:65:A:PHE:HD1  | 11       | 1.32          |
| (1,1855) | 1:5:A:GLN:HG2  | 1:7:A:PHE:HD1   | 10       | 1.31          |
| (1,1855) | 1:5:A:GLN:HG3  | 1:7:A:PHE:HD1   | 10       | 1.31          |
| (1,921)  | 1:44:A:TYR:HE1 | 1:65:A:PHE:HD1  | 6        | 1.31          |
| (1,688)  | 1:67:A:PHE:HD1 | 1:82:A:VAL:HG11 | 12       | 1.31          |

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| Key      | Atom-1         | Atom-2           | Model ID | Violation (Å) |
|----------|----------------|------------------|----------|---------------|
| (1,688)  | 1:67:A:PHE:HD1 | 1:82:A:VAL:HG12  | 12       | 1.31          |
| (1,688)  | 1:67:A:PHE:HD1 | 1:82:A:VAL:HG13  | 12       | 1.31          |
| (1,1356) | 1:74:A:VAL:HA  | 1:101:A:TYR:HE1  | 15       | 1.3           |
| (1,2228) | 1:67:A:PHE:HE1 | 1:71:A:GLN:HE21  | 15       | 1.28          |
| (1,2228) | 1:67:A:PHE:HE1 | 1:71:A:GLN:HE22  | 15       | 1.28          |
| (1,2224) | 1:67:A:PHE:HD1 | 1:69:A:LEU:HD11  | 4        | 1.28          |
| (1,2224) | 1:67:A:PHE:HD1 | 1:69:A:LEU:HD12  | 4        | 1.28          |
| (1,2224) | 1:67:A:PHE:HD1 | 1:69:A:LEU:HD13  | 4        | 1.28          |
| (1,2224) | 1:67:A:PHE:HD1 | 1:69:A:LEU:HD21  | 4        | 1.28          |
| (1,2224) | 1:67:A:PHE:HD1 | 1:69:A:LEU:HD22  | 4        | 1.28          |
| (1,2224) | 1:67:A:PHE:HD1 | 1:69:A:LEU:HD23  | 4        | 1.28          |
| (1,1855) | 1:5:A:GLN:HG2  | 1:7:A:PHE:HD1    | 1        | 1.28          |
| (1,1855) | 1:5:A:GLN:HG3  | 1:7:A:PHE:HD1    | 1        | 1.28          |
| (1,1365) | 1:7:A:PHE:HD1  | 1:23:A:LEU:HA    | 11       | 1.28          |
| (1,926)  | 1:75:A:ILE:H   | 1:101:A:TYR:HE1  | 15       | 1.28          |
| (1,921)  | 1:44:A:TYR:HE1 | 1:65:A:PHE:HD1   | 9        | 1.27          |
| (1,879)  | 1:65:A:PHE:HD1 | 1:67:A:PHE:H     | 9        | 1.27          |
| (1,1356) | 1:74:A:VAL:HA  | 1:101:A:TYR:HE1  | 7        | 1.25          |
| (1,660)  | 1:7:A:PHE:HD1  | 1:23:A:LEU:HB3   | 4        | 1.25          |
| (1,1382) | 1:75:A:ILE:HA  | 1:101:A:TYR:HE1  | 15       | 1.23          |
| (1,1205) | 1:26:A:GLY:HA2 | 1:86:A:ARG:HB2   | 11       | 1.23          |
| (1,651)  | 1:7:A:PHE:HE1  | 1:23:A:LEU:HB2   | 5        | 1.23          |
| (1,1177) | 1:95:A:ILE:HB  | 1:100:A:GLY:HA2  | 13       | 1.22          |
| (1,2227) | 1:67:A:PHE:HE1 | 1:69:A:LEU:HD11  | 8        | 1.21          |
| (1,2227) | 1:67:A:PHE:HE1 | 1:69:A:LEU:HD12  | 8        | 1.21          |
| (1,2227) | 1:67:A:PHE:HE1 | 1:69:A:LEU:HD13  | 8        | 1.21          |
| (1,2227) | 1:67:A:PHE:HE1 | 1:69:A:LEU:HD21  | 8        | 1.21          |
| (1,2227) | 1:67:A:PHE:HE1 | 1:69:A:LEU:HD22  | 8        | 1.21          |
| (1,2227) | 1:67:A:PHE:HE1 | 1:69:A:LEU:HD23  | 8        | 1.21          |
| (1,1855) | 1:5:A:GLN:HG2  | 1:7:A:PHE:HD1    | 15       | 1.21          |
| (1,1855) | 1:5:A:GLN:HG3  | 1:7:A:PHE:HD1    | 15       | 1.21          |
| (1,1728) | 1:5:A:GLN:HG2  | 1:7:A:PHE:HE1    | 18       | 1.21          |
| (1,869)  | 1:78:A:TRP:HZ3 | 1:101:A:TYR:HD1  | 7        | 1.21          |
| (1,687)  | 1:67:A:PHE:HD1 | 1:82:A:VAL:HG21  | 8        | 1.21          |
| (1,687)  | 1:67:A:PHE:HD1 | 1:82:A:VAL:HG22  | 8        | 1.21          |
| (1,687)  | 1:67:A:PHE:HD1 | 1:82:A:VAL:HG23  | 8        | 1.21          |
| (1,687)  | 1:67:A:PHE:HD1 | 1:82:A:VAL:HG21  | 18       | 1.21          |
| (1,687)  | 1:67:A:PHE:HD1 | 1:82:A:VAL:HG22  | 18       | 1.21          |
| (1,687)  | 1:67:A:PHE:HD1 | 1:82:A:VAL:HG23  | 18       | 1.21          |
| (1,1528) | 1:44:A:TYR:HD1 | 1:120:A:ILE:HG21 | 20       | 1.2           |
| (1,1528) | 1:44:A:TYR:HD1 | 1:120:A:ILE:HG22 | 20       | 1.2           |
| (1,1528) | 1:44:A:TYR:HD1 | 1:120:A:ILE:HG23 | 20       | 1.2           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1464) | 1:7:A:PHE:HE1   | 1:23:A:LEU:HB3  | 3        | 1.2           |
| (1,927)  | 1:44:A:TYR:HE1  | 1:65:A:PHE:HE1  | 9        | 1.2           |
| (1,923)  | 1:44:A:TYR:HE1  | 1:66:A:LYS:HA   | 16       | 1.2           |
| (1,921)  | 1:44:A:TYR:HE1  | 1:65:A:PHE:HD1  | 5        | 1.2           |
| (1,921)  | 1:44:A:TYR:HE1  | 1:65:A:PHE:HD1  | 15       | 1.19          |
| (1,1356) | 1:74:A:VAL:HA   | 1:101:A:TYR:HE1 | 3        | 1.18          |
| (1,1370) | 1:67:A:PHE:HD1  | 1:69:A:LEU:HA   | 19       | 1.17          |
| (1,1365) | 1:7:A:PHE:HD1   | 1:23:A:LEU:HA   | 13       | 1.17          |
| (1,902)  | 1:75:A:ILE:H    | 1:101:A:TYR:HD1 | 3        | 1.17          |
| (1,1370) | 1:67:A:PHE:HD1  | 1:69:A:LEU:HA   | 5        | 1.16          |
| (1,687)  | 1:67:A:PHE:HD1  | 1:82:A:VAL:HG21 | 14       | 1.16          |
| (1,687)  | 1:67:A:PHE:HD1  | 1:82:A:VAL:HG22 | 14       | 1.16          |
| (1,687)  | 1:67:A:PHE:HD1  | 1:82:A:VAL:HG23 | 14       | 1.16          |
| (1,1382) | 1:75:A:ILE:HA   | 1:101:A:TYR:HE1 | 7        | 1.15          |
| (1,902)  | 1:75:A:ILE:H    | 1:101:A:TYR:HD1 | 18       | 1.15          |
| (1,902)  | 1:75:A:ILE:H    | 1:101:A:TYR:HD1 | 19       | 1.15          |
| (1,1855) | 1:5:A:GLN:HG2   | 1:7:A:PHE:HD1   | 20       | 1.14          |
| (1,1855) | 1:5:A:GLN:HG3   | 1:7:A:PHE:HD1   | 20       | 1.14          |
| (1,1156) | 1:26:A:GLY:HA2  | 1:89:A:GLU:HB3  | 14       | 1.14          |
| (1,1518) | 1:40:A:VAL:HG21 | 1:67:A:PHE:HE1  | 19       | 1.13          |
| (1,1518) | 1:40:A:VAL:HG22 | 1:67:A:PHE:HE1  | 19       | 1.13          |
| (1,1518) | 1:40:A:VAL:HG23 | 1:67:A:PHE:HE1  | 19       | 1.13          |
| (1,259)  | 1:27:A:ASP:H    | 1:88:A:ASN:HB3  | 14       | 1.13          |
| (1,699)  | 1:75:A:ILE:HG13 | 1:101:A:TYR:HD1 | 17       | 1.12          |
| (1,651)  | 1:7:A:PHE:HE1   | 1:23:A:LEU:HB2  | 8        | 1.12          |
| (1,1855) | 1:5:A:GLN:HG2   | 1:7:A:PHE:HD1   | 17       | 1.11          |
| (1,1855) | 1:5:A:GLN:HG3   | 1:7:A:PHE:HD1   | 17       | 1.11          |
| (1,869)  | 1:78:A:TRP:HZ3  | 1:101:A:TYR:HD1 | 18       | 1.11          |
| (1,717)  | 1:58:A:SER:HA   | 1:59:A:PHE:HD1  | 4        | 1.11          |
| (1,921)  | 1:44:A:TYR:HE1  | 1:65:A:PHE:HD1  | 7        | 1.1           |
| (1,921)  | 1:44:A:TYR:HE1  | 1:65:A:PHE:HD1  | 13       | 1.1           |
| (1,869)  | 1:78:A:TRP:HZ3  | 1:101:A:TYR:HD1 | 3        | 1.1           |
| (1,869)  | 1:78:A:TRP:HZ3  | 1:101:A:TYR:HD1 | 17       | 1.1           |
| (1,650)  | 1:7:A:PHE:HD1   | 1:23:A:LEU:HB2  | 5        | 1.1           |
| (1,2227) | 1:67:A:PHE:HE1  | 1:69:A:LEU:HD11 | 15       | 1.09          |
| (1,2227) | 1:67:A:PHE:HE1  | 1:69:A:LEU:HD12 | 15       | 1.09          |
| (1,2227) | 1:67:A:PHE:HE1  | 1:69:A:LEU:HD13 | 15       | 1.09          |
| (1,2227) | 1:67:A:PHE:HE1  | 1:69:A:LEU:HD21 | 15       | 1.09          |
| (1,2227) | 1:67:A:PHE:HE1  | 1:69:A:LEU:HD22 | 15       | 1.09          |
| (1,2227) | 1:67:A:PHE:HE1  | 1:69:A:LEU:HD23 | 15       | 1.09          |
| (1,2224) | 1:67:A:PHE:HD1  | 1:69:A:LEU:HD11 | 19       | 1.09          |
| (1,2224) | 1:67:A:PHE:HD1  | 1:69:A:LEU:HD12 | 19       | 1.09          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,2224) | 1:67:A:PHE:HD1 | 1:69:A:LEU:HD13 | 19       | 1.09          |
| (1,2224) | 1:67:A:PHE:HD1 | 1:69:A:LEU:HD21 | 19       | 1.09          |
| (1,2224) | 1:67:A:PHE:HD1 | 1:69:A:LEU:HD22 | 19       | 1.09          |
| (1,2224) | 1:67:A:PHE:HD1 | 1:69:A:LEU:HD23 | 19       | 1.09          |
| (1,1729) | 1:5:A:GLN:HG3  | 1:7:A:PHE:HE1   | 5        | 1.09          |
| (1,1464) | 1:7:A:PHE:HE1  | 1:23:A:LEU:HB3  | 2        | 1.09          |
| (1,921)  | 1:44:A:TYR:HE1 | 1:65:A:PHE:HD1  | 17       | 1.09          |
| (1,862)  | 1:78:A:TRP:HH2 | 1:101:A:TYR:HD1 | 8        | 1.09          |
| (1,1686) | 1:67:A:PHE:HE1 | 1:69:A:LEU:HA   | 5        | 1.08          |
| (1,1356) | 1:74:A:VAL:HA  | 1:101:A:TYR:HE1 | 8        | 1.08          |
| (1,927)  | 1:44:A:TYR:HE1 | 1:65:A:PHE:HE1  | 2        | 1.08          |
| (1,921)  | 1:44:A:TYR:HE1 | 1:65:A:PHE:HD1  | 10       | 1.08          |
| (1,902)  | 1:75:A:ILE:H   | 1:101:A:TYR:HD1 | 10       | 1.08          |
| (1,1365) | 1:7:A:PHE:HD1  | 1:23:A:LEU:HA   | 7        | 1.07          |
| (1,1356) | 1:74:A:VAL:HA  | 1:101:A:TYR:HE1 | 14       | 1.07          |
| (1,926)  | 1:75:A:ILE:H   | 1:101:A:TYR:HE1 | 1        | 1.07          |
| (1,902)  | 1:75:A:ILE:H   | 1:101:A:TYR:HD1 | 14       | 1.07          |
| (1,643)  | 1:67:A:PHE:HE1 | 1:74:A:VAL:HG21 | 12       | 1.07          |
| (1,643)  | 1:67:A:PHE:HE1 | 1:74:A:VAL:HG22 | 12       | 1.07          |
| (1,643)  | 1:67:A:PHE:HE1 | 1:74:A:VAL:HG23 | 12       | 1.07          |
| (1,2224) | 1:67:A:PHE:HD1 | 1:69:A:LEU:HD11 | 12       | 1.06          |
| (1,2224) | 1:67:A:PHE:HD1 | 1:69:A:LEU:HD12 | 12       | 1.06          |
| (1,2224) | 1:67:A:PHE:HD1 | 1:69:A:LEU:HD13 | 12       | 1.06          |
| (1,2224) | 1:67:A:PHE:HD1 | 1:69:A:LEU:HD21 | 12       | 1.06          |
| (1,2224) | 1:67:A:PHE:HD1 | 1:69:A:LEU:HD22 | 12       | 1.06          |
| (1,2224) | 1:67:A:PHE:HD1 | 1:69:A:LEU:HD23 | 12       | 1.06          |
| (1,1575) | 1:44:A:TYR:HD1 | 1:66:A:LYS:HA   | 16       | 1.06          |
| (1,1382) | 1:75:A:ILE:HA  | 1:101:A:TYR:HE1 | 20       | 1.06          |
| (1,2224) | 1:67:A:PHE:HD1 | 1:69:A:LEU:HD11 | 11       | 1.05          |
| (1,2224) | 1:67:A:PHE:HD1 | 1:69:A:LEU:HD12 | 11       | 1.05          |
| (1,2224) | 1:67:A:PHE:HD1 | 1:69:A:LEU:HD13 | 11       | 1.05          |
| (1,2224) | 1:67:A:PHE:HD1 | 1:69:A:LEU:HD21 | 11       | 1.05          |
| (1,2224) | 1:67:A:PHE:HD1 | 1:69:A:LEU:HD22 | 11       | 1.05          |
| (1,2224) | 1:67:A:PHE:HD1 | 1:69:A:LEU:HD23 | 11       | 1.05          |
| (1,1870) | 1:7:A:PHE:HD1  | 1:23:A:LEU:HD11 | 7        | 1.05          |
| (1,1870) | 1:7:A:PHE:HD1  | 1:23:A:LEU:HD12 | 7        | 1.05          |
| (1,1870) | 1:7:A:PHE:HD1  | 1:23:A:LEU:HD13 | 7        | 1.05          |
| (1,1870) | 1:7:A:PHE:HD1  | 1:23:A:LEU:HD21 | 7        | 1.05          |
| (1,1870) | 1:7:A:PHE:HD1  | 1:23:A:LEU:HD22 | 7        | 1.05          |
| (1,1870) | 1:7:A:PHE:HD1  | 1:23:A:LEU:HD23 | 7        | 1.05          |
| (1,869)  | 1:78:A:TRP:HZ3 | 1:101:A:TYR:HD1 | 1        | 1.05          |
| (1,717)  | 1:58:A:SER:HA  | 1:59:A:PHE:HD1  | 16       | 1.05          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1855) | 1:5:A:GLN:HG2   | 1:7:A:PHE:HD1   | 12       | 1.04          |
| (1,1855) | 1:5:A:GLN:HG3   | 1:7:A:PHE:HD1   | 12       | 1.04          |
| (1,1518) | 1:40:A:VAL:HG21 | 1:67:A:PHE:HE1  | 12       | 1.04          |
| (1,1518) | 1:40:A:VAL:HG22 | 1:67:A:PHE:HE1  | 12       | 1.04          |
| (1,1518) | 1:40:A:VAL:HG23 | 1:67:A:PHE:HE1  | 12       | 1.04          |
| (1,1464) | 1:7:A:PHE:HE1   | 1:23:A:LEU:HB3  | 19       | 1.04          |
| (1,1356) | 1:74:A:VAL:HA   | 1:101:A:TYR:HE1 | 18       | 1.04          |
| (1,689)  | 1:76:A:LYS:HD3  | 1:99:A:TYR:HE1  | 8        | 1.04          |
| (1,1518) | 1:40:A:VAL:HG21 | 1:67:A:PHE:HE1  | 18       | 1.03          |
| (1,1518) | 1:40:A:VAL:HG22 | 1:67:A:PHE:HE1  | 18       | 1.03          |
| (1,1518) | 1:40:A:VAL:HG23 | 1:67:A:PHE:HE1  | 18       | 1.03          |
| (1,927)  | 1:44:A:TYR:HE1  | 1:65:A:PHE:HE1  | 14       | 1.03          |
| (1,869)  | 1:78:A:TRP:HZ3  | 1:101:A:TYR:HD1 | 6        | 1.03          |
| (1,1382) | 1:75:A:ILE:HA   | 1:101:A:TYR:HE1 | 13       | 1.02          |
| (1,643)  | 1:67:A:PHE:HE1  | 1:74:A:VAL:HG21 | 19       | 1.02          |
| (1,643)  | 1:67:A:PHE:HE1  | 1:74:A:VAL:HG22 | 19       | 1.02          |
| (1,643)  | 1:67:A:PHE:HE1  | 1:74:A:VAL:HG23 | 19       | 1.02          |
| (1,927)  | 1:44:A:TYR:HE1  | 1:65:A:PHE:HE1  | 3        | 1.01          |
| (1,927)  | 1:44:A:TYR:HE1  | 1:65:A:PHE:HE1  | 16       | 1.01          |
| (1,717)  | 1:58:A:SER:HA   | 1:59:A:PHE:HD1  | 15       | 1.01          |
| (1,2227) | 1:67:A:PHE:HE1  | 1:69:A:LEU:HD11 | 16       | 1.0           |
| (1,2227) | 1:67:A:PHE:HE1  | 1:69:A:LEU:HD12 | 16       | 1.0           |
| (1,2227) | 1:67:A:PHE:HE1  | 1:69:A:LEU:HD13 | 16       | 1.0           |
| (1,2227) | 1:67:A:PHE:HE1  | 1:69:A:LEU:HD21 | 16       | 1.0           |
| (1,2227) | 1:67:A:PHE:HE1  | 1:69:A:LEU:HD22 | 16       | 1.0           |
| (1,2227) | 1:67:A:PHE:HE1  | 1:69:A:LEU:HD23 | 16       | 1.0           |
| (1,1177) | 1:95:A:ILE:HB   | 1:100:A:GLY:HA2 | 9        | 1.0           |
| (1,1686) | 1:67:A:PHE:HE1  | 1:69:A:LEU:HA   | 19       | 0.99          |
| (1,643)  | 1:67:A:PHE:HE1  | 1:74:A:VAL:HG21 | 7        | 0.99          |
| (1,643)  | 1:67:A:PHE:HE1  | 1:74:A:VAL:HG22 | 7        | 0.99          |
| (1,643)  | 1:67:A:PHE:HE1  | 1:74:A:VAL:HG23 | 7        | 0.99          |
| (1,1467) | 1:9:A:LYS:HG3   | 1:21:A:THR:H    | 19       | 0.98          |
| (1,650)  | 1:7:A:PHE:HD1   | 1:23:A:LEU:HB2  | 8        | 0.98          |
| (1,2224) | 1:67:A:PHE:HD1  | 1:69:A:LEU:HD11 | 5        | 0.97          |
| (1,2224) | 1:67:A:PHE:HD1  | 1:69:A:LEU:HD12 | 5        | 0.97          |
| (1,2224) | 1:67:A:PHE:HD1  | 1:69:A:LEU:HD13 | 5        | 0.97          |
| (1,2224) | 1:67:A:PHE:HD1  | 1:69:A:LEU:HD21 | 5        | 0.97          |
| (1,2224) | 1:67:A:PHE:HD1  | 1:69:A:LEU:HD22 | 5        | 0.97          |
| (1,2224) | 1:67:A:PHE:HD1  | 1:69:A:LEU:HD23 | 5        | 0.97          |
| (1,1518) | 1:40:A:VAL:HG21 | 1:67:A:PHE:HE1  | 8        | 0.97          |
| (1,1518) | 1:40:A:VAL:HG22 | 1:67:A:PHE:HE1  | 8        | 0.97          |
| (1,1518) | 1:40:A:VAL:HG23 | 1:67:A:PHE:HE1  | 8        | 0.97          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,921)  | 1:44:A:TYR:HE1  | 1:65:A:PHE:HD1  | 12       | 0.97          |
| (1,608)  | 1:78:A:TRP:HH2  | 1:95:A:ILE:HG13 | 8        | 0.97          |
| (1,687)  | 1:67:A:PHE:HD1  | 1:82:A:VAL:HG21 | 7        | 0.96          |
| (1,687)  | 1:67:A:PHE:HD1  | 1:82:A:VAL:HG22 | 7        | 0.96          |
| (1,687)  | 1:67:A:PHE:HD1  | 1:82:A:VAL:HG23 | 7        | 0.96          |
| (1,1518) | 1:40:A:VAL:HG21 | 1:67:A:PHE:HE1  | 7        | 0.95          |
| (1,1518) | 1:40:A:VAL:HG22 | 1:67:A:PHE:HE1  | 7        | 0.95          |
| (1,1518) | 1:40:A:VAL:HG23 | 1:67:A:PHE:HE1  | 7        | 0.95          |
| (1,902)  | 1:75:A:ILE:H    | 1:101:A:TYR:HD1 | 8        | 0.95          |
| (1,2228) | 1:67:A:PHE:HE1  | 1:71:A:GLN:HE21 | 19       | 0.94          |
| (1,2228) | 1:67:A:PHE:HE1  | 1:71:A:GLN:HE22 | 19       | 0.94          |
| (1,1356) | 1:74:A:VAL:HA   | 1:101:A:TYR:HE1 | 19       | 0.94          |
| (1,699)  | 1:75:A:ILE:HG13 | 1:101:A:TYR:HD1 | 5        | 0.94          |
| (1,1518) | 1:40:A:VAL:HG21 | 1:67:A:PHE:HE1  | 15       | 0.93          |
| (1,1518) | 1:40:A:VAL:HG22 | 1:67:A:PHE:HE1  | 15       | 0.93          |
| (1,1518) | 1:40:A:VAL:HG23 | 1:67:A:PHE:HE1  | 15       | 0.93          |
| (1,717)  | 1:58:A:SER:HA   | 1:59:A:PHE:HD1  | 12       | 0.92          |
| (1,644)  | 1:67:A:PHE:HE1  | 1:82:A:VAL:HB   | 7        | 0.92          |
| (1,1382) | 1:75:A:ILE:HA   | 1:101:A:TYR:HE1 | 8        | 0.91          |
| (1,644)  | 1:67:A:PHE:HE1  | 1:82:A:VAL:HB   | 18       | 0.91          |
| (1,2228) | 1:67:A:PHE:HE1  | 1:71:A:GLN:HE21 | 4        | 0.9           |
| (1,2228) | 1:67:A:PHE:HE1  | 1:71:A:GLN:HE22 | 4        | 0.9           |
| (1,1855) | 1:5:A:GLN:HG2   | 1:7:A:PHE:HD1   | 19       | 0.9           |
| (1,1855) | 1:5:A:GLN:HG3   | 1:7:A:PHE:HD1   | 19       | 0.9           |
| (1,862)  | 1:78:A:TRP:HH2  | 1:101:A:TYR:HD1 | 17       | 0.9           |
| (1,2228) | 1:67:A:PHE:HE1  | 1:71:A:GLN:HE21 | 14       | 0.89          |
| (1,2228) | 1:67:A:PHE:HE1  | 1:71:A:GLN:HE22 | 14       | 0.89          |
| (1,927)  | 1:44:A:TYR:HE1  | 1:65:A:PHE:HE1  | 17       | 0.89          |
| (1,921)  | 1:44:A:TYR:HE1  | 1:65:A:PHE:HD1  | 11       | 0.89          |
| (1,2228) | 1:67:A:PHE:HE1  | 1:71:A:GLN:HE21 | 5        | 0.88          |
| (1,2228) | 1:67:A:PHE:HE1  | 1:71:A:GLN:HE22 | 5        | 0.88          |
| (1,2228) | 1:67:A:PHE:HE1  | 1:71:A:GLN:HE21 | 7        | 0.88          |
| (1,2228) | 1:67:A:PHE:HE1  | 1:71:A:GLN:HE22 | 7        | 0.88          |
| (1,869)  | 1:78:A:TRP:HZ3  | 1:101:A:TYR:HD1 | 14       | 0.88          |
| (1,1464) | 1:7:A:PHE:HE1   | 1:23:A:LEU:HB3  | 18       | 0.87          |
| (1,926)  | 1:75:A:ILE:H    | 1:101:A:TYR:HE1 | 6        | 0.87          |
| (1,926)  | 1:75:A:ILE:H    | 1:101:A:TYR:HE1 | 7        | 0.87          |
| (1,2227) | 1:67:A:PHE:HE1  | 1:69:A:LEU:HD11 | 7        | 0.86          |
| (1,2227) | 1:67:A:PHE:HE1  | 1:69:A:LEU:HD12 | 7        | 0.86          |
| (1,2227) | 1:67:A:PHE:HE1  | 1:69:A:LEU:HD13 | 7        | 0.86          |
| (1,2227) | 1:67:A:PHE:HE1  | 1:69:A:LEU:HD21 | 7        | 0.86          |
| (1,2227) | 1:67:A:PHE:HE1  | 1:69:A:LEU:HD22 | 7        | 0.86          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2227) | 1:67:A:PHE:HE1  | 1:69:A:LEU:HD23 | 7        | 0.86          |
| (1,1855) | 1:5:A:GLN:HG2   | 1:7:A:PHE:HD1   | 16       | 0.86          |
| (1,1855) | 1:5:A:GLN:HG3   | 1:7:A:PHE:HD1   | 16       | 0.86          |
| (1,1177) | 1:95:A:ILE:HB   | 1:100:A:GLY:HA2 | 18       | 0.86          |
| (1,1729) | 1:5:A:GLN:HG3   | 1:7:A:PHE:HE1   | 3        | 0.85          |
| (1,1177) | 1:95:A:ILE:HB   | 1:100:A:GLY:HA2 | 19       | 0.85          |
| (1,1382) | 1:75:A:ILE:HA   | 1:101:A:TYR:HE1 | 1        | 0.84          |
| (1,921)  | 1:44:A:TYR:HE1  | 1:65:A:PHE:HD1  | 16       | 0.84          |
| (1,927)  | 1:44:A:TYR:HE1  | 1:65:A:PHE:HE1  | 20       | 0.83          |
| (1,644)  | 1:67:A:PHE:HE1  | 1:82:A:VAL:HB   | 14       | 0.83          |
| (1,1518) | 1:40:A:VAL:HG21 | 1:67:A:PHE:HE1  | 14       | 0.82          |
| (1,1518) | 1:40:A:VAL:HG22 | 1:67:A:PHE:HE1  | 14       | 0.82          |
| (1,1518) | 1:40:A:VAL:HG23 | 1:67:A:PHE:HE1  | 14       | 0.82          |
| (1,926)  | 1:75:A:ILE:H    | 1:101:A:TYR:HE1 | 8        | 0.82          |
| (1,687)  | 1:67:A:PHE:HD1  | 1:82:A:VAL:HG21 | 4        | 0.82          |
| (1,687)  | 1:67:A:PHE:HD1  | 1:82:A:VAL:HG22 | 4        | 0.82          |
| (1,687)  | 1:67:A:PHE:HD1  | 1:82:A:VAL:HG23 | 4        | 0.82          |
| (1,2228) | 1:67:A:PHE:HE1  | 1:71:A:GLN:HE21 | 18       | 0.81          |
| (1,2228) | 1:67:A:PHE:HE1  | 1:71:A:GLN:HE22 | 18       | 0.81          |
| (1,2226) | 1:67:A:PHE:HD1  | 1:73:A:GLU:HB2  | 4        | 0.81          |
| (1,2226) | 1:67:A:PHE:HD1  | 1:73:A:GLU:HB3  | 4        | 0.81          |
| (1,1855) | 1:5:A:GLN:HG2   | 1:7:A:PHE:HD1   | 2        | 0.81          |
| (1,1855) | 1:5:A:GLN:HG3   | 1:7:A:PHE:HD1   | 2        | 0.81          |
| (1,651)  | 1:7:A:PHE:HE1   | 1:23:A:LEU:HB2  | 10       | 0.81          |
| (1,644)  | 1:67:A:PHE:HE1  | 1:82:A:VAL:HB   | 19       | 0.81          |
| (1,687)  | 1:67:A:PHE:HD1  | 1:82:A:VAL:HG21 | 15       | 0.8           |
| (1,687)  | 1:67:A:PHE:HD1  | 1:82:A:VAL:HG22 | 15       | 0.8           |
| (1,687)  | 1:67:A:PHE:HD1  | 1:82:A:VAL:HG23 | 15       | 0.8           |
| (1,1870) | 1:7:A:PHE:HD1   | 1:23:A:LEU:HD11 | 2        | 0.79          |
| (1,1870) | 1:7:A:PHE:HD1   | 1:23:A:LEU:HD12 | 2        | 0.79          |
| (1,1870) | 1:7:A:PHE:HD1   | 1:23:A:LEU:HD13 | 2        | 0.79          |
| (1,1870) | 1:7:A:PHE:HD1   | 1:23:A:LEU:HD21 | 2        | 0.79          |
| (1,1870) | 1:7:A:PHE:HD1   | 1:23:A:LEU:HD22 | 2        | 0.79          |
| (1,1870) | 1:7:A:PHE:HD1   | 1:23:A:LEU:HD23 | 2        | 0.79          |
| (1,1855) | 1:5:A:GLN:HG2   | 1:7:A:PHE:HD1   | 18       | 0.79          |
| (1,1855) | 1:5:A:GLN:HG3   | 1:7:A:PHE:HD1   | 18       | 0.79          |
| (1,1728) | 1:5:A:GLN:HG2   | 1:7:A:PHE:HE1   | 19       | 0.79          |
| (1,717)  | 1:58:A:SER:HA   | 1:59:A:PHE:HD1  | 7        | 0.79          |
| (1,1518) | 1:40:A:VAL:HG21 | 1:67:A:PHE:HE1  | 4        | 0.78          |
| (1,1518) | 1:40:A:VAL:HG22 | 1:67:A:PHE:HE1  | 4        | 0.78          |
| (1,1518) | 1:40:A:VAL:HG23 | 1:67:A:PHE:HE1  | 4        | 0.78          |
| (1,878)  | 1:7:A:PHE:H     | 1:7:A:PHE:HE1   | 6        | 0.78          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,869)  | 1:78:A:TRP:HZ3 | 1:101:A:TYR:HD1 | 8        | 0.78          |
| (1,2227) | 1:67:A:PHE:HE1 | 1:69:A:LEU:HD11 | 14       | 0.77          |
| (1,2227) | 1:67:A:PHE:HE1 | 1:69:A:LEU:HD12 | 14       | 0.77          |
| (1,2227) | 1:67:A:PHE:HE1 | 1:69:A:LEU:HD13 | 14       | 0.77          |
| (1,2227) | 1:67:A:PHE:HE1 | 1:69:A:LEU:HD21 | 14       | 0.77          |
| (1,2227) | 1:67:A:PHE:HE1 | 1:69:A:LEU:HD22 | 14       | 0.77          |
| (1,2227) | 1:67:A:PHE:HE1 | 1:69:A:LEU:HD23 | 14       | 0.77          |
| (1,2227) | 1:67:A:PHE:HE1 | 1:69:A:LEU:HD11 | 18       | 0.77          |
| (1,2227) | 1:67:A:PHE:HE1 | 1:69:A:LEU:HD12 | 18       | 0.77          |
| (1,2227) | 1:67:A:PHE:HE1 | 1:69:A:LEU:HD13 | 18       | 0.77          |
| (1,2227) | 1:67:A:PHE:HE1 | 1:69:A:LEU:HD21 | 18       | 0.77          |
| (1,2227) | 1:67:A:PHE:HE1 | 1:69:A:LEU:HD22 | 18       | 0.77          |
| (1,2227) | 1:67:A:PHE:HE1 | 1:69:A:LEU:HD23 | 18       | 0.77          |
| (1,1177) | 1:95:A:ILE:HB  | 1:100:A:GLY:HA2 | 16       | 0.77          |
| (1,867)  | 1:44:A:TYR:HE1 | 1:66:A:LYS:H    | 20       | 0.77          |
| (1,688)  | 1:67:A:PHE:HD1 | 1:82:A:VAL:HG11 | 11       | 0.77          |
| (1,688)  | 1:67:A:PHE:HD1 | 1:82:A:VAL:HG12 | 11       | 0.77          |
| (1,688)  | 1:67:A:PHE:HD1 | 1:82:A:VAL:HG13 | 11       | 0.77          |
| (1,650)  | 1:7:A:PHE:HD1  | 1:23:A:LEU:HB2  | 10       | 0.77          |
| (1,2226) | 1:67:A:PHE:HD1 | 1:73:A:GLU:HB2  | 5        | 0.76          |
| (1,2226) | 1:67:A:PHE:HD1 | 1:73:A:GLU:HB3  | 5        | 0.76          |
| (1,926)  | 1:75:A:ILE:H   | 1:101:A:TYR:HE1 | 10       | 0.76          |
| (1,717)  | 1:58:A:SER:HA  | 1:59:A:PHE:HD1  | 6        | 0.76          |
| (1,927)  | 1:44:A:TYR:HE1 | 1:65:A:PHE:HE1  | 13       | 0.75          |
| (1,1851) | 1:5:A:GLN:HB2  | 1:7:A:PHE:HD1   | 6        | 0.74          |
| (1,1851) | 1:5:A:GLN:HB3  | 1:7:A:PHE:HD1   | 6        | 0.74          |
| (1,1177) | 1:95:A:ILE:HB  | 1:100:A:GLY:HA2 | 3        | 0.74          |
| (1,1177) | 1:95:A:ILE:HB  | 1:100:A:GLY:HA2 | 20       | 0.74          |
| (1,903)  | 1:44:A:TYR:HD1 | 1:65:A:PHE:HD1  | 20       | 0.74          |
| (1,687)  | 1:67:A:PHE:HD1 | 1:82:A:VAL:HG21 | 19       | 0.73          |
| (1,687)  | 1:67:A:PHE:HD1 | 1:82:A:VAL:HG22 | 19       | 0.73          |
| (1,687)  | 1:67:A:PHE:HD1 | 1:82:A:VAL:HG23 | 19       | 0.73          |
| (1,2228) | 1:67:A:PHE:HE1 | 1:71:A:GLN:HE21 | 12       | 0.71          |
| (1,2228) | 1:67:A:PHE:HE1 | 1:71:A:GLN:HE22 | 12       | 0.71          |
| (1,2227) | 1:67:A:PHE:HE1 | 1:69:A:LEU:HD11 | 4        | 0.7           |
| (1,2227) | 1:67:A:PHE:HE1 | 1:69:A:LEU:HD12 | 4        | 0.7           |
| (1,2227) | 1:67:A:PHE:HE1 | 1:69:A:LEU:HD13 | 4        | 0.7           |
| (1,2227) | 1:67:A:PHE:HE1 | 1:69:A:LEU:HD21 | 4        | 0.7           |
| (1,2227) | 1:67:A:PHE:HE1 | 1:69:A:LEU:HD22 | 4        | 0.7           |
| (1,2227) | 1:67:A:PHE:HE1 | 1:69:A:LEU:HD23 | 4        | 0.7           |
| (1,878)  | 1:7:A:PHE:H    | 1:7:A:PHE:HE1   | 3        | 0.7           |
| (1,1870) | 1:7:A:PHE:HD1  | 1:23:A:LEU:HD11 | 12       | 0.69          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1870) | 1:7:A:PHE:HD1   | 1:23:A:LEU:HD12 | 12       | 0.69          |
| (1,1870) | 1:7:A:PHE:HD1   | 1:23:A:LEU:HD13 | 12       | 0.69          |
| (1,1870) | 1:7:A:PHE:HD1   | 1:23:A:LEU:HD21 | 12       | 0.69          |
| (1,1870) | 1:7:A:PHE:HD1   | 1:23:A:LEU:HD22 | 12       | 0.69          |
| (1,1870) | 1:7:A:PHE:HD1   | 1:23:A:LEU:HD23 | 12       | 0.69          |
| (1,1177) | 1:95:A:ILE:HB   | 1:100:A:GLY:HA2 | 11       | 0.69          |
| (1,921)  | 1:44:A:TYR:HE1  | 1:65:A:PHE:HD1  | 20       | 0.69          |
| (1,1575) | 1:44:A:TYR:HD1  | 1:66:A:LYS:HA   | 20       | 0.68          |
| (1,1205) | 1:26:A:GLY:HA2  | 1:86:A:ARG:HB2  | 2        | 0.68          |
| (1,927)  | 1:44:A:TYR:HE1  | 1:65:A:PHE:HE1  | 7        | 0.68          |
| (1,872)  | 1:65:A:PHE:HE1  | 1:66:A:LYS:H    | 19       | 0.68          |
| (1,1518) | 1:40:A:VAL:HG21 | 1:67:A:PHE:HE1  | 16       | 0.67          |
| (1,1518) | 1:40:A:VAL:HG22 | 1:67:A:PHE:HE1  | 16       | 0.67          |
| (1,1518) | 1:40:A:VAL:HG23 | 1:67:A:PHE:HE1  | 16       | 0.67          |
| (1,927)  | 1:44:A:TYR:HE1  | 1:65:A:PHE:HE1  | 6        | 0.67          |
| (1,1852) | 1:5:A:GLN:HB2   | 1:7:A:PHE:HE1   | 14       | 0.65          |
| (1,1852) | 1:5:A:GLN:HB3   | 1:7:A:PHE:HE1   | 14       | 0.65          |
| (1,1728) | 1:5:A:GLN:HG2   | 1:7:A:PHE:HE1   | 6        | 0.65          |
| (1,1365) | 1:7:A:PHE:HD1   | 1:23:A:LEU:HA   | 12       | 0.65          |
| (1,1177) | 1:95:A:ILE:HB   | 1:100:A:GLY:HA2 | 15       | 0.65          |
| (1,869)  | 1:78:A:TRP:HZ3  | 1:101:A:TYR:HD1 | 10       | 0.65          |
| (1,2228) | 1:67:A:PHE:HE1  | 1:71:A:GLN:HE21 | 16       | 0.64          |
| (1,2228) | 1:67:A:PHE:HE1  | 1:71:A:GLN:HE22 | 16       | 0.64          |
| (1,927)  | 1:44:A:TYR:HE1  | 1:65:A:PHE:HE1  | 15       | 0.63          |
| (1,878)  | 1:7:A:PHE:H     | 1:7:A:PHE:HE1   | 10       | 0.63          |
| (1,645)  | 1:7:A:PHE:HD1   | 1:23:A:LEU:HD21 | 2        | 0.63          |
| (1,645)  | 1:7:A:PHE:HD1   | 1:23:A:LEU:HD22 | 2        | 0.63          |
| (1,645)  | 1:7:A:PHE:HD1   | 1:23:A:LEU:HD23 | 2        | 0.63          |
| (1,1365) | 1:7:A:PHE:HD1   | 1:23:A:LEU:HA   | 2        | 0.62          |
| (1,927)  | 1:44:A:TYR:HE1  | 1:65:A:PHE:HE1  | 5        | 0.62          |
| (1,2226) | 1:67:A:PHE:HD1  | 1:73:A:GLU:HB2  | 15       | 0.61          |
| (1,2226) | 1:67:A:PHE:HD1  | 1:73:A:GLU:HB3  | 15       | 0.61          |
| (1,927)  | 1:44:A:TYR:HE1  | 1:65:A:PHE:HE1  | 8        | 0.61          |
| (1,687)  | 1:67:A:PHE:HD1  | 1:82:A:VAL:HG21 | 5        | 0.6           |
| (1,687)  | 1:67:A:PHE:HD1  | 1:82:A:VAL:HG22 | 5        | 0.6           |
| (1,687)  | 1:67:A:PHE:HD1  | 1:82:A:VAL:HG23 | 5        | 0.6           |
| (1,573)  | 1:87:A:LYS:HG2  | 1:88:A:ASN:HD21 | 8        | 0.6           |
| (1,1852) | 1:5:A:GLN:HB2   | 1:7:A:PHE:HE1   | 5        | 0.59          |
| (1,1852) | 1:5:A:GLN:HB3   | 1:7:A:PHE:HE1   | 5        | 0.59          |
| (1,1537) | 1:75:A:ILE:HG21 | 1:101:A:TYR:HE1 | 5        | 0.59          |
| (1,1537) | 1:75:A:ILE:HG22 | 1:101:A:TYR:HE1 | 5        | 0.59          |
| (1,1537) | 1:75:A:ILE:HG23 | 1:101:A:TYR:HE1 | 5        | 0.59          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1574) | 1:43:A:HIS:HA   | 1:44:A:TYR:HD1  | 16       | 0.58          |
| (1,1464) | 1:7:A:PHE:HE1   | 1:23:A:LEU:HB3  | 4        | 0.58          |
| (1,1219) | 1:46:A:GLY:HA3  | 1:117:A:LEU:HB3 | 9        | 0.58          |
| (1,2068) | 1:36:A:LYS:HD3  | 1:70:A:GLU:HG2  | 18       | 0.56          |
| (1,2068) | 1:36:A:LYS:HD3  | 1:70:A:GLU:HG3  | 18       | 0.56          |
| (1,1531) | 1:67:A:PHE:HD1  | 1:74:A:VAL:HG21 | 5        | 0.56          |
| (1,1531) | 1:67:A:PHE:HD1  | 1:74:A:VAL:HG22 | 5        | 0.56          |
| (1,1531) | 1:67:A:PHE:HD1  | 1:74:A:VAL:HG23 | 5        | 0.56          |
| (1,699)  | 1:75:A:ILE:HG13 | 1:101:A:TYR:HD1 | 15       | 0.56          |
| (1,2043) | 1:35:A:LYS:HB3  | 1:38:A:ASN:HB2  | 4        | 0.55          |
| (1,2043) | 1:35:A:LYS:HB3  | 1:38:A:ASN:HB3  | 4        | 0.55          |
| (1,927)  | 1:44:A:TYR:HE1  | 1:65:A:PHE:HE1  | 12       | 0.55          |
| (1,1729) | 1:5:A:GLN:HG3   | 1:7:A:PHE:HE1   | 8        | 0.54          |
| (1,1356) | 1:74:A:VAL:HA   | 1:101:A:TYR:HE1 | 4        | 0.54          |
| (1,927)  | 1:44:A:TYR:HE1  | 1:65:A:PHE:HE1  | 10       | 0.54          |
| (1,927)  | 1:44:A:TYR:HE1  | 1:65:A:PHE:HE1  | 11       | 0.54          |
| (1,1870) | 1:7:A:PHE:HD1   | 1:23:A:LEU:HD11 | 18       | 0.53          |
| (1,1870) | 1:7:A:PHE:HD1   | 1:23:A:LEU:HD12 | 18       | 0.53          |
| (1,1870) | 1:7:A:PHE:HD1   | 1:23:A:LEU:HD13 | 18       | 0.53          |
| (1,1870) | 1:7:A:PHE:HD1   | 1:23:A:LEU:HD21 | 18       | 0.53          |
| (1,1870) | 1:7:A:PHE:HD1   | 1:23:A:LEU:HD22 | 18       | 0.53          |
| (1,1870) | 1:7:A:PHE:HD1   | 1:23:A:LEU:HD23 | 18       | 0.53          |
| (1,1855) | 1:5:A:GLN:HG2   | 1:7:A:PHE:HD1   | 5        | 0.53          |
| (1,1855) | 1:5:A:GLN:HG3   | 1:7:A:PHE:HD1   | 5        | 0.53          |
| (1,1852) | 1:5:A:GLN:HB2   | 1:7:A:PHE:HE1   | 2        | 0.53          |
| (1,1852) | 1:5:A:GLN:HB3   | 1:7:A:PHE:HE1   | 2        | 0.53          |
| (1,1852) | 1:5:A:GLN:HB2   | 1:7:A:PHE:HE1   | 12       | 0.53          |
| (1,1852) | 1:5:A:GLN:HB3   | 1:7:A:PHE:HE1   | 12       | 0.53          |
| (1,1382) | 1:75:A:ILE:HA   | 1:101:A:TYR:HE1 | 10       | 0.53          |
| (1,660)  | 1:7:A:PHE:HD1   | 1:23:A:LEU:HB3  | 5        | 0.53          |
| (1,1574) | 1:43:A:HIS:HA   | 1:44:A:TYR:HD1  | 20       | 0.52          |
| (1,1382) | 1:75:A:ILE:HA   | 1:101:A:TYR:HE1 | 6        | 0.52          |
| (1,926)  | 1:75:A:ILE:H    | 1:101:A:TYR:HE1 | 19       | 0.52          |
| (1,2228) | 1:67:A:PHE:HE1  | 1:71:A:GLN:HE21 | 8        | 0.51          |
| (1,2228) | 1:67:A:PHE:HE1  | 1:71:A:GLN:HE22 | 8        | 0.51          |
| (1,2227) | 1:67:A:PHE:HE1  | 1:69:A:LEU:HD11 | 11       | 0.51          |
| (1,2227) | 1:67:A:PHE:HE1  | 1:69:A:LEU:HD12 | 11       | 0.51          |
| (1,2227) | 1:67:A:PHE:HE1  | 1:69:A:LEU:HD13 | 11       | 0.51          |
| (1,2227) | 1:67:A:PHE:HE1  | 1:69:A:LEU:HD21 | 11       | 0.51          |
| (1,2227) | 1:67:A:PHE:HE1  | 1:69:A:LEU:HD22 | 11       | 0.51          |
| (1,2227) | 1:67:A:PHE:HE1  | 1:69:A:LEU:HD23 | 11       | 0.51          |
| (1,1156) | 1:26:A:GLY:HA2  | 1:89:A:GLU:HB3  | 11       | 0.51          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,321)  | 1:44:A:TYR:HD1  | 1:65:A:PHE:H    | 16       | 0.51          |
| (1,2226) | 1:67:A:PHE:HD1  | 1:73:A:GLU:HB2  | 18       | 0.5           |
| (1,2226) | 1:67:A:PHE:HD1  | 1:73:A:GLU:HB3  | 18       | 0.5           |
| (1,1531) | 1:67:A:PHE:HD1  | 1:74:A:VAL:HG21 | 18       | 0.5           |
| (1,1531) | 1:67:A:PHE:HD1  | 1:74:A:VAL:HG22 | 18       | 0.5           |
| (1,1531) | 1:67:A:PHE:HD1  | 1:74:A:VAL:HG23 | 18       | 0.5           |
| (1,254)  | 1:27:A:ASP:H    | 1:28:A:GLU:HB3  | 6        | 0.5           |
| (1,1855) | 1:5:A:GLN:HG2   | 1:7:A:PHE:HD1   | 3        | 0.49          |
| (1,1855) | 1:5:A:GLN:HG3   | 1:7:A:PHE:HD1   | 3        | 0.49          |
| (1,1537) | 1:75:A:ILE:HG21 | 1:101:A:TYR:HE1 | 17       | 0.49          |
| (1,1537) | 1:75:A:ILE:HG22 | 1:101:A:TYR:HE1 | 17       | 0.49          |
| (1,1537) | 1:75:A:ILE:HG23 | 1:101:A:TYR:HE1 | 17       | 0.49          |
| (1,1382) | 1:75:A:ILE:HA   | 1:101:A:TYR:HE1 | 14       | 0.49          |
| (1,926)  | 1:75:A:ILE:H    | 1:101:A:TYR:HE1 | 14       | 0.49          |
| (1,926)  | 1:75:A:ILE:H    | 1:101:A:TYR:HE1 | 18       | 0.49          |
| (1,1382) | 1:75:A:ILE:HA   | 1:101:A:TYR:HE1 | 19       | 0.48          |
| (1,1365) | 1:7:A:PHE:HD1   | 1:23:A:LEU:HA   | 19       | 0.48          |
| (1,926)  | 1:75:A:ILE:H    | 1:101:A:TYR:HE1 | 4        | 0.47          |
| (1,1390) | 1:26:A:GLY:HA2  | 1:89:A:GLU:H    | 14       | 0.46          |
| (1,1365) | 1:7:A:PHE:HD1   | 1:23:A:LEU:HA   | 6        | 0.46          |
| (1,1155) | 1:26:A:GLY:HA2  | 1:86:A:ARG:HB3  | 14       | 0.46          |
| (1,926)  | 1:75:A:ILE:H    | 1:101:A:TYR:HE1 | 3        | 0.46          |
| (1,923)  | 1:44:A:TYR:HE1  | 1:66:A:LYS:HA   | 20       | 0.46          |
| (1,608)  | 1:78:A:TRP:HH2  | 1:95:A:ILE:HG13 | 17       | 0.46          |
| (1,2228) | 1:67:A:PHE:HE1  | 1:71:A:GLN:HE21 | 11       | 0.45          |
| (1,2228) | 1:67:A:PHE:HE1  | 1:71:A:GLN:HE22 | 11       | 0.45          |
| (1,2227) | 1:67:A:PHE:HE1  | 1:69:A:LEU:HD11 | 19       | 0.44          |
| (1,2227) | 1:67:A:PHE:HE1  | 1:69:A:LEU:HD12 | 19       | 0.44          |
| (1,2227) | 1:67:A:PHE:HE1  | 1:69:A:LEU:HD13 | 19       | 0.44          |
| (1,2227) | 1:67:A:PHE:HE1  | 1:69:A:LEU:HD21 | 19       | 0.44          |
| (1,2227) | 1:67:A:PHE:HE1  | 1:69:A:LEU:HD22 | 19       | 0.44          |
| (1,2227) | 1:67:A:PHE:HE1  | 1:69:A:LEU:HD23 | 19       | 0.44          |
| (1,699)  | 1:75:A:ILE:HG13 | 1:101:A:TYR:HD1 | 20       | 0.44          |
| (1,644)  | 1:67:A:PHE:HE1  | 1:82:A:VAL:HB   | 4        | 0.44          |
| (1,927)  | 1:44:A:TYR:HE1  | 1:65:A:PHE:HE1  | 18       | 0.43          |
| (1,2227) | 1:67:A:PHE:HE1  | 1:69:A:LEU:HD11 | 12       | 0.41          |
| (1,2227) | 1:67:A:PHE:HE1  | 1:69:A:LEU:HD12 | 12       | 0.41          |
| (1,2227) | 1:67:A:PHE:HE1  | 1:69:A:LEU:HD13 | 12       | 0.41          |
| (1,2227) | 1:67:A:PHE:HE1  | 1:69:A:LEU:HD21 | 12       | 0.41          |
| (1,2227) | 1:67:A:PHE:HE1  | 1:69:A:LEU:HD22 | 12       | 0.41          |
| (1,2227) | 1:67:A:PHE:HE1  | 1:69:A:LEU:HD23 | 12       | 0.41          |
| (1,521)  | 1:75:A:ILE:HG12 | 1:76:A:LYS:H    | 15       | 0.41          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1219) | 1:46:A:GLY:HA3  | 1:117:A:LEU:HB3 | 16       | 0.4           |
| (1,1852) | 1:5:A:GLN:HB2   | 1:7:A:PHE:HE1   | 19       | 0.39          |
| (1,1852) | 1:5:A:GLN:HB3   | 1:7:A:PHE:HE1   | 19       | 0.39          |
| (1,1467) | 1:9:A:LYS:HG3   | 1:21:A:THR:H    | 4        | 0.39          |
| (1,1365) | 1:7:A:PHE:HD1   | 1:23:A:LEU:HA   | 18       | 0.39          |
| (1,2226) | 1:67:A:PHE:HD1  | 1:73:A:GLU:HB2  | 14       | 0.38          |
| (1,2226) | 1:67:A:PHE:HD1  | 1:73:A:GLU:HB3  | 14       | 0.38          |
| (1,878)  | 1:7:A:PHE:H     | 1:7:A:PHE:HE1   | 4        | 0.37          |
| (1,1467) | 1:9:A:LYS:HG3   | 1:21:A:THR:H    | 5        | 0.36          |
| (1,1365) | 1:7:A:PHE:HD1   | 1:23:A:LEU:HA   | 3        | 0.36          |
| (1,903)  | 1:44:A:TYR:HD1  | 1:65:A:PHE:HD1  | 16       | 0.36          |
| (1,656)  | 1:7:A:PHE:HD1   | 1:23:A:LEU:HD11 | 7        | 0.36          |
| (1,656)  | 1:7:A:PHE:HD1   | 1:23:A:LEU:HD12 | 7        | 0.36          |
| (1,656)  | 1:7:A:PHE:HD1   | 1:23:A:LEU:HD13 | 7        | 0.36          |
| (1,1156) | 1:26:A:GLY:HA2  | 1:89:A:GLU:HB3  | 2        | 0.35          |
| (1,521)  | 1:75:A:ILE:HG12 | 1:76:A:LYS:H    | 20       | 0.35          |
| (1,254)  | 1:27:A:ASP:H    | 1:28:A:GLU:HB3  | 9        | 0.35          |
| (1,2227) | 1:67:A:PHE:HE1  | 1:69:A:LEU:HD11 | 5        | 0.33          |
| (1,2227) | 1:67:A:PHE:HE1  | 1:69:A:LEU:HD12 | 5        | 0.33          |
| (1,2227) | 1:67:A:PHE:HE1  | 1:69:A:LEU:HD13 | 5        | 0.33          |
| (1,2227) | 1:67:A:PHE:HE1  | 1:69:A:LEU:HD21 | 5        | 0.33          |
| (1,2227) | 1:67:A:PHE:HE1  | 1:69:A:LEU:HD22 | 5        | 0.33          |
| (1,2227) | 1:67:A:PHE:HE1  | 1:69:A:LEU:HD23 | 5        | 0.33          |
| (1,1531) | 1:67:A:PHE:HD1  | 1:74:A:VAL:HG21 | 11       | 0.33          |
| (1,1531) | 1:67:A:PHE:HD1  | 1:74:A:VAL:HG22 | 11       | 0.33          |
| (1,1531) | 1:67:A:PHE:HD1  | 1:74:A:VAL:HG23 | 11       | 0.33          |
| (1,878)  | 1:7:A:PHE:H     | 1:7:A:PHE:HE1   | 19       | 0.33          |
| (1,1503) | 1:42:A:VAL:HG11 | 1:67:A:PHE:HD1  | 15       | 0.32          |
| (1,1503) | 1:42:A:VAL:HG12 | 1:67:A:PHE:HD1  | 15       | 0.32          |
| (1,1503) | 1:42:A:VAL:HG13 | 1:67:A:PHE:HD1  | 15       | 0.32          |
| (1,1382) | 1:75:A:ILE:HA   | 1:101:A:TYR:HE1 | 4        | 0.32          |
| (1,2211) | 1:62:A:ASN:HD21 | 1:64:A:PRO:HD2  | 4        | 0.31          |
| (1,2211) | 1:62:A:ASN:HD21 | 1:64:A:PRO:HD3  | 4        | 0.31          |
| (1,1503) | 1:42:A:VAL:HG11 | 1:67:A:PHE:HD1  | 16       | 0.31          |
| (1,1503) | 1:42:A:VAL:HG12 | 1:67:A:PHE:HD1  | 16       | 0.31          |
| (1,1503) | 1:42:A:VAL:HG13 | 1:67:A:PHE:HD1  | 16       | 0.31          |
| (1,1177) | 1:95:A:ILE:HB   | 1:100:A:GLY:HA2 | 1        | 0.31          |
| (1,989)  | 1:12:A:LEU:HA   | 1:17:A:GLY:HA2  | 15       | 0.31          |
| (1,259)  | 1:27:A:ASP:H    | 1:88:A:ASN:HB3  | 16       | 0.31          |
| (1,1179) | 1:76:A:LYS:HD3  | 1:99:A:TYR:HA   | 8        | 0.3           |
| (1,521)  | 1:75:A:ILE:HG12 | 1:76:A:LYS:H    | 1        | 0.3           |
| (1,1219) | 1:46:A:GLY:HA3  | 1:117:A:LEU:HB3 | 5        | 0.29          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1219) | 1:46:A:GLY:HA3  | 1:117:A:LEU:HB3  | 20       | 0.29          |
| (1,660)  | 1:7:A:PHE:HD1   | 1:23:A:LEU:HB3   | 8        | 0.29          |
| (1,644)  | 1:67:A:PHE:HE1  | 1:82:A:VAL:HB    | 5        | 0.29          |
| (1,368)  | 1:93:A:VAL:H    | 1:118:A:PHE:HB3  | 13       | 0.29          |
| (1,1382) | 1:75:A:ILE:HA   | 1:101:A:TYR:HE1  | 3        | 0.28          |
| (1,521)  | 1:75:A:ILE:HG12 | 1:76:A:LYS:H     | 11       | 0.28          |
| (1,1855) | 1:5:A:GLN:HG2   | 1:7:A:PHE:HD1    | 8        | 0.27          |
| (1,1855) | 1:5:A:GLN:HG3   | 1:7:A:PHE:HD1    | 8        | 0.27          |
| (1,1852) | 1:5:A:GLN:HB2   | 1:7:A:PHE:HE1    | 13       | 0.27          |
| (1,1852) | 1:5:A:GLN:HB3   | 1:7:A:PHE:HE1    | 13       | 0.27          |
| (1,1509) | 1:123:A:LEU:H   | 1:123:A:LEU:HD21 | 1        | 0.27          |
| (1,1509) | 1:123:A:LEU:H   | 1:123:A:LEU:HD22 | 1        | 0.27          |
| (1,1509) | 1:123:A:LEU:H   | 1:123:A:LEU:HD23 | 1        | 0.27          |
| (1,1503) | 1:42:A:VAL:HG11 | 1:67:A:PHE:HD1   | 8        | 0.27          |
| (1,1503) | 1:42:A:VAL:HG12 | 1:67:A:PHE:HD1   | 8        | 0.27          |
| (1,1503) | 1:42:A:VAL:HG13 | 1:67:A:PHE:HD1   | 8        | 0.27          |
| (1,1464) | 1:7:A:PHE:HE1   | 1:23:A:LEU:HB3   | 5        | 0.26          |
| (1,1509) | 1:123:A:LEU:H   | 1:123:A:LEU:HD21 | 2        | 0.25          |
| (1,1509) | 1:123:A:LEU:H   | 1:123:A:LEU:HD22 | 2        | 0.25          |
| (1,1509) | 1:123:A:LEU:H   | 1:123:A:LEU:HD23 | 2        | 0.25          |
| (1,1219) | 1:46:A:GLY:HA3  | 1:117:A:LEU:HB3  | 8        | 0.25          |
| (1,991)  | 1:85:A:MET:HA   | 1:120:A:ILE:HG21 | 17       | 0.25          |
| (1,991)  | 1:85:A:MET:HA   | 1:120:A:ILE:HG22 | 17       | 0.25          |
| (1,991)  | 1:85:A:MET:HA   | 1:120:A:ILE:HG23 | 17       | 0.25          |
| (1,642)  | 1:67:A:PHE:HE1  | 1:74:A:VAL:HG11  | 5        | 0.25          |
| (1,642)  | 1:67:A:PHE:HE1  | 1:74:A:VAL:HG12  | 5        | 0.25          |
| (1,642)  | 1:67:A:PHE:HE1  | 1:74:A:VAL:HG13  | 5        | 0.25          |
| (1,1531) | 1:67:A:PHE:HD1  | 1:74:A:VAL:HG21  | 14       | 0.24          |
| (1,1531) | 1:67:A:PHE:HD1  | 1:74:A:VAL:HG22  | 14       | 0.24          |
| (1,1531) | 1:67:A:PHE:HD1  | 1:74:A:VAL:HG23  | 14       | 0.24          |
| (1,1200) | 1:34:A:PRO:HA   | 1:122:A:LEU:HG   | 1        | 0.24          |
| (1,642)  | 1:67:A:PHE:HE1  | 1:74:A:VAL:HG11  | 4        | 0.24          |
| (1,642)  | 1:67:A:PHE:HE1  | 1:74:A:VAL:HG12  | 4        | 0.24          |
| (1,642)  | 1:67:A:PHE:HE1  | 1:74:A:VAL:HG13  | 4        | 0.24          |
| (1,259)  | 1:27:A:ASP:H    | 1:88:A:ASN:HB3   | 19       | 0.24          |
| (1,1852) | 1:5:A:GLN:HB2   | 1:7:A:PHE:HE1    | 10       | 0.23          |
| (1,1852) | 1:5:A:GLN:HB3   | 1:7:A:PHE:HE1    | 10       | 0.23          |
| (1,1509) | 1:123:A:LEU:H   | 1:123:A:LEU:HD21 | 6        | 0.23          |
| (1,1509) | 1:123:A:LEU:H   | 1:123:A:LEU:HD22 | 6        | 0.23          |
| (1,1509) | 1:123:A:LEU:H   | 1:123:A:LEU:HD23 | 6        | 0.23          |
| (1,1503) | 1:42:A:VAL:HG11 | 1:67:A:PHE:HD1   | 7        | 0.23          |
| (1,1503) | 1:42:A:VAL:HG12 | 1:67:A:PHE:HD1   | 7        | 0.23          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1503) | 1:42:A:VAL:HG13 | 1:67:A:PHE:HD1   | 7        | 0.23          |
| (1,869)  | 1:78:A:TRP:HZ3  | 1:101:A:TYR:HD1  | 5        | 0.23          |
| (1,653)  | 1:7:A:PHE:HD1   | 1:21:A:THR:HG21  | 2        | 0.23          |
| (1,653)  | 1:7:A:PHE:HD1   | 1:21:A:THR:HG22  | 2        | 0.23          |
| (1,653)  | 1:7:A:PHE:HD1   | 1:21:A:THR:HG23  | 2        | 0.23          |
| (1,521)  | 1:75:A:ILE:HG12 | 1:76:A:LYS:H     | 13       | 0.23          |
| (1,521)  | 1:75:A:ILE:HG12 | 1:76:A:LYS:H     | 18       | 0.23          |
| (1,1870) | 1:7:A:PHE:HD1   | 1:23:A:LEU:HD11  | 16       | 0.22          |
| (1,1870) | 1:7:A:PHE:HD1   | 1:23:A:LEU:HD12  | 16       | 0.22          |
| (1,1870) | 1:7:A:PHE:HD1   | 1:23:A:LEU:HD13  | 16       | 0.22          |
| (1,1870) | 1:7:A:PHE:HD1   | 1:23:A:LEU:HD21  | 16       | 0.22          |
| (1,1870) | 1:7:A:PHE:HD1   | 1:23:A:LEU:HD22  | 16       | 0.22          |
| (1,1870) | 1:7:A:PHE:HD1   | 1:23:A:LEU:HD23  | 16       | 0.22          |
| (1,699)  | 1:75:A:ILE:HG13 | 1:101:A:TYR:HD1  | 13       | 0.22          |
| (1,162)  | 1:36:A:LYS:HD2  | 1:38:A:ASN:H     | 16       | 0.22          |
| (1,2226) | 1:67:A:PHE:HD1  | 1:73:A:GLU:HB2   | 16       | 0.21          |
| (1,2226) | 1:67:A:PHE:HD1  | 1:73:A:GLU:HB3   | 16       | 0.21          |
| (1,2226) | 1:67:A:PHE:HD1  | 1:73:A:GLU:HB2   | 19       | 0.21          |
| (1,2226) | 1:67:A:PHE:HD1  | 1:73:A:GLU:HB3   | 19       | 0.21          |
| (1,1509) | 1:123:A:LEU:H   | 1:123:A:LEU:HD21 | 15       | 0.21          |
| (1,1509) | 1:123:A:LEU:H   | 1:123:A:LEU:HD22 | 15       | 0.21          |
| (1,1509) | 1:123:A:LEU:H   | 1:123:A:LEU:HD23 | 15       | 0.21          |
| (1,1219) | 1:46:A:GLY:HA3  | 1:117:A:LEU:HB3  | 2        | 0.21          |
| (1,1200) | 1:34:A:PRO:HA   | 1:122:A:LEU:HG   | 20       | 0.21          |
| (1,2065) | 1:36:A:LYS:HG2  | 1:70:A:GLU:HB2   | 12       | 0.2           |
| (1,2065) | 1:36:A:LYS:HG3  | 1:70:A:GLU:HB2   | 12       | 0.2           |
| (1,878)  | 1:7:A:PHE:H     | 1:7:A:PHE:HE1    | 8        | 0.2           |
| (1,1)    | 1:92:A:LEU:HB3  | 1:93:A:VAL:H     | 17       | 0.2           |
| (1,1881) | 1:9:A:LYS:H     | 1:9:A:LYS:HD2    | 5        | 0.19          |
| (1,1881) | 1:9:A:LYS:H     | 1:9:A:LYS:HD3    | 5        | 0.19          |
| (1,1870) | 1:7:A:PHE:HD1   | 1:23:A:LEU:HD11  | 15       | 0.19          |
| (1,1870) | 1:7:A:PHE:HD1   | 1:23:A:LEU:HD12  | 15       | 0.19          |
| (1,1870) | 1:7:A:PHE:HD1   | 1:23:A:LEU:HD13  | 15       | 0.19          |
| (1,1870) | 1:7:A:PHE:HD1   | 1:23:A:LEU:HD21  | 15       | 0.19          |
| (1,1870) | 1:7:A:PHE:HD1   | 1:23:A:LEU:HD22  | 15       | 0.19          |
| (1,1870) | 1:7:A:PHE:HD1   | 1:23:A:LEU:HD23  | 15       | 0.19          |
| (1,1855) | 1:5:A:GLN:HG2   | 1:7:A:PHE:HD1    | 7        | 0.19          |
| (1,1855) | 1:5:A:GLN:HG3   | 1:7:A:PHE:HD1    | 7        | 0.19          |
| (1,1200) | 1:34:A:PRO:HA   | 1:122:A:LEU:HG   | 8        | 0.19          |
| (1,1200) | 1:34:A:PRO:HA   | 1:122:A:LEU:HG   | 10       | 0.19          |
| (1,642)  | 1:67:A:PHE:HE1  | 1:74:A:VAL:HG11  | 14       | 0.19          |
| (1,642)  | 1:67:A:PHE:HE1  | 1:74:A:VAL:HG12  | 14       | 0.19          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,642)  | 1:67:A:PHE:HE1  | 1:74:A:VAL:HG13  | 14       | 0.19          |
| (1,84)   | 1:50:A:SER:H    | 1:117:A:LEU:HD21 | 17       | 0.19          |
| (1,84)   | 1:50:A:SER:H    | 1:117:A:LEU:HD22 | 17       | 0.19          |
| (1,84)   | 1:50:A:SER:H    | 1:117:A:LEU:HD23 | 17       | 0.19          |
| (1,2241) | 1:69:A:LEU:HA   | 1:71:A:GLN:HE21  | 10       | 0.18          |
| (1,2241) | 1:69:A:LEU:HA   | 1:71:A:GLN:HE22  | 10       | 0.18          |
| (1,1503) | 1:42:A:VAL:HG11 | 1:67:A:PHE:HD1   | 11       | 0.18          |
| (1,1503) | 1:42:A:VAL:HG12 | 1:67:A:PHE:HD1   | 11       | 0.18          |
| (1,1503) | 1:42:A:VAL:HG13 | 1:67:A:PHE:HD1   | 11       | 0.18          |
| (1,1219) | 1:46:A:GLY:HA3  | 1:117:A:LEU:HB3  | 4        | 0.18          |
| (1,843)  | 1:57:A:SER:H    | 1:62:A:ASN:H     | 3        | 0.18          |
| (1,1)    | 1:92:A:LEU:HB3  | 1:93:A:VAL:H     | 4        | 0.18          |
| (1,2527) | 1:125:A:PHE:HD1 | 1:126:A:ARG:HG2  | 11       | 0.17          |
| (1,2527) | 1:125:A:PHE:HD1 | 1:126:A:ARG:HG3  | 11       | 0.17          |
| (1,1509) | 1:123:A:LEU:H   | 1:123:A:LEU:HD21 | 16       | 0.17          |
| (1,1509) | 1:123:A:LEU:H   | 1:123:A:LEU:HD22 | 16       | 0.17          |
| (1,1509) | 1:123:A:LEU:H   | 1:123:A:LEU:HD23 | 16       | 0.17          |
| (1,1503) | 1:42:A:VAL:HG11 | 1:67:A:PHE:HD1   | 19       | 0.17          |
| (1,1503) | 1:42:A:VAL:HG12 | 1:67:A:PHE:HD1   | 19       | 0.17          |
| (1,1503) | 1:42:A:VAL:HG13 | 1:67:A:PHE:HD1   | 19       | 0.17          |
| (1,1000) | 1:47:A:LYS:HB2  | 1:54:A:VAL:HA    | 8        | 0.17          |
| (1,991)  | 1:85:A:MET:HA   | 1:120:A:ILE:HG21 | 3        | 0.17          |
| (1,991)  | 1:85:A:MET:HA   | 1:120:A:ILE:HG22 | 3        | 0.17          |
| (1,991)  | 1:85:A:MET:HA   | 1:120:A:ILE:HG23 | 3        | 0.17          |
| (1,104)  | 1:36:A:LYS:HD2  | 1:37:A:GLY:H     | 1        | 0.17          |
| (1,57)   | 1:35:A:LYS:HB3  | 1:38:A:ASN:HD22  | 7        | 0.17          |
| (1,1)    | 1:92:A:LEU:HB3  | 1:93:A:VAL:H     | 7        | 0.17          |
| (1,2105) | 1:42:A:VAL:HA   | 1:66:A:LYS:HD2   | 20       | 0.16          |
| (1,2105) | 1:42:A:VAL:HA   | 1:66:A:LYS:HD3   | 20       | 0.16          |
| (1,1944) | 1:20:A:LYS:HD2  | 1:120:A:ILE:HD11 | 7        | 0.16          |
| (1,1944) | 1:20:A:LYS:HD2  | 1:120:A:ILE:HD12 | 7        | 0.16          |
| (1,1944) | 1:20:A:LYS:HD2  | 1:120:A:ILE:HD13 | 7        | 0.16          |
| (1,1944) | 1:20:A:LYS:HD3  | 1:120:A:ILE:HD11 | 7        | 0.16          |
| (1,1944) | 1:20:A:LYS:HD3  | 1:120:A:ILE:HD12 | 7        | 0.16          |
| (1,1944) | 1:20:A:LYS:HD3  | 1:120:A:ILE:HD13 | 7        | 0.16          |
| (1,1944) | 1:20:A:LYS:HD2  | 1:120:A:ILE:HD11 | 11       | 0.16          |
| (1,1944) | 1:20:A:LYS:HD2  | 1:120:A:ILE:HD12 | 11       | 0.16          |
| (1,1944) | 1:20:A:LYS:HD2  | 1:120:A:ILE:HD13 | 11       | 0.16          |
| (1,1944) | 1:20:A:LYS:HD3  | 1:120:A:ILE:HD11 | 11       | 0.16          |
| (1,1944) | 1:20:A:LYS:HD3  | 1:120:A:ILE:HD12 | 11       | 0.16          |
| (1,1944) | 1:20:A:LYS:HD3  | 1:120:A:ILE:HD13 | 11       | 0.16          |
| (1,1875) | 1:8:A:GLU:HA    | 1:9:A:LYS:HD2    | 5        | 0.16          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1875) | 1:8:A:GLU:HA    | 1:9:A:LYS:HD3    | 5        | 0.16          |
| (1,1870) | 1:7:A:PHE:HD1   | 1:23:A:LEU:HD11  | 4        | 0.16          |
| (1,1870) | 1:7:A:PHE:HD1   | 1:23:A:LEU:HD12  | 4        | 0.16          |
| (1,1870) | 1:7:A:PHE:HD1   | 1:23:A:LEU:HD13  | 4        | 0.16          |
| (1,1870) | 1:7:A:PHE:HD1   | 1:23:A:LEU:HD21  | 4        | 0.16          |
| (1,1870) | 1:7:A:PHE:HD1   | 1:23:A:LEU:HD22  | 4        | 0.16          |
| (1,1870) | 1:7:A:PHE:HD1   | 1:23:A:LEU:HD23  | 4        | 0.16          |
| (1,1672) | 1:76:A:LYS:HA   | 1:76:A:LYS:HD3   | 8        | 0.16          |
| (1,1503) | 1:42:A:VAL:HG11 | 1:67:A:PHE:HD1   | 12       | 0.16          |
| (1,1503) | 1:42:A:VAL:HG12 | 1:67:A:PHE:HD1   | 12       | 0.16          |
| (1,1503) | 1:42:A:VAL:HG13 | 1:67:A:PHE:HD1   | 12       | 0.16          |
| (1,1367) | 1:50:A:SER:HA   | 1:116:A:LEU:HA   | 3        | 0.16          |
| (1,1367) | 1:50:A:SER:HA   | 1:116:A:LEU:HA   | 19       | 0.16          |
| (1,1365) | 1:7:A:PHE:HD1   | 1:23:A:LEU:HA    | 4        | 0.16          |
| (1,1200) | 1:34:A:PRO:HA   | 1:122:A:LEU:HG   | 3        | 0.16          |
| (1,1200) | 1:34:A:PRO:HA   | 1:122:A:LEU:HG   | 9        | 0.16          |
| (1,1200) | 1:34:A:PRO:HA   | 1:122:A:LEU:HG   | 12       | 0.16          |
| (1,878)  | 1:7:A:PHE:H     | 1:7:A:PHE:HE1    | 5        | 0.16          |
| (1,799)  | 1:68:A:HIS:H    | 1:73:A:GLU:H     | 13       | 0.16          |
| (1,642)  | 1:67:A:PHE:HE1  | 1:74:A:VAL:HG11  | 18       | 0.16          |
| (1,642)  | 1:67:A:PHE:HE1  | 1:74:A:VAL:HG12  | 18       | 0.16          |
| (1,642)  | 1:67:A:PHE:HE1  | 1:74:A:VAL:HG13  | 18       | 0.16          |
| (1,256)  | 1:27:A:ASP:H    | 1:86:A:ARG:HB2   | 18       | 0.16          |
| (1,2527) | 1:125:A:PHE:HD1 | 1:126:A:ARG:HG2  | 20       | 0.15          |
| (1,2527) | 1:125:A:PHE:HD1 | 1:126:A:ARG:HG3  | 20       | 0.15          |
| (1,2421) | 1:97:A:SER:HB2  | 1:113:A:ASN:HD21 | 8        | 0.15          |
| (1,2421) | 1:97:A:SER:HB2  | 1:113:A:ASN:HD22 | 8        | 0.15          |
| (1,2421) | 1:97:A:SER:HB3  | 1:113:A:ASN:HD21 | 8        | 0.15          |
| (1,2421) | 1:97:A:SER:HB3  | 1:113:A:ASN:HD22 | 8        | 0.15          |
| (1,2283) | 1:76:A:LYS:HA   | 1:76:A:LYS:HE2   | 4        | 0.15          |
| (1,2283) | 1:76:A:LYS:HA   | 1:76:A:LYS:HE3   | 4        | 0.15          |
| (1,2226) | 1:67:A:PHE:HD1  | 1:73:A:GLU:HB2   | 12       | 0.15          |
| (1,2226) | 1:67:A:PHE:HD1  | 1:73:A:GLU:HB3   | 12       | 0.15          |
| (1,1870) | 1:7:A:PHE:HD1   | 1:23:A:LEU:HD11  | 19       | 0.15          |
| (1,1870) | 1:7:A:PHE:HD1   | 1:23:A:LEU:HD12  | 19       | 0.15          |
| (1,1870) | 1:7:A:PHE:HD1   | 1:23:A:LEU:HD13  | 19       | 0.15          |
| (1,1870) | 1:7:A:PHE:HD1   | 1:23:A:LEU:HD21  | 19       | 0.15          |
| (1,1870) | 1:7:A:PHE:HD1   | 1:23:A:LEU:HD22  | 19       | 0.15          |
| (1,1870) | 1:7:A:PHE:HD1   | 1:23:A:LEU:HD23  | 19       | 0.15          |
| (1,1523) | 1:75:A:ILE:H    | 1:75:A:ILE:HD11  | 10       | 0.15          |
| (1,1523) | 1:75:A:ILE:H    | 1:75:A:ILE:HD12  | 10       | 0.15          |
| (1,1523) | 1:75:A:ILE:H    | 1:75:A:ILE:HD13  | 10       | 0.15          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1509) | 1:123:A:LEU:H   | 1:123:A:LEU:HD21 | 8        | 0.15          |
| (1,1509) | 1:123:A:LEU:H   | 1:123:A:LEU:HD22 | 8        | 0.15          |
| (1,1509) | 1:123:A:LEU:H   | 1:123:A:LEU:HD23 | 8        | 0.15          |
| (1,1437) | 1:9:A:LYS:HA    | 1:22:A:ILE:HB    | 16       | 0.15          |
| (1,1367) | 1:50:A:SER:HA   | 1:116:A:LEU:HA   | 8        | 0.15          |
| (1,1367) | 1:50:A:SER:HA   | 1:116:A:LEU:HA   | 18       | 0.15          |
| (1,1085) | 1:78:A:TRP:HB3  | 1:82:A:VAL:HA    | 5        | 0.15          |
| (1,162)  | 1:36:A:LYS:HD2  | 1:38:A:ASN:H     | 7        | 0.15          |
| (1,1)    | 1:92:A:LEU:HB3  | 1:93:A:VAL:H     | 3        | 0.15          |
| (1,2404) | 1:94:A:ARG:HD2  | 1:116:A:LEU:HA   | 19       | 0.14          |
| (1,2404) | 1:94:A:ARG:HD3  | 1:116:A:LEU:HA   | 19       | 0.14          |
| (1,2054) | 1:36:A:LYS:HA   | 1:70:A:GLU:HG2   | 12       | 0.14          |
| (1,2054) | 1:36:A:LYS:HA   | 1:70:A:GLU:HG3   | 12       | 0.14          |
| (1,1875) | 1:8:A:GLU:HA    | 1:9:A:LYS:HD2    | 4        | 0.14          |
| (1,1875) | 1:8:A:GLU:HA    | 1:9:A:LYS:HD3    | 4        | 0.14          |
| (1,1870) | 1:7:A:PHE:HD1   | 1:23:A:LEU:HD11  | 6        | 0.14          |
| (1,1870) | 1:7:A:PHE:HD1   | 1:23:A:LEU:HD12  | 6        | 0.14          |
| (1,1870) | 1:7:A:PHE:HD1   | 1:23:A:LEU:HD13  | 6        | 0.14          |
| (1,1870) | 1:7:A:PHE:HD1   | 1:23:A:LEU:HD21  | 6        | 0.14          |
| (1,1870) | 1:7:A:PHE:HD1   | 1:23:A:LEU:HD22  | 6        | 0.14          |
| (1,1870) | 1:7:A:PHE:HD1   | 1:23:A:LEU:HD23  | 6        | 0.14          |
| (1,1851) | 1:5:A:GLN:HB2   | 1:7:A:PHE:HD1    | 14       | 0.14          |
| (1,1851) | 1:5:A:GLN:HB3   | 1:7:A:PHE:HD1    | 14       | 0.14          |
| (1,1523) | 1:75:A:ILE:H    | 1:75:A:ILE:HD11  | 8        | 0.14          |
| (1,1523) | 1:75:A:ILE:H    | 1:75:A:ILE:HD12  | 8        | 0.14          |
| (1,1523) | 1:75:A:ILE:H    | 1:75:A:ILE:HD13  | 8        | 0.14          |
| (1,1085) | 1:78:A:TRP:HB3  | 1:82:A:VAL:HA    | 19       | 0.14          |
| (1,162)  | 1:36:A:LYS:HD2  | 1:38:A:ASN:H     | 2        | 0.14          |
| (1,2527) | 1:125:A:PHE:HD1 | 1:126:A:ARG:HG2  | 10       | 0.13          |
| (1,2527) | 1:125:A:PHE:HD1 | 1:126:A:ARG:HG3  | 10       | 0.13          |
| (1,2527) | 1:125:A:PHE:HD1 | 1:126:A:ARG:HG2  | 12       | 0.13          |
| (1,2527) | 1:125:A:PHE:HD1 | 1:126:A:ARG:HG3  | 12       | 0.13          |
| (1,2463) | 1:109:A:SER:HB2 | 1:116:A:LEU:HG   | 20       | 0.13          |
| (1,2463) | 1:109:A:SER:HB3 | 1:116:A:LEU:HG   | 20       | 0.13          |
| (1,2241) | 1:69:A:LEU:HA   | 1:71:A:GLN:HE21  | 8        | 0.13          |
| (1,2241) | 1:69:A:LEU:HA   | 1:71:A:GLN:HE22  | 8        | 0.13          |
| (1,1334) | 1:74:A:VAL:HB   | 1:120:A:ILE:HD11 | 11       | 0.13          |
| (1,1334) | 1:74:A:VAL:HB   | 1:120:A:ILE:HD12 | 11       | 0.13          |
| (1,1334) | 1:74:A:VAL:HB   | 1:120:A:ILE:HD13 | 11       | 0.13          |
| (1,1200) | 1:34:A:PRO:HA   | 1:122:A:LEU:HG   | 18       | 0.13          |
| (1,1085) | 1:78:A:TRP:HB3  | 1:82:A:VAL:HA    | 15       | 0.13          |
| (1,1022) | 1:52:A:GLY:HA3  | 1:117:A:LEU:HD11 | 2        | 0.13          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1022) | 1:52:A:GLY:HA3  | 1:117:A:LEU:HD12 | 2        | 0.13          |
| (1,1022) | 1:52:A:GLY:HA3  | 1:117:A:LEU:HD13 | 2        | 0.13          |
| (1,792)  | 1:90:A:LYS:HA   | 1:121:A:GLU:H    | 2        | 0.13          |
| (1,730)  | 1:87:A:LYS:HE3  | 1:125:A:PHE:HD1  | 8        | 0.13          |
| (1,729)  | 1:51:A:THR:H    | 1:117:A:LEU:HD11 | 20       | 0.13          |
| (1,729)  | 1:51:A:THR:H    | 1:117:A:LEU:HD12 | 20       | 0.13          |
| (1,729)  | 1:51:A:THR:H    | 1:117:A:LEU:HD13 | 20       | 0.13          |
| (1,699)  | 1:75:A:ILE:HG13 | 1:101:A:TYR:HD1  | 4        | 0.13          |
| (1,645)  | 1:7:A:PHE:HD1   | 1:23:A:LEU:HD21  | 12       | 0.13          |
| (1,645)  | 1:7:A:PHE:HD1   | 1:23:A:LEU:HD22  | 12       | 0.13          |
| (1,645)  | 1:7:A:PHE:HD1   | 1:23:A:LEU:HD23  | 12       | 0.13          |
| (1,521)  | 1:75:A:ILE:HG12 | 1:76:A:LYS:H     | 9        | 0.13          |
| (1,521)  | 1:75:A:ILE:HG12 | 1:76:A:LYS:H     | 12       | 0.13          |
| (1,400)  | 1:28:A:GLU:HG2  | 1:30:A:GLU:H     | 16       | 0.13          |
| (1,256)  | 1:27:A:ASP:H    | 1:86:A:ARG:HB2   | 2        | 0.13          |
| (1,256)  | 1:27:A:ASP:H    | 1:86:A:ARG:HB2   | 4        | 0.13          |
| (1,84)   | 1:50:A:SER:H    | 1:117:A:LEU:HD21 | 12       | 0.13          |
| (1,84)   | 1:50:A:SER:H    | 1:117:A:LEU:HD22 | 12       | 0.13          |
| (1,84)   | 1:50:A:SER:H    | 1:117:A:LEU:HD23 | 12       | 0.13          |
| (1,2527) | 1:125:A:PHE:HD1 | 1:126:A:ARG:HG2  | 4        | 0.12          |
| (1,2527) | 1:125:A:PHE:HD1 | 1:126:A:ARG:HG3  | 4        | 0.12          |
| (1,2527) | 1:125:A:PHE:HD1 | 1:126:A:ARG:HG2  | 8        | 0.12          |
| (1,2527) | 1:125:A:PHE:HD1 | 1:126:A:ARG:HG3  | 8        | 0.12          |
| (1,2288) | 1:76:A:LYS:HG3  | 1:79:A:ASP:HB2   | 2        | 0.12          |
| (1,2288) | 1:76:A:LYS:HG3  | 1:79:A:ASP:HB3   | 2        | 0.12          |
| (1,2241) | 1:69:A:LEU:HA   | 1:71:A:GLN:HE21  | 7        | 0.12          |
| (1,2241) | 1:69:A:LEU:HA   | 1:71:A:GLN:HE22  | 7        | 0.12          |
| (1,2241) | 1:69:A:LEU:HA   | 1:71:A:GLN:HE21  | 9        | 0.12          |
| (1,2241) | 1:69:A:LEU:HA   | 1:71:A:GLN:HE22  | 9        | 0.12          |
| (1,2241) | 1:69:A:LEU:HA   | 1:71:A:GLN:HE21  | 17       | 0.12          |
| (1,2241) | 1:69:A:LEU:HA   | 1:71:A:GLN:HE22  | 17       | 0.12          |
| (1,2237) | 1:68:A:HIS:HB2  | 1:71:A:GLN:HE21  | 13       | 0.12          |
| (1,2237) | 1:68:A:HIS:HB2  | 1:71:A:GLN:HE22  | 13       | 0.12          |
| (1,2237) | 1:68:A:HIS:HB3  | 1:71:A:GLN:HE21  | 13       | 0.12          |
| (1,2237) | 1:68:A:HIS:HB3  | 1:71:A:GLN:HE22  | 13       | 0.12          |
| (1,2231) | 1:68:A:HIS:HA   | 1:71:A:GLN:HG2   | 13       | 0.12          |
| (1,2231) | 1:68:A:HIS:HA   | 1:71:A:GLN:HG3   | 13       | 0.12          |
| (1,2146) | 1:49:A:GLU:HB2  | 1:117:A:LEU:HG   | 20       | 0.12          |
| (1,2146) | 1:49:A:GLU:HB3  | 1:117:A:LEU:HG   | 20       | 0.12          |
| (1,2103) | 1:42:A:VAL:H    | 1:66:A:LYS:HE2   | 11       | 0.12          |
| (1,2103) | 1:42:A:VAL:H    | 1:66:A:LYS:HE3   | 11       | 0.12          |
| (1,2081) | 1:39:A:GLU:HA   | 1:126:A:ARG:HD2  | 5        | 0.12          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2081) | 1:39:A:GLU:HA   | 1:126:A:ARG:HD3  | 5        | 0.12          |
| (1,1870) | 1:7:A:PHE:HD1   | 1:23:A:LEU:HD11  | 1        | 0.12          |
| (1,1870) | 1:7:A:PHE:HD1   | 1:23:A:LEU:HD12  | 1        | 0.12          |
| (1,1870) | 1:7:A:PHE:HD1   | 1:23:A:LEU:HD13  | 1        | 0.12          |
| (1,1870) | 1:7:A:PHE:HD1   | 1:23:A:LEU:HD21  | 1        | 0.12          |
| (1,1870) | 1:7:A:PHE:HD1   | 1:23:A:LEU:HD22  | 1        | 0.12          |
| (1,1870) | 1:7:A:PHE:HD1   | 1:23:A:LEU:HD23  | 1        | 0.12          |
| (1,1371) | 1:50:A:SER:HB3  | 1:116:A:LEU:HA   | 13       | 0.12          |
| (1,1367) | 1:50:A:SER:HA   | 1:116:A:LEU:HA   | 1        | 0.12          |
| (1,1215) | 1:66:A:LYS:HD3  | 1:67:A:PHE:HA    | 7        | 0.12          |
| (1,1200) | 1:34:A:PRO:HA   | 1:122:A:LEU:HG   | 4        | 0.12          |
| (1,1200) | 1:34:A:PRO:HA   | 1:122:A:LEU:HG   | 16       | 0.12          |
| (1,1160) | 1:111:A:PRO:HA  | 1:116:A:LEU:HB2  | 1        | 0.12          |
| (1,1085) | 1:78:A:TRP:HB3  | 1:82:A:VAL:HA    | 10       | 0.12          |
| (1,768)  | 1:75:A:ILE:HB   | 1:78:A:TRP:HE3   | 5        | 0.12          |
| (1,645)  | 1:7:A:PHE:HD1   | 1:23:A:LEU:HD21  | 7        | 0.12          |
| (1,645)  | 1:7:A:PHE:HD1   | 1:23:A:LEU:HD22  | 7        | 0.12          |
| (1,645)  | 1:7:A:PHE:HD1   | 1:23:A:LEU:HD23  | 7        | 0.12          |
| (1,400)  | 1:28:A:GLU:HG2  | 1:30:A:GLU:H     | 10       | 0.12          |
| (1,84)   | 1:50:A:SER:H    | 1:117:A:LEU:HD21 | 18       | 0.12          |
| (1,84)   | 1:50:A:SER:H    | 1:117:A:LEU:HD22 | 18       | 0.12          |
| (1,84)   | 1:50:A:SER:H    | 1:117:A:LEU:HD23 | 18       | 0.12          |
| (1,2527) | 1:125:A:PHE:HD1 | 1:126:A:ARG:HG2  | 14       | 0.11          |
| (1,2527) | 1:125:A:PHE:HD1 | 1:126:A:ARG:HG3  | 14       | 0.11          |
| (1,2527) | 1:125:A:PHE:HD1 | 1:126:A:ARG:HG2  | 16       | 0.11          |
| (1,2527) | 1:125:A:PHE:HD1 | 1:126:A:ARG:HG3  | 16       | 0.11          |
| (1,2404) | 1:94:A:ARG:HD2  | 1:116:A:LEU:HA   | 17       | 0.11          |
| (1,2404) | 1:94:A:ARG:HD3  | 1:116:A:LEU:HA   | 17       | 0.11          |
| (1,2377) | 1:90:A:LYS:HE2  | 1:119:A:GLU:HB3  | 19       | 0.11          |
| (1,2377) | 1:90:A:LYS:HE3  | 1:119:A:GLU:HB3  | 19       | 0.11          |
| (1,2105) | 1:42:A:VAL:HA   | 1:66:A:LYS:HD2   | 3        | 0.11          |
| (1,2105) | 1:42:A:VAL:HA   | 1:66:A:LYS:HD3   | 3        | 0.11          |
| (1,2006) | 1:29:A:GLY:H    | 1:33:A:ILE:HG12  | 8        | 0.11          |
| (1,2006) | 1:29:A:GLY:H    | 1:33:A:ILE:HG13  | 8        | 0.11          |
| (1,1910) | 1:12:A:LEU:HD11 | 1:16:A:GLY:HA2   | 12       | 0.11          |
| (1,1910) | 1:12:A:LEU:HD12 | 1:16:A:GLY:HA2   | 12       | 0.11          |
| (1,1910) | 1:12:A:LEU:HD13 | 1:16:A:GLY:HA2   | 12       | 0.11          |
| (1,1910) | 1:12:A:LEU:HD21 | 1:16:A:GLY:HA2   | 12       | 0.11          |
| (1,1910) | 1:12:A:LEU:HD22 | 1:16:A:GLY:HA2   | 12       | 0.11          |
| (1,1910) | 1:12:A:LEU:HD23 | 1:16:A:GLY:HA2   | 12       | 0.11          |
| (1,1870) | 1:7:A:PHE:HD1   | 1:23:A:LEU:HD11  | 3        | 0.11          |
| (1,1870) | 1:7:A:PHE:HD1   | 1:23:A:LEU:HD12  | 3        | 0.11          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1870) | 1:7:A:PHE:HD1   | 1:23:A:LEU:HD13  | 3        | 0.11          |
| (1,1870) | 1:7:A:PHE:HD1   | 1:23:A:LEU:HD21  | 3        | 0.11          |
| (1,1870) | 1:7:A:PHE:HD1   | 1:23:A:LEU:HD22  | 3        | 0.11          |
| (1,1870) | 1:7:A:PHE:HD1   | 1:23:A:LEU:HD23  | 3        | 0.11          |
| (1,1855) | 1:5:A:GLN:HG2   | 1:7:A:PHE:HD1    | 4        | 0.11          |
| (1,1855) | 1:5:A:GLN:HG3   | 1:7:A:PHE:HD1    | 4        | 0.11          |
| (1,1553) | 1:90:A:LYS:HE3  | 1:91:A:CYS:HA    | 12       | 0.11          |
| (1,1523) | 1:75:A:ILE:H    | 1:75:A:ILE:HD11  | 7        | 0.11          |
| (1,1523) | 1:75:A:ILE:H    | 1:75:A:ILE:HD12  | 7        | 0.11          |
| (1,1523) | 1:75:A:ILE:H    | 1:75:A:ILE:HD13  | 7        | 0.11          |
| (1,1523) | 1:75:A:ILE:H    | 1:75:A:ILE:HD11  | 15       | 0.11          |
| (1,1523) | 1:75:A:ILE:H    | 1:75:A:ILE:HD12  | 15       | 0.11          |
| (1,1523) | 1:75:A:ILE:H    | 1:75:A:ILE:HD13  | 15       | 0.11          |
| (1,1523) | 1:75:A:ILE:H    | 1:75:A:ILE:HD11  | 16       | 0.11          |
| (1,1523) | 1:75:A:ILE:H    | 1:75:A:ILE:HD12  | 16       | 0.11          |
| (1,1523) | 1:75:A:ILE:H    | 1:75:A:ILE:HD13  | 16       | 0.11          |
| (1,1437) | 1:9:A:LYS:HA    | 1:22:A:ILE:HB    | 12       | 0.11          |
| (1,1367) | 1:50:A:SER:HA   | 1:116:A:LEU:HA   | 7        | 0.11          |
| (1,1367) | 1:50:A:SER:HA   | 1:116:A:LEU:HA   | 10       | 0.11          |
| (1,1367) | 1:50:A:SER:HA   | 1:116:A:LEU:HA   | 15       | 0.11          |
| (1,1085) | 1:78:A:TRP:HB3  | 1:82:A:VAL:HA    | 2        | 0.11          |
| (1,991)  | 1:85:A:MET:HA   | 1:120:A:ILE:HG21 | 7        | 0.11          |
| (1,991)  | 1:85:A:MET:HA   | 1:120:A:ILE:HG22 | 7        | 0.11          |
| (1,991)  | 1:85:A:MET:HA   | 1:120:A:ILE:HG23 | 7        | 0.11          |
| (1,891)  | 1:33:A:ILE:H    | 1:86:A:ARG:HA    | 5        | 0.11          |
| (1,799)  | 1:68:A:HIS:H    | 1:73:A:GLU:H     | 9        | 0.11          |
| (1,717)  | 1:58:A:SER:HA   | 1:59:A:PHE:HD1   | 14       | 0.11          |
| (1,699)  | 1:75:A:ILE:HG13 | 1:101:A:TYR:HD1  | 8        | 0.11          |
| (1,521)  | 1:75:A:ILE:HG12 | 1:76:A:LYS:H     | 6        | 0.11          |
| (1,521)  | 1:75:A:ILE:HG12 | 1:76:A:LYS:H     | 14       | 0.11          |
| (1,390)  | 1:12:A:LEU:H    | 1:19:A:ILE:HD11  | 3        | 0.11          |
| (1,390)  | 1:12:A:LEU:H    | 1:19:A:ILE:HD12  | 3        | 0.11          |
| (1,390)  | 1:12:A:LEU:H    | 1:19:A:ILE:HD13  | 3        | 0.11          |
| (1,256)  | 1:27:A:ASP:H    | 1:86:A:ARG:HB2   | 11       | 0.11          |
| (1,91)   | 1:75:A:ILE:H    | 1:75:A:ILE:HG12  | 2        | 0.11          |
| (1,1)    | 1:92:A:LEU:HB3  | 1:93:A:VAL:H     | 1        | 0.11          |
| (1,2527) | 1:125:A:PHE:HD1 | 1:126:A:ARG:HG2  | 9        | 0.1           |
| (1,2527) | 1:125:A:PHE:HD1 | 1:126:A:ARG:HG3  | 9        | 0.1           |
| (1,2527) | 1:125:A:PHE:HD1 | 1:126:A:ARG:HG2  | 17       | 0.1           |
| (1,2527) | 1:125:A:PHE:HD1 | 1:126:A:ARG:HG3  | 17       | 0.1           |
| (1,2446) | 1:107:A:GLY:HA2 | 1:111:A:PRO:HG3  | 15       | 0.1           |
| (1,2446) | 1:107:A:GLY:HA3 | 1:111:A:PRO:HG3  | 15       | 0.1           |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2300) | 1:81:A:CYS:HB2  | 1:84:A:SER:HB2   | 8        | 0.1           |
| (1,2300) | 1:81:A:CYS:HB2  | 1:84:A:SER:HB3   | 8        | 0.1           |
| (1,2241) | 1:69:A:LEU:HA   | 1:71:A:GLN:HE21  | 16       | 0.1           |
| (1,2241) | 1:69:A:LEU:HA   | 1:71:A:GLN:HE22  | 16       | 0.1           |
| (1,2226) | 1:67:A:PHE:HD1  | 1:73:A:GLU:HB2   | 11       | 0.1           |
| (1,2226) | 1:67:A:PHE:HD1  | 1:73:A:GLU:HB3   | 11       | 0.1           |
| (1,2146) | 1:49:A:GLU:HB2  | 1:117:A:LEU:HG   | 7        | 0.1           |
| (1,2146) | 1:49:A:GLU:HB3  | 1:117:A:LEU:HG   | 7        | 0.1           |
| (1,1910) | 1:12:A:LEU:HD11 | 1:16:A:GLY:HA2   | 2        | 0.1           |
| (1,1910) | 1:12:A:LEU:HD12 | 1:16:A:GLY:HA2   | 2        | 0.1           |
| (1,1910) | 1:12:A:LEU:HD13 | 1:16:A:GLY:HA2   | 2        | 0.1           |
| (1,1910) | 1:12:A:LEU:HD21 | 1:16:A:GLY:HA2   | 2        | 0.1           |
| (1,1910) | 1:12:A:LEU:HD22 | 1:16:A:GLY:HA2   | 2        | 0.1           |
| (1,1910) | 1:12:A:LEU:HD23 | 1:16:A:GLY:HA2   | 2        | 0.1           |
| (1,1632) | 1:7:A:PHE:HB2   | 1:21:A:THR:HA    | 9        | 0.1           |
| (1,1390) | 1:26:A:GLY:HA2  | 1:89:A:GLU:H     | 16       | 0.1           |
| (1,1367) | 1:50:A:SER:HA   | 1:116:A:LEU:HA   | 17       | 0.1           |
| (1,1334) | 1:74:A:VAL:HB   | 1:120:A:ILE:HD11 | 1        | 0.1           |
| (1,1334) | 1:74:A:VAL:HB   | 1:120:A:ILE:HD12 | 1        | 0.1           |
| (1,1334) | 1:74:A:VAL:HB   | 1:120:A:ILE:HD13 | 1        | 0.1           |
| (1,1334) | 1:74:A:VAL:HB   | 1:120:A:ILE:HD11 | 18       | 0.1           |
| (1,1334) | 1:74:A:VAL:HB   | 1:120:A:ILE:HD12 | 18       | 0.1           |
| (1,1334) | 1:74:A:VAL:HB   | 1:120:A:ILE:HD13 | 18       | 0.1           |
| (1,1200) | 1:34:A:PRO:HA   | 1:122:A:LEU:HG   | 13       | 0.1           |
| (1,843)  | 1:57:A:SER:H    | 1:62:A:ASN:H     | 4        | 0.1           |
| (1,799)  | 1:68:A:HIS:H    | 1:73:A:GLU:H     | 16       | 0.1           |
| (1,699)  | 1:75:A:ILE:HG13 | 1:101:A:TYR:HD1  | 7        | 0.1           |
| (1,521)  | 1:75:A:ILE:HG12 | 1:76:A:LYS:H     | 4        | 0.1           |

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

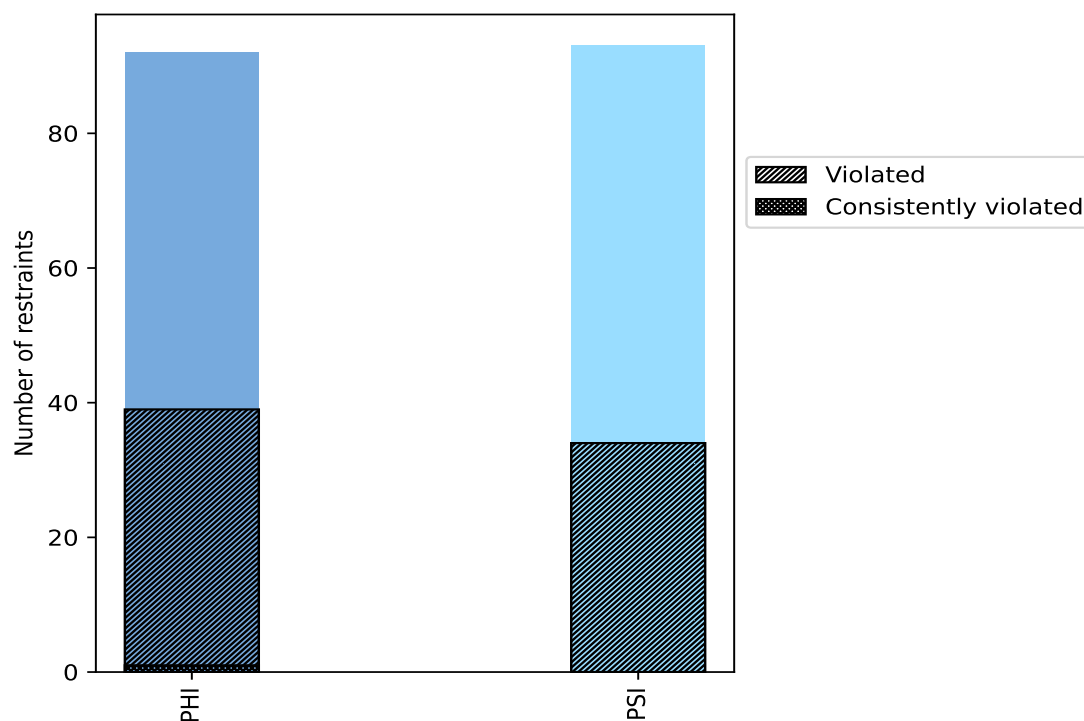
### 10.1 Summary of dihedral-angle violations [i](#)

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

| Angle type | Count | % <sup>1</sup> | Violated <sup>3</sup> |                |                | Consistently Violated <sup>4</sup> |                |                |
|------------|-------|----------------|-----------------------|----------------|----------------|------------------------------------|----------------|----------------|
|            |       |                | Count                 | % <sup>2</sup> | % <sup>1</sup> | Count                              | % <sup>2</sup> | % <sup>1</sup> |
| PHI        | 92    | 49.7           | 39                    | 42.4           | 21.1           | 1                                  | 1.1            | 0.5            |
| PSI        | 93    | 50.3           | 34                    | 36.6           | 18.4           | 0                                  | 0.0            | 0.0            |
| Total      | 185   | 100.0          | 73                    | 39.5           | 39.5           | 1                                  | 0.5            | 0.5            |

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

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



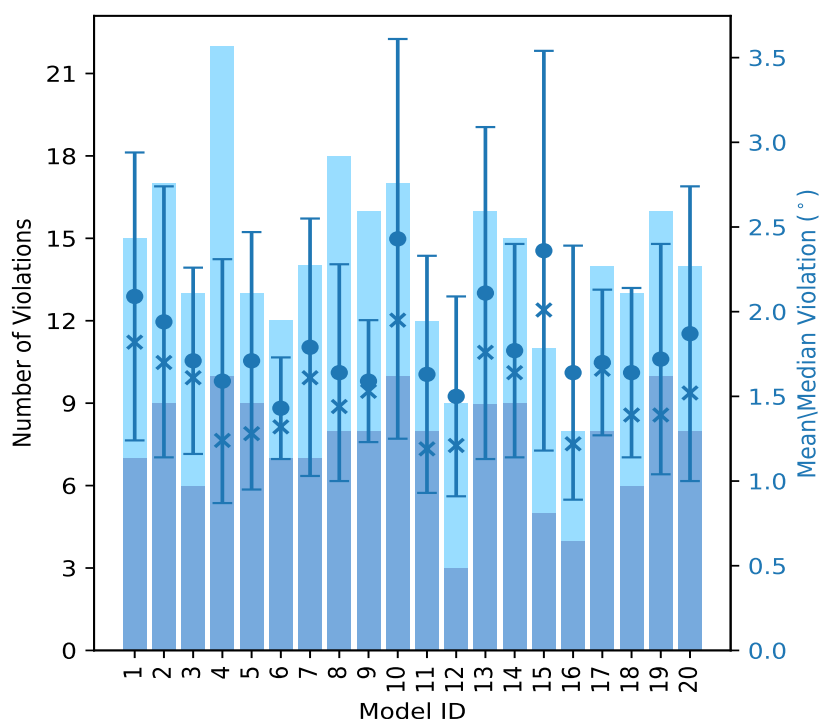
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

## 10.2 Dihedral-angle violation statistics for each model

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

| Model ID | Number of violations |     |       | Mean (°) | Max (°) | SD (°) | Median (°) |
|----------|----------------------|-----|-------|----------|---------|--------|------------|
|          | PHI                  | PSI | Total |          |         |        |            |
| 1        | 7                    | 8   | 15    | 2.09     | 3.88    | 0.85   | 1.82       |
| 2        | 9                    | 8   | 17    | 1.94     | 4.37    | 0.8    | 1.7        |
| 3        | 6                    | 7   | 13    | 1.71     | 3.22    | 0.55   | 1.61       |
| 4        | 10                   | 12  | 22    | 1.59     | 3.47    | 0.72   | 1.24       |
| 5        | 9                    | 4   | 13    | 1.71     | 3.37    | 0.76   | 1.28       |
| 6        | 7                    | 5   | 12    | 1.43     | 2.11    | 0.3    | 1.32       |
| 7        | 7                    | 7   | 14    | 1.79     | 4.1     | 0.76   | 1.61       |
| 8        | 8                    | 10  | 18    | 1.64     | 3.65    | 0.64   | 1.44       |
| 9        | 8                    | 8   | 16    | 1.59     | 2.58    | 0.36   | 1.53       |
| 10       | 10                   | 7   | 17    | 2.43     | 4.68    | 1.18   | 1.95       |
| 11       | 8                    | 4   | 12    | 1.63     | 2.96    | 0.7    | 1.19       |
| 12       | 3                    | 6   | 9     | 1.5      | 2.78    | 0.59   | 1.21       |
| 13       | 9                    | 7   | 16    | 2.11     | 4.85    | 0.98   | 1.76       |
| 14       | 9                    | 6   | 15    | 1.77     | 3.36    | 0.63   | 1.64       |
| 15       | 5                    | 6   | 11    | 2.36     | 4.57    | 1.18   | 2.01       |
| 16       | 4                    | 4   | 8     | 1.64     | 3.0     | 0.75   | 1.22       |
| 17       | 8                    | 6   | 14    | 1.7      | 2.57    | 0.43   | 1.66       |
| 18       | 6                    | 7   | 13    | 1.64     | 2.71    | 0.5    | 1.39       |
| 19       | 10                   | 6   | 16    | 1.72     | 3.28    | 0.68   | 1.39       |
| 20       | 8                    | 6   | 14    | 1.87     | 4.07    | 0.87   | 1.52       |

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



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

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

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

| Number of violated restraints |     |       | Fraction of the ensemble |      |
|-------------------------------|-----|-------|--------------------------|------|
| PHI                           | PSI | Total | Count <sup>1</sup>       | %    |
| 16                            | 11  | 27    | 1                        | 5.0  |
| 5                             | 7   | 12    | 2                        | 10.0 |
| 4                             | 5   | 9     | 3                        | 15.0 |
| 4                             | 2   | 6     | 4                        | 20.0 |
| 1                             | 1   | 2     | 5                        | 25.0 |
| 1                             | 1   | 2     | 6                        | 30.0 |
| 1                             | 0   | 1     | 7                        | 35.0 |
| 2                             | 2   | 4     | 8                        | 40.0 |
| 1                             | 1   | 2     | 9                        | 45.0 |
| 0                             | 1   | 1     | 10                       | 50.0 |
| 2                             | 2   | 4     | 11                       | 55.0 |

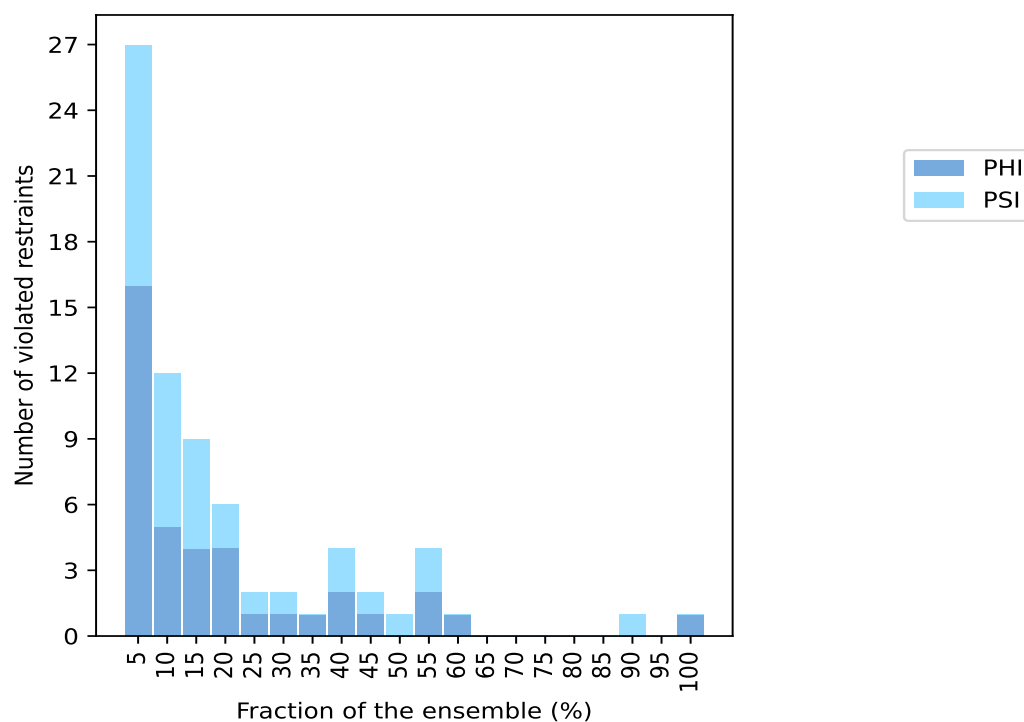
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| Number of violated restraints |     |       | Fraction of the ensemble |       |
|-------------------------------|-----|-------|--------------------------|-------|
| PHI                           | PSI | Total | Count <sup>1</sup>       | %     |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

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

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

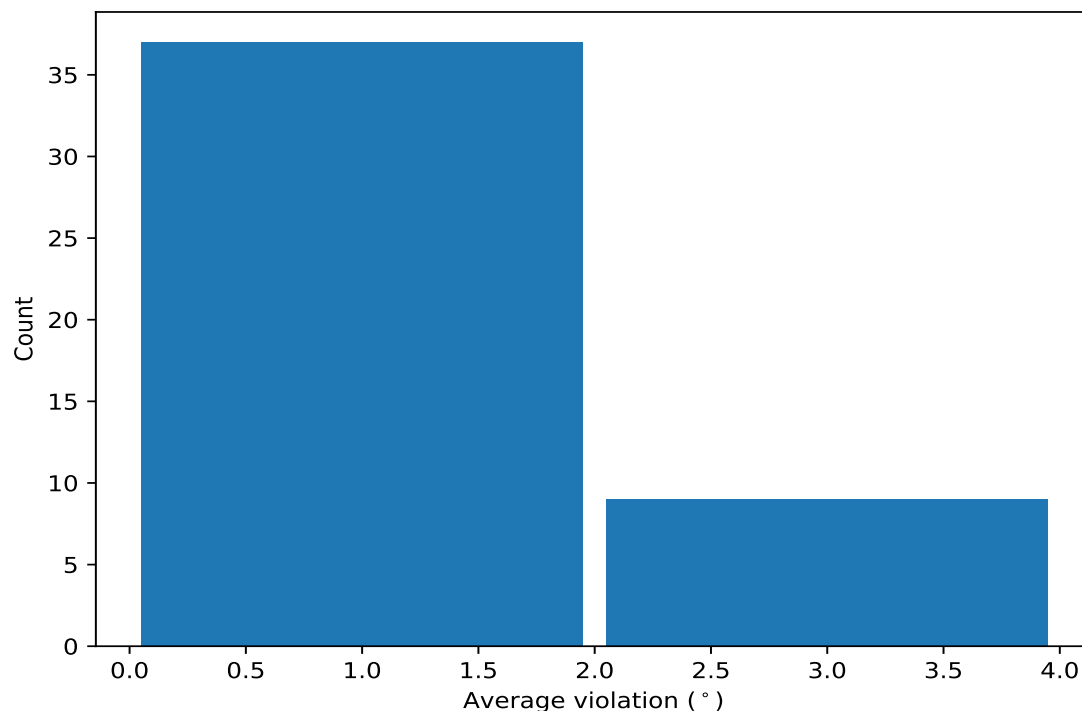


## 10.4 Most violated dihedral-angle restraints in the ensemble [i](#)

### 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 |
|---------|---------------|----------------|----------------|---------------|---------------------|------|-----------------|--------|
| (1,17)  | 1:15:A:ASP:C  | 1:16:A:GLY:N   | 1:16:A:GLY:CA  | 1:16:A:GLY:C  | 20                  | 2.69 | 0.73            | 2.93   |
| (1,161) | 1:109:A:SER:N | 1:109:A:SER:CA | 1:109:A:SER:C  | 1:110:A:ILE:N | 18                  | 2.75 | 1.03            | 2.76   |
| (1,109) | 1:74:A:VAL:C  | 1:75:A:ILE:N   | 1:75:A:ILE:CA  | 1:75:A:ILE:C  | 12                  | 2.05 | 1.1             | 1.64   |
| (1,100) | 1:68:A:HIS:N  | 1:68:A:HIS:CA  | 1:68:A:HIS:C   | 1:69:A:LEU:N  | 11                  | 2.23 | 1.02            | 2.01   |
| (1,7)   | 1:9:A:LYS:C   | 1:10:A:VAL:N   | 1:10:A:VAL:CA  | 1:10:A:VAL:C  | 11                  | 1.82 | 0.56            | 1.73   |
| (1,113) | 1:77:A:GLY:N  | 1:77:A:GLY:CA  | 1:77:A:GLY:C   | 1:78:A:TRP:N  | 11                  | 1.54 | 0.44            | 1.42   |
| (1,114) | 1:77:A:GLY:C  | 1:78:A:TRP:N   | 1:78:A:TRP:CA  | 1:78:A:TRP:C  | 11                  | 1.36 | 0.31            | 1.23   |
| (1,40)  | 1:32:A:ASN:N  | 1:32:A:ASN:CA  | 1:32:A:ASN:C   | 1:33:A:ILE:N  | 10                  | 2.58 | 0.81            | 2.39   |
| (1,172) | 1:119:A:GLU:C | 1:120:A:ILE:N  | 1:120:A:ILE:CA | 1:120:A:ILE:C | 9                   | 1.77 | 0.49            | 1.54   |
| (1,123) | 1:82:A:VAL:N  | 1:82:A:VAL:CA  | 1:82:A:VAL:C   | 1:83:A:SER:N  | 9                   | 1.39 | 0.28            | 1.37   |
| (1,159) | 1:108:A:GLU:N | 1:108:A:GLU:CA | 1:108:A:GLU:C  | 1:109:A:SER:N | 8                   | 1.74 | 0.49            | 1.73   |
| (1,117) | 1:79:A:ASP:N  | 1:79:A:ASP:CA  | 1:79:A:ASP:C   | 1:80:A:ILE:N  | 8                   | 1.53 | 0.34            | 1.49   |
| (1,61)  | 1:44:A:TYR:C  | 1:45:A:VAL:N   | 1:45:A:VAL:CA  | 1:45:A:VAL:C  | 8                   | 1.43 | 0.27            | 1.4    |
| (1,148) | 1:97:A:SER:C  | 1:98:A:MET:N   | 1:98:A:MET:CA  | 1:98:A:MET:C  | 8                   | 1.41 | 0.34            | 1.4    |
| (1,93)  | 1:64:A:PRO:C  | 1:65:A:PHE:N   | 1:65:A:PHE:CA  | 1:65:A:PHE:C  | 7                   | 1.53 | 0.31            | 1.49   |
| (1,85)  | 1:58:A:SER:C  | 1:59:A:PHE:N   | 1:59:A:PHE:CA  | 1:59:A:PHE:C  | 6                   | 2.18 | 0.56            | 2.08   |
| (1,143) | 1:94:A:ARG:N  | 1:94:A:ARG:CA  | 1:94:A:ARG:C   | 1:95:A:ILE:N  | 6                   | 1.52 | 0.23            | 1.56   |
| (1,8)   | 1:10:A:VAL:N  | 1:10:A:VAL:CA  | 1:10:A:VAL:C   | 1:11:A:GLU:N  | 5                   | 1.5  | 0.45            | 1.27   |
| (1,77)  | 1:54:A:VAL:C  | 1:55:A:PHE:N   | 1:55:A:PHE:CA  | 1:55:A:PHE:C  | 5                   | 1.34 | 0.37            | 1.15   |
| (1,64)  | 1:47:A:LYS:N  | 1:47:A:LYS:CA  | 1:47:A:LYS:C   | 1:48:A:LEU:N  | 4                   | 1.85 | 0.38            | 2.02   |

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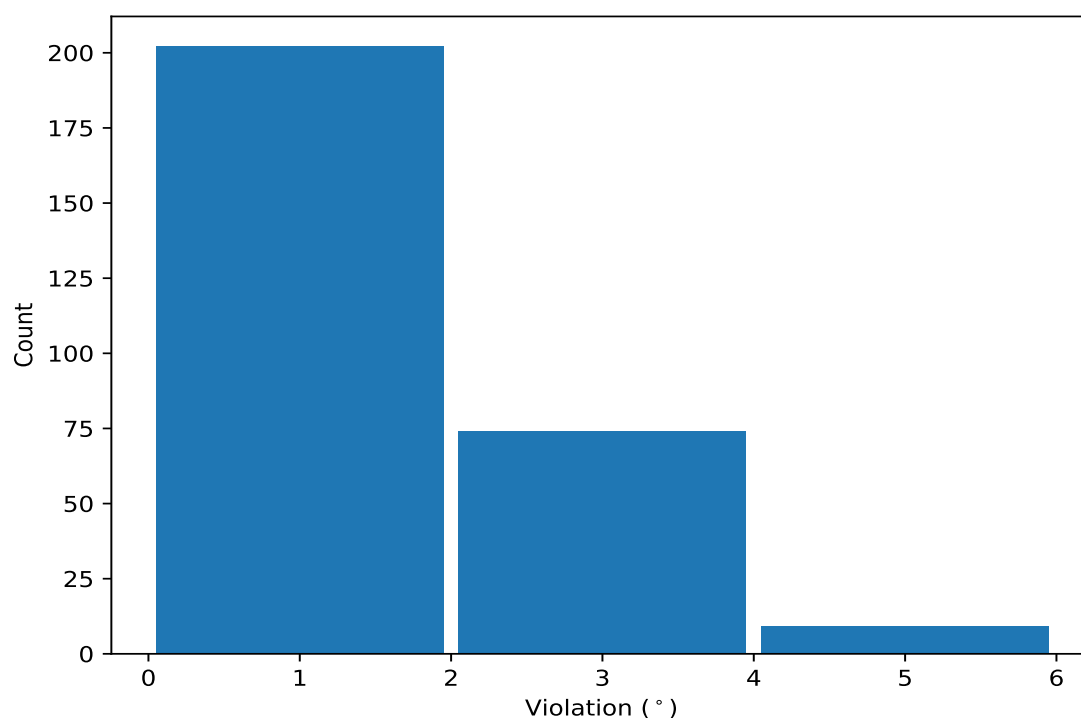
| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Models <sup>1</sup> | Mean | SD <sup>2</sup> | Median |
|---------|---------------|----------------|----------------|---------------|---------------------|------|-----------------|--------|
| (1,84)  | 1:58:A:SER:N  | 1:58:A:SER:CA  | 1:58:A:SER:C   | 1:59:A:PHE:N  | 4                   | 1.83 | 0.4             | 1.66   |
| (1,83)  | 1:57:A:SER:C  | 1:58:A:SER:N   | 1:58:A:SER:CA  | 1:58:A:SER:C  | 4                   | 1.81 | 0.52            | 1.98   |
| (1,105) | 1:71:A:GLN:C  | 1:72:A:GLY:N   | 1:72:A:GLY:CA  | 1:72:A:GLY:C  | 4                   | 1.81 | 0.78            | 1.48   |
| (1,132) | 1:88:A:ASN:C  | 1:89:A:GLU:N   | 1:89:A:GLU:CA  | 1:89:A:GLU:C  | 4                   | 1.38 | 0.27            | 1.38   |
| (1,21)  | 1:18:A:VAL:C  | 1:19:A:ILE:N   | 1:19:A:ILE:CA  | 1:19:A:ILE:C  | 4                   | 1.2  | 0.17            | 1.14   |
| (1,81)  | 1:56:A:ASP:C  | 1:57:A:SER:N   | 1:57:A:SER:CA  | 1:57:A:SER:C  | 3                   | 1.86 | 0.52            | 1.59   |
| (1,38)  | 1:31:A:GLU:N  | 1:31:A:GLU:CA  | 1:31:A:GLU:C   | 1:32:A:ASN:N  | 3                   | 1.68 | 0.42            | 1.65   |
| (1,180) | 1:124:A:SER:C | 1:125:A:PHE:N  | 1:125:A:PHE:CA | 1:125:A:PHE:C | 3                   | 1.47 | 0.33            | 1.59   |
| (1,185) | 1:127:A:GLU:N | 1:127:A:GLU:CA | 1:127:A:GLU:C  | 1:128:A:LEU:N | 3                   | 1.45 | 0.48            | 1.23   |
| (1,24)  | 1:20:A:LYS:N  | 1:20:A:LYS:CA  | 1:20:A:LYS:C   | 1:21:A:THR:N  | 3                   | 1.45 | 0.52            | 1.14   |
| (1,120) | 1:80:A:ILE:C  | 1:81:A:CYS:N   | 1:81:A:CYS:CA  | 1:81:A:CYS:C  | 3                   | 1.44 | 0.43            | 1.19   |
| (1,47)  | 1:36:A:LYS:C  | 1:37:A:GLY:N   | 1:37:A:GLY:CA  | 1:37:A:GLY:C  | 3                   | 1.38 | 0.11            | 1.35   |
| (1,94)  | 1:65:A:PHE:N  | 1:65:A:PHE:CA  | 1:65:A:PHE:C   | 1:66:A:LYS:N  | 3                   | 1.31 | 0.11            | 1.34   |
| (1,177) | 1:122:A:LEU:N | 1:122:A:LEU:CA | 1:122:A:LEU:C  | 1:123:A:LEU:N | 3                   | 1.28 | 0.11            | 1.3    |
| (1,46)  | 1:36:A:LYS:N  | 1:36:A:LYS:CA  | 1:36:A:LYS:C   | 1:37:A:GLY:N  | 2                   | 3.41 | 0.47            | 3.41   |
| (1,36)  | 1:30:A:GLU:N  | 1:30:A:GLU:CA  | 1:30:A:GLU:C   | 1:31:A:GLU:N  | 2                   | 2.86 | 1.82            | 2.86   |
| (1,108) | 1:74:A:VAL:N  | 1:74:A:VAL:CA  | 1:74:A:VAL:C   | 1:75:A:ILE:N  | 2                   | 2.33 | 0.97            | 2.33   |
| (1,127) | 1:85:A:MET:N  | 1:85:A:MET:CA  | 1:85:A:MET:C   | 1:86:A:ARG:N  | 2                   | 1.58 | 0.3             | 1.58   |
| (1,16)  | 1:15:A:ASP:N  | 1:15:A:ASP:CA  | 1:15:A:ASP:C   | 1:16:A:GLY:N  | 2                   | 1.5  | 0.19            | 1.5    |
| (1,140) | 1:92:A:LEU:C  | 1:93:A:VAL:N   | 1:93:A:VAL:CA  | 1:93:A:VAL:C  | 2                   | 1.3  | 0.02            | 1.3    |
| (1,106) | 1:72:A:GLY:N  | 1:72:A:GLY:CA  | 1:72:A:GLY:C   | 1:73:A:GLU:N  | 2                   | 1.23 | 0.02            | 1.23   |
| (1,112) | 1:76:A:LYS:C  | 1:77:A:GLY:N   | 1:77:A:GLY:CA  | 1:77:A:GLY:C  | 2                   | 1.18 | 0.04            | 1.18   |
| (1,160) | 1:108:A:GLU:C | 1:109:A:SER:N  | 1:109:A:SER:CA | 1:109:A:SER:C | 2                   | 1.18 | 0.03            | 1.18   |
| (1,69)  | 1:49:A:GLU:C  | 1:50:A:SER:N   | 1:50:A:SER:CA  | 1:50:A:SER:C  | 2                   | 1.16 | 0.04            | 1.16   |
| (1,149) | 1:98:A:MET:N  | 1:98:A:MET:CA  | 1:98:A:MET:C   | 1:99:A:TYR:N  | 2                   | 1.14 | 0.08            | 1.14   |
| (1,35)  | 1:29:A:GLY:C  | 1:30:A:GLU:N   | 1:30:A:GLU:CA  | 1:30:A:GLU:C  | 2                   | 1.03 | 0.03            | 1.03   |

<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 (°) |
|---------|---------------|----------------|---------------|---------------|----------|---------------|
| (1,100) | 1:68:A:HIS:N  | 1:68:A:HIS:CA  | 1:68:A:HIS:C  | 1:69:A:LEU:N  | 13       | 4.85          |
| (1,36)  | 1:30:A:GLU:N  | 1:30:A:GLU:CA  | 1:30:A:GLU:C  | 1:31:A:GLU:N  | 10       | 4.68          |
| (1,161) | 1:109:A:SER:N | 1:109:A:SER:CA | 1:109:A:SER:C | 1:110:A:ILE:N | 15       | 4.57          |
| (1,161) | 1:109:A:SER:N | 1:109:A:SER:CA | 1:109:A:SER:C | 1:110:A:ILE:N | 10       | 4.47          |
| (1,17)  | 1:15:A:ASP:C  | 1:16:A:GLY:N   | 1:16:A:GLY:CA | 1:16:A:GLY:C  | 15       | 4.44          |
| (1,109) | 1:74:A:VAL:C  | 1:75:A:ILE:N   | 1:75:A:ILE:CA | 1:75:A:ILE:C  | 10       | 4.43          |
| (1,109) | 1:74:A:VAL:C  | 1:75:A:ILE:N   | 1:75:A:ILE:CA | 1:75:A:ILE:C  | 2        | 4.37          |
| (1,40)  | 1:32:A:ASN:N  | 1:32:A:ASN:CA  | 1:32:A:ASN:C  | 1:33:A:ILE:N  | 7        | 4.1           |
| (1,161) | 1:109:A:SER:N | 1:109:A:SER:CA | 1:109:A:SER:C | 1:110:A:ILE:N | 20       | 4.07          |
| (1,46)  | 1:36:A:LYS:N  | 1:36:A:LYS:CA  | 1:36:A:LYS:C  | 1:37:A:GLY:N  | 1        | 3.88          |
| (1,161) | 1:109:A:SER:N | 1:109:A:SER:CA | 1:109:A:SER:C | 1:110:A:ILE:N | 8        | 3.65          |
| (1,40)  | 1:32:A:ASN:N  | 1:32:A:ASN:CA  | 1:32:A:ASN:C  | 1:33:A:ILE:N  | 1        | 3.48          |
| (1,37)  | 1:30:A:GLU:C  | 1:31:A:GLU:N   | 1:31:A:GLU:CA | 1:31:A:GLU:C  | 10       | 3.47          |
| (1,17)  | 1:15:A:ASP:C  | 1:16:A:GLY:N   | 1:16:A:GLY:CA | 1:16:A:GLY:C  | 4        | 3.47          |
| (1,161) | 1:109:A:SER:N | 1:109:A:SER:CA | 1:109:A:SER:C | 1:110:A:ILE:N | 5        | 3.37          |
| (1,17)  | 1:15:A:ASP:C  | 1:16:A:GLY:N   | 1:16:A:GLY:CA | 1:16:A:GLY:C  | 14       | 3.36          |
| (1,108) | 1:74:A:VAL:N  | 1:74:A:VAL:CA  | 1:74:A:VAL:C  | 1:75:A:ILE:N  | 2        | 3.3           |
| (1,17)  | 1:15:A:ASP:C  | 1:16:A:GLY:N   | 1:16:A:GLY:CA | 1:16:A:GLY:C  | 19       | 3.28          |
| (1,161) | 1:109:A:SER:N | 1:109:A:SER:CA | 1:109:A:SER:C | 1:110:A:ILE:N | 4        | 3.27          |
| (1,85)  | 1:58:A:SER:C  | 1:59:A:PHE:N   | 1:59:A:PHE:CA | 1:59:A:PHE:C  | 20       | 3.22          |
| (1,40)  | 1:32:A:ASN:N  | 1:32:A:ASN:CA  | 1:32:A:ASN:C  | 1:33:A:ILE:N  | 3        | 3.22          |

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| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,100) | 1:68:A:HIS:N  | 1:68:A:HIS:CA  | 1:68:A:HIS:C   | 1:69:A:LEU:N  | 10       | 3.16          |
| (1,17)  | 1:15:A:ASP:C  | 1:16:A:GLY:N   | 1:16:A:GLY:CA  | 1:16:A:GLY:C  | 13       | 3.16          |
| (1,105) | 1:71:A:GLN:C  | 1:72:A:GLY:N   | 1:72:A:GLY:CA  | 1:72:A:GLY:C  | 13       | 3.13          |
| (1,17)  | 1:15:A:ASP:C  | 1:16:A:GLY:N   | 1:16:A:GLY:CA  | 1:16:A:GLY:C  | 5        | 3.09          |
| (1,17)  | 1:15:A:ASP:C  | 1:16:A:GLY:N   | 1:16:A:GLY:CA  | 1:16:A:GLY:C  | 20       | 3.07          |
| (1,161) | 1:109:A:SER:N | 1:109:A:SER:CA | 1:109:A:SER:C  | 1:110:A:ILE:N | 1        | 3.04          |
| (1,17)  | 1:15:A:ASP:C  | 1:16:A:GLY:N   | 1:16:A:GLY:CA  | 1:16:A:GLY:C  | 1        | 3.03          |
| (1,17)  | 1:15:A:ASP:C  | 1:16:A:GLY:N   | 1:16:A:GLY:CA  | 1:16:A:GLY:C  | 10       | 3.0           |
| (1,17)  | 1:15:A:ASP:C  | 1:16:A:GLY:N   | 1:16:A:GLY:CA  | 1:16:A:GLY:C  | 16       | 3.0           |
| (1,161) | 1:109:A:SER:N | 1:109:A:SER:CA | 1:109:A:SER:C  | 1:110:A:ILE:N | 11       | 2.96          |
| (1,40)  | 1:32:A:ASN:N  | 1:32:A:ASN:CA  | 1:32:A:ASN:C   | 1:33:A:ILE:N  | 15       | 2.96          |
| (1,46)  | 1:36:A:LYS:N  | 1:36:A:LYS:CA  | 1:36:A:LYS:C   | 1:37:A:GLY:N  | 4        | 2.94          |
| (1,102) | 1:69:A:LEU:N  | 1:69:A:LEU:CA  | 1:69:A:LEU:C   | 1:70:A:GLU:N  | 13       | 2.93          |
| (1,17)  | 1:15:A:ASP:C  | 1:16:A:GLY:N   | 1:16:A:GLY:CA  | 1:16:A:GLY:C  | 11       | 2.86          |
| (1,161) | 1:109:A:SER:N | 1:109:A:SER:CA | 1:109:A:SER:C  | 1:110:A:ILE:N | 12       | 2.78          |
| (1,161) | 1:109:A:SER:N | 1:109:A:SER:CA | 1:109:A:SER:C  | 1:110:A:ILE:N | 16       | 2.75          |
| (1,100) | 1:68:A:HIS:N  | 1:68:A:HIS:CA  | 1:68:A:HIS:C   | 1:69:A:LEU:N  | 8        | 2.73          |
| (1,161) | 1:109:A:SER:N | 1:109:A:SER:CA | 1:109:A:SER:C  | 1:110:A:ILE:N | 13       | 2.72          |
| (1,159) | 1:108:A:GLU:N | 1:108:A:GLU:CA | 1:108:A:GLU:C  | 1:109:A:SER:N | 18       | 2.71          |
| (1,7)   | 1:9:A:LYS:C   | 1:10:A:VAL:N   | 1:10:A:VAL:CA  | 1:10:A:VAL:C  | 15       | 2.61          |
| (1,113) | 1:77:A:GLY:N  | 1:77:A:GLY:CA  | 1:77:A:GLY:C   | 1:78:A:TRP:N  | 15       | 2.59          |
| (1,81)  | 1:56:A:ASP:C  | 1:57:A:SER:N   | 1:57:A:SER:CA  | 1:57:A:SER:C  | 9        | 2.58          |
| (1,7)   | 1:9:A:LYS:C   | 1:10:A:VAL:N   | 1:10:A:VAL:CA  | 1:10:A:VAL:C  | 17       | 2.57          |
| (1,40)  | 1:32:A:ASN:N  | 1:32:A:ASN:CA  | 1:32:A:ASN:C   | 1:33:A:ILE:N  | 11       | 2.53          |
| (1,84)  | 1:58:A:SER:N  | 1:58:A:SER:CA  | 1:58:A:SER:C   | 1:59:A:PHE:N  | 19       | 2.5           |
| (1,161) | 1:109:A:SER:N | 1:109:A:SER:CA | 1:109:A:SER:C  | 1:110:A:ILE:N | 14       | 2.45          |
| (1,85)  | 1:58:A:SER:C  | 1:59:A:PHE:N   | 1:59:A:PHE:CA  | 1:59:A:PHE:C  | 19       | 2.44          |
| (1,172) | 1:119:A:GLU:C | 1:120:A:ILE:N  | 1:120:A:ILE:CA | 1:120:A:ILE:C | 19       | 2.42          |
| (1,172) | 1:119:A:GLU:C | 1:120:A:ILE:N  | 1:120:A:ILE:CA | 1:120:A:ILE:C | 2        | 2.41          |
| (1,172) | 1:119:A:GLU:C | 1:120:A:ILE:N  | 1:120:A:ILE:CA | 1:120:A:ILE:C | 5        | 2.35          |
| (1,100) | 1:68:A:HIS:N  | 1:68:A:HIS:CA  | 1:68:A:HIS:C   | 1:69:A:LEU:N  | 7        | 2.35          |
| (1,17)  | 1:15:A:ASP:C  | 1:16:A:GLY:N   | 1:16:A:GLY:CA  | 1:16:A:GLY:C  | 12       | 2.35          |
| (1,83)  | 1:57:A:SER:C  | 1:58:A:SER:N   | 1:58:A:SER:CA  | 1:58:A:SER:C  | 7        | 2.3           |
| (1,17)  | 1:15:A:ASP:C  | 1:16:A:GLY:N   | 1:16:A:GLY:CA  | 1:16:A:GLY:C  | 17       | 2.3           |
| (1,7)   | 1:9:A:LYS:C   | 1:10:A:VAL:N   | 1:10:A:VAL:CA  | 1:10:A:VAL:C  | 10       | 2.29          |
| (1,40)  | 1:32:A:ASN:N  | 1:32:A:ASN:CA  | 1:32:A:ASN:C   | 1:33:A:ILE:N  | 8        | 2.26          |
| (1,17)  | 1:15:A:ASP:C  | 1:16:A:GLY:N   | 1:16:A:GLY:CA  | 1:16:A:GLY:C  | 18       | 2.26          |
| (1,7)   | 1:9:A:LYS:C   | 1:10:A:VAL:N   | 1:10:A:VAL:CA  | 1:10:A:VAL:C  | 2        | 2.26          |
| (1,161) | 1:109:A:SER:N | 1:109:A:SER:CA | 1:109:A:SER:C  | 1:110:A:ILE:N | 19       | 2.25          |
| (1,83)  | 1:57:A:SER:C  | 1:58:A:SER:N   | 1:58:A:SER:CA  | 1:58:A:SER:C  | 19       | 2.24          |
| (1,85)  | 1:58:A:SER:C  | 1:59:A:PHE:N   | 1:59:A:PHE:CA  | 1:59:A:PHE:C  | 10       | 2.22          |
| (1,8)   | 1:10:A:VAL:N  | 1:10:A:VAL:CA  | 1:10:A:VAL:C   | 1:11:A:GLU:N  | 14       | 2.21          |
| (1,38)  | 1:31:A:GLU:N  | 1:31:A:GLU:CA  | 1:31:A:GLU:C   | 1:32:A:ASN:N  | 14       | 2.2           |
| (1,64)  | 1:47:A:LYS:N  | 1:47:A:LYS:CA  | 1:47:A:LYS:C   | 1:48:A:LEU:N  | 18       | 2.18          |
| (1,24)  | 1:20:A:LYS:N  | 1:20:A:LYS:CA  | 1:20:A:LYS:C   | 1:21:A:THR:N  | 17       | 2.18          |
| (1,17)  | 1:15:A:ASP:C  | 1:16:A:GLY:N   | 1:16:A:GLY:CA  | 1:16:A:GLY:C  | 2        | 2.18          |
| (1,7)   | 1:9:A:LYS:C   | 1:10:A:VAL:N   | 1:10:A:VAL:CA  | 1:10:A:VAL:C  | 1        | 2.18          |
| (1,113) | 1:77:A:GLY:N  | 1:77:A:GLY:CA  | 1:77:A:GLY:C   | 1:78:A:TRP:N  | 1        | 2.17          |
| (1,109) | 1:74:A:VAL:C  | 1:75:A:ILE:N   | 1:75:A:ILE:CA  | 1:75:A:ILE:C  | 3        | 2.17          |
| (1,159) | 1:108:A:GLU:N | 1:108:A:GLU:CA | 1:108:A:GLU:C  | 1:109:A:SER:N | 5        | 2.13          |
| (1,40)  | 1:32:A:ASN:N  | 1:32:A:ASN:CA  | 1:32:A:ASN:C   | 1:33:A:ILE:N  | 14       | 2.13          |

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| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,185) | 1:127:A:GLU:N | 1:127:A:GLU:CA | 1:127:A:GLU:C  | 1:128:A:LEU:N | 18       | 2.12          |
| (1,17)  | 1:15:A:ASP:C  | 1:16:A:GLY:N   | 1:16:A:GLY:CA  | 1:16:A:GLY:C  | 6        | 2.11          |
| (1,117) | 1:79:A:ASP:N  | 1:79:A:ASP:CA  | 1:79:A:ASP:C   | 1:80:A:ILE:N  | 4        | 2.1           |
| (1,109) | 1:74:A:VAL:C  | 1:75:A:ILE:N   | 1:75:A:ILE:CA  | 1:75:A:ILE:C  | 14       | 2.1           |
| (1,100) | 1:68:A:HIS:N  | 1:68:A:HIS:CA  | 1:68:A:HIS:C   | 1:69:A:LEU:N  | 4        | 2.1           |
| (1,40)  | 1:32:A:ASN:N  | 1:32:A:ASN:CA  | 1:32:A:ASN:C   | 1:33:A:ILE:N  | 9        | 2.09          |
| (1,148) | 1:97:A:SER:C  | 1:98:A:MET:N   | 1:98:A:MET:CA  | 1:98:A:MET:C  | 2        | 2.06          |
| (1,64)  | 1:47:A:LYS:N  | 1:47:A:LYS:CA  | 1:47:A:LYS:C   | 1:48:A:LEU:N  | 1        | 2.06          |
| (1,120) | 1:80:A:ILE:C  | 1:81:A:CYS:N   | 1:81:A:CYS:CA  | 1:81:A:CYS:C  | 13       | 2.05          |
| (1,77)  | 1:54:A:VAL:C  | 1:55:A:PHE:N   | 1:55:A:PHE:CA  | 1:55:A:PHE:C  | 3        | 2.04          |
| (1,100) | 1:68:A:HIS:N  | 1:68:A:HIS:CA  | 1:68:A:HIS:C   | 1:69:A:LEU:N  | 15       | 2.01          |
| (1,17)  | 1:15:A:ASP:C  | 1:16:A:GLY:N   | 1:16:A:GLY:CA  | 1:16:A:GLY:C  | 7        | 1.98          |
| (1,64)  | 1:47:A:LYS:N  | 1:47:A:LYS:CA  | 1:47:A:LYS:C   | 1:48:A:LEU:N  | 3        | 1.97          |
| (1,93)  | 1:64:A:PRO:C  | 1:65:A:PHE:N   | 1:65:A:PHE:CA  | 1:65:A:PHE:C  | 10       | 1.95          |
| (1,85)  | 1:58:A:SER:C  | 1:59:A:PHE:N   | 1:59:A:PHE:CA  | 1:59:A:PHE:C  | 7        | 1.95          |
| (1,17)  | 1:15:A:ASP:C  | 1:16:A:GLY:N   | 1:16:A:GLY:CA  | 1:16:A:GLY:C  | 8        | 1.91          |
| (1,93)  | 1:64:A:PRO:C  | 1:65:A:PHE:N   | 1:65:A:PHE:CA  | 1:65:A:PHE:C  | 17       | 1.9           |
| (1,172) | 1:119:A:GLU:C | 1:120:A:ILE:N  | 1:120:A:ILE:CA | 1:120:A:ILE:C | 14       | 1.89          |
| (1,127) | 1:85:A:MET:N  | 1:85:A:MET:CA  | 1:85:A:MET:C   | 1:86:A:ARG:N  | 13       | 1.88          |
| (1,143) | 1:94:A:ARG:N  | 1:94:A:ARG:CA  | 1:94:A:ARG:C   | 1:95:A:ILE:N  | 17       | 1.87          |
| (1,123) | 1:82:A:VAL:N  | 1:82:A:VAL:CA  | 1:82:A:VAL:C   | 1:83:A:SER:N  | 20       | 1.87          |
| (1,117) | 1:79:A:ASP:N  | 1:79:A:ASP:CA  | 1:79:A:ASP:C   | 1:80:A:ILE:N  | 9        | 1.86          |
| (1,114) | 1:77:A:GLY:C  | 1:78:A:TRP:N   | 1:78:A:TRP:CA  | 1:78:A:TRP:C  | 19       | 1.86          |
| (1,100) | 1:68:A:HIS:N  | 1:68:A:HIS:CA  | 1:68:A:HIS:C   | 1:69:A:LEU:N  | 6        | 1.85          |
| (1,8)   | 1:10:A:VAL:N  | 1:10:A:VAL:CA  | 1:10:A:VAL:C   | 1:11:A:GLU:N  | 2        | 1.85          |
| (1,61)  | 1:44:A:TYR:C  | 1:45:A:VAL:N   | 1:45:A:VAL:CA  | 1:45:A:VAL:C  | 11       | 1.84          |
| (1,117) | 1:79:A:ASP:N  | 1:79:A:ASP:CA  | 1:79:A:ASP:C   | 1:80:A:ILE:N  | 17       | 1.82          |
| (1,85)  | 1:58:A:SER:C  | 1:59:A:PHE:N   | 1:59:A:PHE:CA  | 1:59:A:PHE:C  | 1        | 1.82          |
| (1,161) | 1:109:A:SER:N | 1:109:A:SER:CA | 1:109:A:SER:C  | 1:110:A:ILE:N | 3        | 1.8           |
| (1,159) | 1:108:A:GLU:N | 1:108:A:GLU:CA | 1:108:A:GLU:C  | 1:109:A:SER:N | 9        | 1.8           |
| (1,84)  | 1:58:A:SER:N  | 1:58:A:SER:CA  | 1:58:A:SER:C   | 1:59:A:PHE:N  | 7        | 1.8           |
| (1,180) | 1:124:A:SER:C | 1:125:A:PHE:N  | 1:125:A:PHE:CA | 1:125:A:PHE:C | 10       | 1.79          |
| (1,114) | 1:77:A:GLY:C  | 1:78:A:TRP:N   | 1:78:A:TRP:CA  | 1:78:A:TRP:C  | 13       | 1.79          |
| (1,61)  | 1:44:A:TYR:C  | 1:45:A:VAL:N   | 1:45:A:VAL:CA  | 1:45:A:VAL:C  | 16       | 1.78          |
| (1,159) | 1:108:A:GLU:N | 1:108:A:GLU:CA | 1:108:A:GLU:C  | 1:109:A:SER:N | 2        | 1.77          |
| (1,114) | 1:77:A:GLY:C  | 1:78:A:TRP:N   | 1:78:A:TRP:CA  | 1:78:A:TRP:C  | 15       | 1.77          |
| (1,109) | 1:74:A:VAL:C  | 1:75:A:ILE:N   | 1:75:A:ILE:CA  | 1:75:A:ILE:C  | 17       | 1.73          |
| (1,93)  | 1:64:A:PRO:C  | 1:65:A:PHE:N   | 1:65:A:PHE:CA  | 1:65:A:PHE:C  | 5        | 1.73          |
| (1,7)   | 1:9:A:LYS:C   | 1:10:A:VAL:N   | 1:10:A:VAL:CA  | 1:10:A:VAL:C  | 13       | 1.73          |
| (1,137) | 1:91:A:CYS:N  | 1:91:A:CYS:CA  | 1:91:A:CYS:C   | 1:92:A:LEU:N  | 7        | 1.72          |
| (1,113) | 1:77:A:GLY:N  | 1:77:A:GLY:CA  | 1:77:A:GLY:C   | 1:78:A:TRP:N  | 9        | 1.71          |
| (1,83)  | 1:57:A:SER:C  | 1:58:A:SER:N   | 1:58:A:SER:CA  | 1:58:A:SER:C  | 20       | 1.71          |
| (1,132) | 1:88:A:ASN:C  | 1:89:A:GLU:N   | 1:89:A:GLU:CA  | 1:89:A:GLU:C  | 2        | 1.7           |
| (1,159) | 1:108:A:GLU:N | 1:108:A:GLU:CA | 1:108:A:GLU:C  | 1:109:A:SER:N | 8        | 1.69          |
| (1,123) | 1:82:A:VAL:N  | 1:82:A:VAL:CA  | 1:82:A:VAL:C   | 1:83:A:SER:N  | 4        | 1.69          |
| (1,16)  | 1:15:A:ASP:N  | 1:15:A:ASP:CA  | 1:15:A:ASP:C   | 1:16:A:GLY:N  | 10       | 1.69          |
| (1,181) | 1:125:A:PHE:N | 1:125:A:PHE:CA | 1:125:A:PHE:C  | 1:126:A:ARG:N | 18       | 1.68          |
| (1,109) | 1:74:A:VAL:C  | 1:75:A:ILE:N   | 1:75:A:ILE:CA  | 1:75:A:ILE:C  | 18       | 1.68          |
| (1,38)  | 1:31:A:GLU:N  | 1:31:A:GLU:CA  | 1:31:A:GLU:C   | 1:32:A:ASN:N  | 10       | 1.65          |
| (1,148) | 1:97:A:SER:C  | 1:98:A:MET:N   | 1:98:A:MET:CA  | 1:98:A:MET:C  | 8        | 1.64          |
| (1,103) | 1:70:A:GLU:C  | 1:71:A:GLN:N   | 1:71:A:GLN:CA  | 1:71:A:GLN:C  | 14       | 1.64          |

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| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,17)  | 1:15:A:ASP:C  | 1:16:A:GLY:N   | 1:16:A:GLY:CA  | 1:16:A:GLY:C  | 3        | 1.64          |
| (1,40)  | 1:32:A:ASN:N  | 1:32:A:ASN:CA  | 1:32:A:ASN:C   | 1:33:A:ILE:N  | 2        | 1.63          |
| (1,7)   | 1:9:A:LYS:C   | 1:10:A:VAL:N   | 1:10:A:VAL:CA  | 1:10:A:VAL:C  | 14       | 1.63          |
| (1,159) | 1:108:A:GLU:N | 1:108:A:GLU:CA | 1:108:A:GLU:C  | 1:109:A:SER:N | 20       | 1.62          |
| (1,143) | 1:94:A:ARG:N  | 1:94:A:ARG:CA  | 1:94:A:ARG:C   | 1:95:A:ILE:N  | 2        | 1.62          |
| (1,132) | 1:88:A:ASN:C  | 1:89:A:GLU:N   | 1:89:A:GLU:CA  | 1:89:A:GLU:C  | 1        | 1.61          |
| (1,109) | 1:74:A:VAL:C  | 1:75:A:ILE:N   | 1:75:A:ILE:CA  | 1:75:A:ILE:C  | 9        | 1.61          |
| (1,100) | 1:68:A:HIS:N  | 1:68:A:HIS:CA  | 1:68:A:HIS:C   | 1:69:A:LEU:N  | 3        | 1.61          |
| (1,109) | 1:74:A:VAL:C  | 1:75:A:ILE:N   | 1:75:A:ILE:CA  | 1:75:A:ILE:C  | 13       | 1.6           |
| (1,105) | 1:71:A:GLN:C  | 1:72:A:GLY:N   | 1:72:A:GLY:CA  | 1:72:A:GLY:C  | 15       | 1.6           |
| (1,180) | 1:124:A:SER:C | 1:125:A:PHE:N  | 1:125:A:PHE:CA | 1:125:A:PHE:C | 4        | 1.59          |
| (1,117) | 1:79:A:ASP:N  | 1:79:A:ASP:CA  | 1:79:A:ASP:C   | 1:80:A:ILE:N  | 1        | 1.59          |
| (1,81)  | 1:56:A:ASP:C  | 1:57:A:SER:N   | 1:57:A:SER:CA  | 1:57:A:SER:C  | 6        | 1.59          |
| (1,50)  | 1:39:A:GLU:N  | 1:39:A:GLU:CA  | 1:39:A:GLU:C   | 1:40:A:VAL:N  | 4        | 1.59          |
| (1,148) | 1:97:A:SER:C  | 1:98:A:MET:N   | 1:98:A:MET:CA  | 1:98:A:MET:C  | 10       | 1.58          |
| (1,148) | 1:97:A:SER:C  | 1:98:A:MET:N   | 1:98:A:MET:CA  | 1:98:A:MET:C  | 17       | 1.58          |
| (1,114) | 1:77:A:GLY:C  | 1:78:A:TRP:N   | 1:78:A:TRP:CA  | 1:78:A:TRP:C  | 8        | 1.58          |
| (1,143) | 1:94:A:ARG:N  | 1:94:A:ARG:CA  | 1:94:A:ARG:C   | 1:95:A:ILE:N  | 6        | 1.57          |
| (1,61)  | 1:44:A:TYR:C  | 1:45:A:VAL:N   | 1:45:A:VAL:CA  | 1:45:A:VAL:C  | 13       | 1.57          |
| (1,143) | 1:94:A:ARG:N  | 1:94:A:ARG:CA  | 1:94:A:ARG:C   | 1:95:A:ILE:N  | 8        | 1.56          |
| (1,123) | 1:82:A:VAL:N  | 1:82:A:VAL:CA  | 1:82:A:VAL:C   | 1:83:A:SER:N  | 2        | 1.56          |
| (1,55)  | 1:41:A:THR:C  | 1:42:A:VAL:N   | 1:42:A:VAL:CA  | 1:42:A:VAL:C  | 4        | 1.56          |
| (1,172) | 1:119:A:GLU:C | 1:120:A:ILE:N  | 1:120:A:ILE:CA | 1:120:A:ILE:C | 1        | 1.54          |
| (1,152) | 1:102:A:GLY:C | 1:103:A:ASP:N  | 1:103:A:ASP:CA | 1:103:A:ASP:C | 9        | 1.53          |
| (1,123) | 1:82:A:VAL:N  | 1:82:A:VAL:CA  | 1:82:A:VAL:C   | 1:83:A:SER:N  | 9        | 1.53          |
| (1,84)  | 1:58:A:SER:N  | 1:58:A:SER:CA  | 1:58:A:SER:C   | 1:59:A:PHE:N  | 20       | 1.53          |
| (1,47)  | 1:36:A:LYS:C  | 1:37:A:GLY:N   | 1:37:A:GLY:CA  | 1:37:A:GLY:C  | 9        | 1.53          |
| (1,172) | 1:119:A:GLU:C | 1:120:A:ILE:N  | 1:120:A:ILE:CA | 1:120:A:ILE:C | 8        | 1.52          |
| (1,156) | 1:105:A:GLY:C | 1:106:A:CYS:N  | 1:106:A:CYS:CA | 1:106:A:CYS:C | 10       | 1.52          |
| (1,113) | 1:77:A:GLY:N  | 1:77:A:GLY:CA  | 1:77:A:GLY:C   | 1:78:A:TRP:N  | 3        | 1.51          |
| (1,172) | 1:119:A:GLU:C | 1:120:A:ILE:N  | 1:120:A:ILE:CA | 1:120:A:ILE:C | 20       | 1.5           |
| (1,161) | 1:109:A:SER:N | 1:109:A:SER:CA | 1:109:A:SER:C  | 1:110:A:ILE:N | 7        | 1.5           |
| (1,145) | 1:95:A:ILE:N  | 1:95:A:ILE:CA  | 1:95:A:ILE:C   | 1:96:A:GLU:N  | 17       | 1.5           |
| (1,109) | 1:74:A:VAL:C  | 1:75:A:ILE:N   | 1:75:A:ILE:CA  | 1:75:A:ILE:C  | 6        | 1.5           |
| (1,84)  | 1:58:A:SER:N  | 1:58:A:SER:CA  | 1:58:A:SER:C   | 1:59:A:PHE:N  | 9        | 1.5           |
| (1,93)  | 1:64:A:PRO:C  | 1:65:A:PHE:N   | 1:65:A:PHE:CA  | 1:65:A:PHE:C  | 9        | 1.49          |
| (1,100) | 1:68:A:HIS:N  | 1:68:A:HIS:CA  | 1:68:A:HIS:C   | 1:69:A:LEU:N  | 12       | 1.48          |
| (1,21)  | 1:18:A:VAL:C  | 1:19:A:ILE:N   | 1:19:A:ILE:CA  | 1:19:A:ILE:C  | 17       | 1.48          |
| (1,61)  | 1:44:A:TYR:C  | 1:45:A:VAL:N   | 1:45:A:VAL:CA  | 1:45:A:VAL:C  | 1        | 1.47          |
| (1,113) | 1:77:A:GLY:N  | 1:77:A:GLY:CA  | 1:77:A:GLY:C   | 1:78:A:TRP:N  | 20       | 1.46          |
| (1,86)  | 1:59:A:PHE:N  | 1:59:A:PHE:CA  | 1:59:A:PHE:C   | 1:60:A:ASP:N  | 1        | 1.45          |
| (1,63)  | 1:46:A:GLY:C  | 1:47:A:LYS:N   | 1:47:A:LYS:CA  | 1:47:A:LYS:C  | 7        | 1.45          |
| (1,9)   | 1:10:A:VAL:C  | 1:11:A:GLU:N   | 1:11:A:GLU:CA  | 1:11:A:GLU:C  | 2        | 1.45          |
| (1,94)  | 1:65:A:PHE:N  | 1:65:A:PHE:CA  | 1:65:A:PHE:C   | 1:66:A:LYS:N  | 13       | 1.43          |
| (1,113) | 1:77:A:GLY:N  | 1:77:A:GLY:CA  | 1:77:A:GLY:C   | 1:78:A:TRP:N  | 13       | 1.42          |
| (1,85)  | 1:58:A:SER:C  | 1:59:A:PHE:N   | 1:59:A:PHE:CA  | 1:59:A:PHE:C  | 11       | 1.42          |
| (1,177) | 1:122:A:LEU:N | 1:122:A:LEU:CA | 1:122:A:LEU:C  | 1:123:A:LEU:N | 2        | 1.4           |
| (1,81)  | 1:56:A:ASP:C  | 1:57:A:SER:N   | 1:57:A:SER:CA  | 1:57:A:SER:C  | 3        | 1.4           |
| (1,117) | 1:79:A:ASP:N  | 1:79:A:ASP:CA  | 1:79:A:ASP:C   | 1:80:A:ILE:N  | 19       | 1.39          |
| (1,77)  | 1:54:A:VAL:C  | 1:55:A:PHE:N   | 1:55:A:PHE:CA  | 1:55:A:PHE:C  | 18       | 1.39          |
| (1,40)  | 1:32:A:ASN:N  | 1:32:A:ASN:CA  | 1:32:A:ASN:C   | 1:33:A:ILE:N  | 19       | 1.39          |

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| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,100) | 1:68:A:HIS:N  | 1:68:A:HIS:CA  | 1:68:A:HIS:C   | 1:69:A:LEU:N  | 9        | 1.38          |
| (1,123) | 1:82:A:VAL:N  | 1:82:A:VAL:CA  | 1:82:A:VAL:C   | 1:83:A:SER:N  | 18       | 1.37          |
| (1,105) | 1:71:A:GLN:C  | 1:72:A:GLY:N   | 1:72:A:GLY:CA  | 1:72:A:GLY:C  | 3        | 1.37          |
| (1,113) | 1:77:A:GLY:N  | 1:77:A:GLY:CA  | 1:77:A:GLY:C   | 1:78:A:TRP:N  | 18       | 1.36          |
| (1,109) | 1:74:A:VAL:C  | 1:75:A:ILE:N   | 1:75:A:ILE:CA  | 1:75:A:ILE:C  | 8        | 1.36          |
| (1,108) | 1:74:A:VAL:N  | 1:74:A:VAL:CA  | 1:74:A:VAL:C   | 1:75:A:ILE:N  | 3        | 1.36          |
| (1,143) | 1:94:A:ARG:N  | 1:94:A:ARG:CA  | 1:94:A:ARG:C   | 1:95:A:ILE:N  | 7        | 1.35          |
| (1,47)  | 1:36:A:LYS:C  | 1:37:A:GLY:N   | 1:37:A:GLY:CA  | 1:37:A:GLY:C  | 20       | 1.35          |
| (1,94)  | 1:65:A:PHE:N  | 1:65:A:PHE:CA  | 1:65:A:PHE:C   | 1:66:A:LYS:N  | 6        | 1.34          |
| (1,57)  | 1:42:A:VAL:C  | 1:43:A:HIS:N   | 1:43:A:HIS:CA  | 1:43:A:HIS:C  | 5        | 1.34          |
| (1,113) | 1:77:A:GLY:N  | 1:77:A:GLY:CA  | 1:77:A:GLY:C   | 1:78:A:TRP:N  | 19       | 1.33          |
| (1,61)  | 1:44:A:TYR:C  | 1:45:A:VAL:N   | 1:45:A:VAL:CA  | 1:45:A:VAL:C  | 20       | 1.33          |
| (1,59)  | 1:43:A:HIS:C  | 1:44:A:TYR:N   | 1:44:A:TYR:CA  | 1:44:A:TYR:C  | 16       | 1.33          |
| (1,140) | 1:92:A:LEU:C  | 1:93:A:VAL:N   | 1:93:A:VAL:CA  | 1:93:A:VAL:C  | 2        | 1.31          |
| (1,7)   | 1:9:A:LYS:C   | 1:10:A:VAL:N   | 1:10:A:VAL:CA  | 1:10:A:VAL:C  | 8        | 1.31          |
| (1,177) | 1:122:A:LEU:N | 1:122:A:LEU:CA | 1:122:A:LEU:C  | 1:123:A:LEU:N | 12       | 1.3           |
| (1,161) | 1:109:A:SER:N | 1:109:A:SER:CA | 1:109:A:SER:C  | 1:110:A:ILE:N | 9        | 1.3           |
| (1,113) | 1:77:A:GLY:N  | 1:77:A:GLY:CA  | 1:77:A:GLY:C   | 1:78:A:TRP:N  | 4        | 1.3           |
| (1,16)  | 1:15:A:ASP:N  | 1:15:A:ASP:CA  | 1:15:A:ASP:C   | 1:16:A:GLY:N  | 8        | 1.3           |
| (1,161) | 1:109:A:SER:N | 1:109:A:SER:CA | 1:109:A:SER:C  | 1:110:A:ILE:N | 6        | 1.29          |
| (1,140) | 1:92:A:LEU:C  | 1:93:A:VAL:N   | 1:93:A:VAL:CA  | 1:93:A:VAL:C  | 5        | 1.28          |
| (1,114) | 1:77:A:GLY:C  | 1:78:A:TRP:N   | 1:78:A:TRP:CA  | 1:78:A:TRP:C  | 17       | 1.28          |
| (1,80)  | 1:56:A:ASP:N  | 1:56:A:ASP:CA  | 1:56:A:ASP:C   | 1:57:A:SER:N  | 8        | 1.28          |
| (1,127) | 1:85:A:MET:N  | 1:85:A:MET:CA  | 1:85:A:MET:C   | 1:86:A:ARG:N  | 18       | 1.27          |
| (1,61)  | 1:44:A:TYR:C  | 1:45:A:VAL:N   | 1:45:A:VAL:CA  | 1:45:A:VAL:C  | 5        | 1.27          |
| (1,53)  | 1:40:A:VAL:C  | 1:41:A:THR:N   | 1:41:A:THR:CA  | 1:41:A:THR:C  | 13       | 1.27          |
| (1,47)  | 1:36:A:LYS:C  | 1:37:A:GLY:N   | 1:37:A:GLY:CA  | 1:37:A:GLY:C  | 4        | 1.27          |
| (1,17)  | 1:15:A:ASP:C  | 1:16:A:GLY:N   | 1:16:A:GLY:CA  | 1:16:A:GLY:C  | 9        | 1.27          |
| (1,8)   | 1:10:A:VAL:N  | 1:10:A:VAL:CA  | 1:10:A:VAL:C   | 1:11:A:GLU:N  | 15       | 1.27          |
| (1,123) | 1:82:A:VAL:N  | 1:82:A:VAL:CA  | 1:82:A:VAL:C   | 1:83:A:SER:N  | 5        | 1.26          |
| (1,93)  | 1:64:A:PRO:C  | 1:65:A:PHE:N   | 1:65:A:PHE:CA  | 1:65:A:PHE:C  | 7        | 1.26          |
| (1,174) | 1:120:A:ILE:C | 1:121:A:GLU:N  | 1:121:A:GLU:CA | 1:121:A:GLU:C | 7        | 1.25          |
| (1,106) | 1:72:A:GLY:N  | 1:72:A:GLY:CA  | 1:72:A:GLY:C   | 1:73:A:GLU:N  | 17       | 1.24          |
| (1,185) | 1:127:A:GLU:N | 1:127:A:GLU:CA | 1:127:A:GLU:C  | 1:128:A:LEU:N | 14       | 1.23          |
| (1,149) | 1:98:A:MET:N  | 1:98:A:MET:CA  | 1:98:A:MET:C   | 1:99:A:TYR:N  | 20       | 1.23          |
| (1,114) | 1:77:A:GLY:C  | 1:78:A:TRP:N   | 1:78:A:TRP:CA  | 1:78:A:TRP:C  | 6        | 1.23          |
| (1,161) | 1:109:A:SER:N | 1:109:A:SER:CA | 1:109:A:SER:C  | 1:110:A:ILE:N | 17       | 1.22          |
| (1,112) | 1:76:A:LYS:C  | 1:77:A:GLY:N   | 1:77:A:GLY:CA  | 1:77:A:GLY:C  | 14       | 1.22          |
| (1,160) | 1:108:A:GLU:C | 1:109:A:SER:N  | 1:109:A:SER:CA | 1:109:A:SER:C | 11       | 1.21          |
| (1,148) | 1:97:A:SER:C  | 1:98:A:MET:N   | 1:98:A:MET:CA  | 1:98:A:MET:C  | 14       | 1.21          |
| (1,117) | 1:79:A:ASP:N  | 1:79:A:ASP:CA  | 1:79:A:ASP:C   | 1:80:A:ILE:N  | 12       | 1.21          |
| (1,106) | 1:72:A:GLY:N  | 1:72:A:GLY:CA  | 1:72:A:GLY:C   | 1:73:A:GLU:N  | 4        | 1.21          |
| (1,93)  | 1:64:A:PRO:C  | 1:65:A:PHE:N   | 1:65:A:PHE:CA  | 1:65:A:PHE:C  | 19       | 1.21          |
| (1,69)  | 1:49:A:GLU:C  | 1:50:A:SER:N   | 1:50:A:SER:CA  | 1:50:A:SER:C  | 6        | 1.2           |
| (1,64)  | 1:47:A:LYS:N  | 1:47:A:LYS:CA  | 1:47:A:LYS:C   | 1:48:A:LEU:N  | 4        | 1.2           |
| (1,120) | 1:80:A:ILE:C  | 1:81:A:CYS:N   | 1:81:A:CYS:CA  | 1:81:A:CYS:C  | 8        | 1.19          |
| (1,54)  | 1:41:A:THR:N  | 1:41:A:THR:CA  | 1:41:A:THR:C   | 1:42:A:VAL:N  | 10       | 1.19          |
| (1,7)   | 1:9:A:LYS:C   | 1:10:A:VAL:N   | 1:10:A:VAL:CA  | 1:10:A:VAL:C  | 5        | 1.19          |
| (1,38)  | 1:31:A:GLU:N  | 1:31:A:GLU:CA  | 1:31:A:GLU:C   | 1:32:A:ASN:N  | 11       | 1.18          |
| (1,94)  | 1:65:A:PHE:N  | 1:65:A:PHE:CA  | 1:65:A:PHE:C   | 1:66:A:LYS:N  | 4        | 1.17          |
| (1,93)  | 1:64:A:PRO:C  | 1:65:A:PHE:N   | 1:65:A:PHE:CA  | 1:65:A:PHE:C  | 2        | 1.17          |

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| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,132) | 1:88:A:ASN:C  | 1:89:A:GLU:N   | 1:89:A:GLU:CA  | 1:89:A:GLU:C  | 9        | 1.16          |
| (1,21)  | 1:18:A:VAL:C  | 1:19:A:ILE:N   | 1:19:A:ILE:CA  | 1:19:A:ILE:C  | 6        | 1.16          |
| (1,160) | 1:108:A:GLU:C | 1:109:A:SER:N  | 1:109:A:SER:CA | 1:109:A:SER:C | 19       | 1.15          |
| (1,117) | 1:79:A:ASP:N  | 1:79:A:ASP:CA  | 1:79:A:ASP:C   | 1:80:A:ILE:N  | 15       | 1.15          |
| (1,105) | 1:71:A:GLN:C  | 1:72:A:GLY:N   | 1:72:A:GLY:CA  | 1:72:A:GLY:C  | 6        | 1.15          |
| (1,77)  | 1:54:A:VAL:C  | 1:55:A:PHE:N   | 1:55:A:PHE:CA  | 1:55:A:PHE:C  | 20       | 1.15          |
| (1,61)  | 1:44:A:TYR:C  | 1:45:A:VAL:N   | 1:45:A:VAL:CA  | 1:45:A:VAL:C  | 14       | 1.15          |
| (1,48)  | 1:37:A:GLY:N  | 1:37:A:GLY:CA  | 1:37:A:GLY:C   | 1:38:A:ASN:N  | 11       | 1.15          |
| (1,8)   | 1:10:A:VAL:N  | 1:10:A:VAL:CA  | 1:10:A:VAL:C   | 1:11:A:GLU:N  | 13       | 1.15          |
| (1,177) | 1:122:A:LEU:N | 1:122:A:LEU:CA | 1:122:A:LEU:C  | 1:123:A:LEU:N | 8        | 1.14          |
| (1,172) | 1:119:A:GLU:C | 1:120:A:ILE:N  | 1:120:A:ILE:CA | 1:120:A:ILE:C | 10       | 1.14          |
| (1,143) | 1:94:A:ARG:N  | 1:94:A:ARG:CA  | 1:94:A:ARG:C   | 1:95:A:ILE:N  | 4        | 1.14          |
| (1,112) | 1:76:A:LYS:C  | 1:77:A:GLY:N   | 1:77:A:GLY:CA  | 1:77:A:GLY:C  | 11       | 1.14          |
| (1,24)  | 1:20:A:LYS:N  | 1:20:A:LYS:CA  | 1:20:A:LYS:C   | 1:21:A:THR:N  | 12       | 1.14          |
| (1,172) | 1:119:A:GLU:C | 1:120:A:ILE:N  | 1:120:A:ILE:CA | 1:120:A:ILE:C | 11       | 1.13          |
| (1,159) | 1:108:A:GLU:N | 1:108:A:GLU:CA | 1:108:A:GLU:C  | 1:109:A:SER:N | 6        | 1.13          |
| (1,117) | 1:79:A:ASP:N  | 1:79:A:ASP:CA  | 1:79:A:ASP:C   | 1:80:A:ILE:N  | 8        | 1.13          |
| (1,114) | 1:77:A:GLY:C  | 1:78:A:TRP:N   | 1:78:A:TRP:CA  | 1:78:A:TRP:C  | 18       | 1.13          |
| (1,91)  | 1:62:A:ASN:C  | 1:63:A:VAL:N   | 1:63:A:VAL:CA  | 1:63:A:VAL:C  | 9        | 1.13          |
| (1,23)  | 1:19:A:ILE:C  | 1:20:A:LYS:N   | 1:20:A:LYS:CA  | 1:20:A:LYS:C  | 8        | 1.13          |
| (1,21)  | 1:18:A:VAL:C  | 1:19:A:ILE:N   | 1:19:A:ILE:CA  | 1:19:A:ILE:C  | 20       | 1.13          |
| (1,7)   | 1:9:A:LYS:C   | 1:10:A:VAL:N   | 1:10:A:VAL:CA  | 1:10:A:VAL:C  | 18       | 1.13          |
| (1,148) | 1:97:A:SER:C  | 1:98:A:MET:N   | 1:98:A:MET:CA  | 1:98:A:MET:C  | 4        | 1.12          |
| (1,114) | 1:77:A:GLY:C  | 1:78:A:TRP:N   | 1:78:A:TRP:CA  | 1:78:A:TRP:C  | 12       | 1.12          |
| (1,69)  | 1:49:A:GLU:C  | 1:50:A:SER:N   | 1:50:A:SER:CA  | 1:50:A:SER:C  | 4        | 1.12          |
| (1,114) | 1:77:A:GLY:C  | 1:78:A:TRP:N   | 1:78:A:TRP:CA  | 1:78:A:TRP:C  | 16       | 1.11          |
| (1,14)  | 1:14:A:ALA:N  | 1:14:A:ALA:CA  | 1:14:A:ALA:C   | 1:15:A:ASP:N  | 14       | 1.11          |
| (1,123) | 1:82:A:VAL:N  | 1:82:A:VAL:CA  | 1:82:A:VAL:C   | 1:83:A:SER:N  | 16       | 1.09          |
| (1,113) | 1:77:A:GLY:N  | 1:77:A:GLY:CA  | 1:77:A:GLY:C   | 1:78:A:TRP:N  | 5        | 1.09          |
| (1,95)  | 1:65:A:PHE:C  | 1:66:A:LYS:N   | 1:66:A:LYS:CA  | 1:66:A:LYS:C  | 3        | 1.09          |
| (1,67)  | 1:48:A:LEU:C  | 1:49:A:GLU:N   | 1:49:A:GLU:CA  | 1:49:A:GLU:C  | 11       | 1.09          |
| (1,123) | 1:82:A:VAL:N  | 1:82:A:VAL:CA  | 1:82:A:VAL:C   | 1:83:A:SER:N  | 8        | 1.08          |
| (1,120) | 1:80:A:ILE:C  | 1:81:A:CYS:N   | 1:81:A:CYS:CA  | 1:81:A:CYS:C  | 17       | 1.08          |
| (1,132) | 1:88:A:ASN:C  | 1:89:A:GLU:N   | 1:89:A:GLU:CA  | 1:89:A:GLU:C  | 18       | 1.07          |
| (1,77)  | 1:54:A:VAL:C  | 1:55:A:PHE:N   | 1:55:A:PHE:CA  | 1:55:A:PHE:C  | 5        | 1.07          |
| (1,7)   | 1:9:A:LYS:C   | 1:10:A:VAL:N   | 1:10:A:VAL:CA  | 1:10:A:VAL:C  | 11       | 1.07          |
| (1,159) | 1:108:A:GLU:N | 1:108:A:GLU:CA | 1:108:A:GLU:C  | 1:109:A:SER:N | 12       | 1.06          |
| (1,149) | 1:98:A:MET:N  | 1:98:A:MET:CA  | 1:98:A:MET:C   | 1:99:A:TYR:N  | 16       | 1.06          |
| (1,148) | 1:97:A:SER:C  | 1:98:A:MET:N   | 1:98:A:MET:CA  | 1:98:A:MET:C  | 5        | 1.06          |
| (1,138) | 1:91:A:CYS:C  | 1:92:A:LEU:N   | 1:92:A:LEU:CA  | 1:92:A:LEU:C  | 4        | 1.06          |
| (1,123) | 1:82:A:VAL:N  | 1:82:A:VAL:CA  | 1:82:A:VAL:C   | 1:83:A:SER:N  | 19       | 1.06          |
| (1,35)  | 1:29:A:GLY:C  | 1:30:A:GLU:N   | 1:30:A:GLU:CA  | 1:30:A:GLU:C  | 13       | 1.06          |
| (1,22)  | 1:19:A:ILE:N  | 1:19:A:ILE:CA  | 1:19:A:ILE:C   | 1:20:A:LYS:N  | 4        | 1.06          |
| (1,148) | 1:97:A:SER:C  | 1:98:A:MET:N   | 1:98:A:MET:CA  | 1:98:A:MET:C  | 1        | 1.05          |
| (1,114) | 1:77:A:GLY:C  | 1:78:A:TRP:N   | 1:78:A:TRP:CA  | 1:78:A:TRP:C  | 4        | 1.04          |
| (1,114) | 1:77:A:GLY:C  | 1:78:A:TRP:N   | 1:78:A:TRP:CA  | 1:78:A:TRP:C  | 7        | 1.04          |
| (1,113) | 1:77:A:GLY:N  | 1:77:A:GLY:CA  | 1:77:A:GLY:C   | 1:78:A:TRP:N  | 10       | 1.04          |
| (1,109) | 1:74:A:VAL:C  | 1:75:A:ILE:N   | 1:75:A:ILE:CA  | 1:75:A:ILE:C  | 12       | 1.04          |
| (1,21)  | 1:18:A:VAL:C  | 1:19:A:ILE:N   | 1:19:A:ILE:CA  | 1:19:A:ILE:C  | 14       | 1.04          |
| (1,8)   | 1:10:A:VAL:N  | 1:10:A:VAL:CA  | 1:10:A:VAL:C   | 1:11:A:GLU:N  | 1        | 1.04          |
| (1,77)  | 1:54:A:VAL:C  | 1:55:A:PHE:N   | 1:55:A:PHE:CA  | 1:55:A:PHE:C  | 19       | 1.03          |

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*Continued from previous page...*

| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,36)  | 1:30:A:GLU:N  | 1:30:A:GLU:CA  | 1:30:A:GLU:C   | 1:31:A:GLU:N  | 3        | 1.03          |
| (1,180) | 1:124:A:SER:C | 1:125:A:PHE:N  | 1:125:A:PHE:CA | 1:125:A:PHE:C | 19       | 1.02          |
| (1,109) | 1:74:A:VAL:C  | 1:75:A:ILE:N   | 1:75:A:ILE:CA  | 1:75:A:ILE:C  | 4        | 1.02          |
| (1,61)  | 1:44:A:TYR:C  | 1:45:A:VAL:N   | 1:45:A:VAL:CA  | 1:45:A:VAL:C  | 19       | 1.02          |
| (1,24)  | 1:20:A:LYS:N  | 1:20:A:LYS:CA  | 1:20:A:LYS:C   | 1:21:A:THR:N  | 16       | 1.02          |
| (1,185) | 1:127:A:GLU:N | 1:127:A:GLU:CA | 1:127:A:GLU:C  | 1:128:A:LEU:N | 7        | 1.01          |
| (1,100) | 1:68:A:HIS:N  | 1:68:A:HIS:CA  | 1:68:A:HIS:C   | 1:69:A:LEU:N  | 2        | 1.0           |
| (1,83)  | 1:57:A:SER:C  | 1:58:A:SER:N   | 1:58:A:SER:CA  | 1:58:A:SER:C  | 4        | 1.0           |
| (1,35)  | 1:29:A:GLY:C  | 1:30:A:GLU:N   | 1:30:A:GLU:CA  | 1:30:A:GLU:C  | 15       | 1.0           |