



# Full wwPDB NMR Structure Validation Report ⓘ

Dec 25, 2024 – 08:14 PM EST

PDB ID : 8U9O  
BMRB ID : 52129  
Title : Solution structure of RsgI9 CRE domain from C. thermocellum  
Authors : Takayesu, A.; Mahoney, B.J.; Clubb, R.T.  
Deposited on : 2023-09-19

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
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) : 2.40

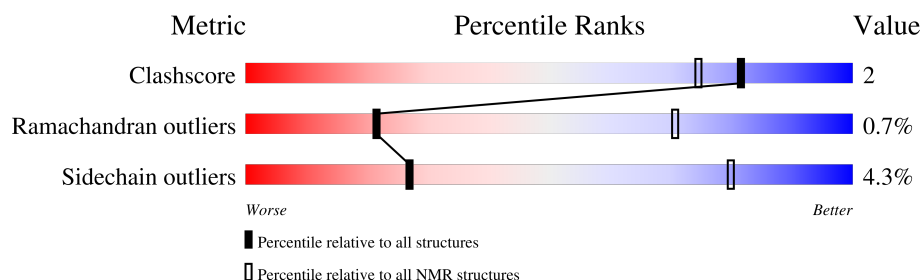
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 81%.

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            | 210492                      | 14027                     |
| Ramachandran outliers | 207382                      | 12486                     |
| Sidechain outliers    | 206894                      | 12463                     |

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     | 22     |                  |
| 2   | B     | 155    |                  |

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 7 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

| Well-defined (core) protein residues |                                   |                   |              |
|--------------------------------------|-----------------------------------|-------------------|--------------|
| Well-defined core                    | Residue range (total)             | Backbone RMSD (Å) | Medoid model |
| 1                                    | A:179-A:188, B:189-B:340<br>(162) | 0.78              | 7            |

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

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

The models can be grouped into 4 clusters and 3 single-model clusters were found.

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

### 3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2669 atoms, of which 1342 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Anti-sigma-I factor RsgI9.

| Mol | Chain | Residues | Atoms |    |    |    |    | Trace |
|-----|-------|----------|-------|----|----|----|----|-------|
| 1   | A     | 12       | Total | C  | H  | N  | O  | 0     |
|     |       |          | 171   | 57 | 79 | 13 | 22 |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| A     | 177     | GLY      | ASP    | conflict | UNP A3DC20 |

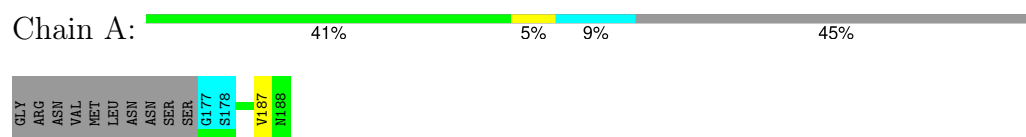
- Molecule 2 is a protein called Anti-sigma-I factor RsgI9.

| Mol | Chain | Residues | Atoms |     |      |     |     |   | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|-------|
| 2   | B     | 155      | Total | C   | H    | N   | O   | S | 0     |
|     |       |          | 2498  | 769 | 1263 | 203 | 259 | 4 |       |

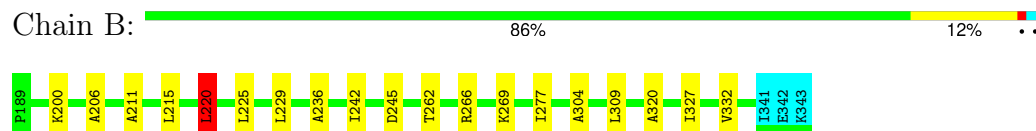


### 4.2.2 Score per residue for model 2

- Molecule 1: Anti-sigma-I factor RsgI9

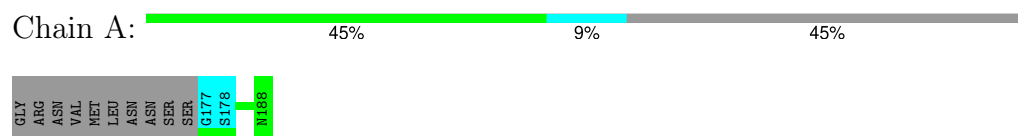


- Molecule 2: Anti-sigma-I factor RsgI9

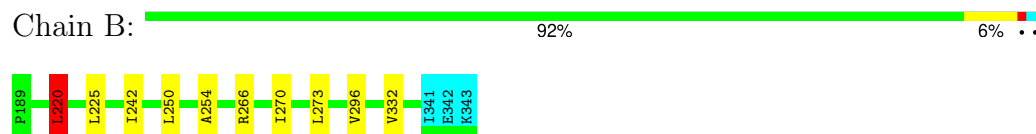


### 4.2.3 Score per residue for model 3

- Molecule 1: Anti-sigma-I factor RsgI9

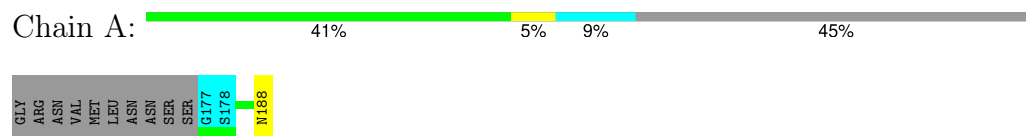


- Molecule 2: Anti-sigma-I factor RsgI9

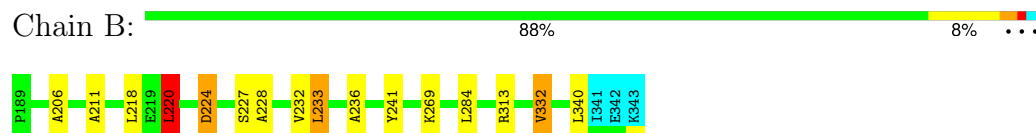


### 4.2.4 Score per residue for model 4

- Molecule 1: Anti-sigma-I factor RsgI9

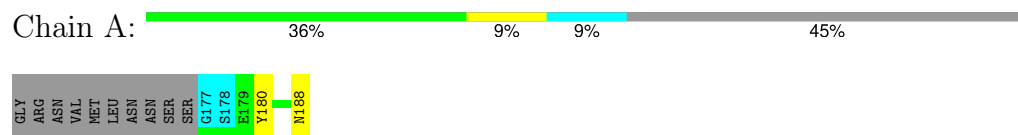


- Molecule 2: Anti-sigma-I factor RsgI9

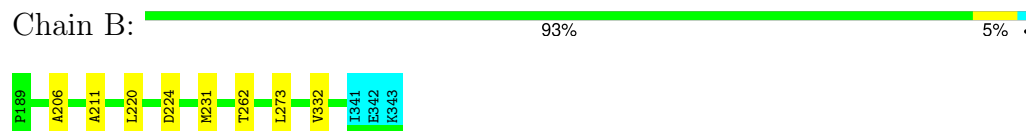


### 4.2.5 Score per residue for model 5

- Molecule 1: Anti-sigma-I factor RsgI9

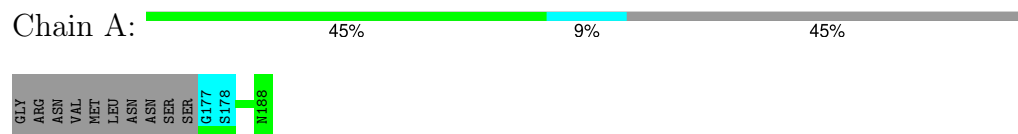


- Molecule 2: Anti-sigma-I factor RsgI9

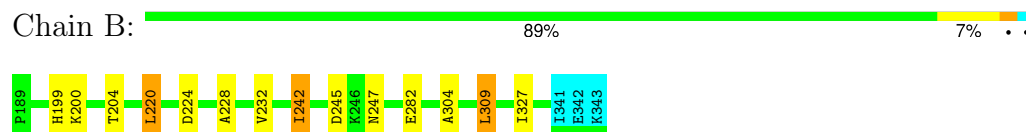


### 4.2.6 Score per residue for model 6

- Molecule 1: Anti-sigma-I factor RsgI9

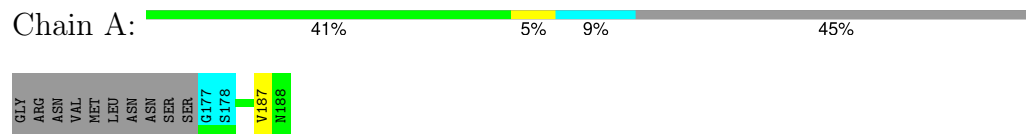


- Molecule 2: Anti-sigma-I factor RsgI9

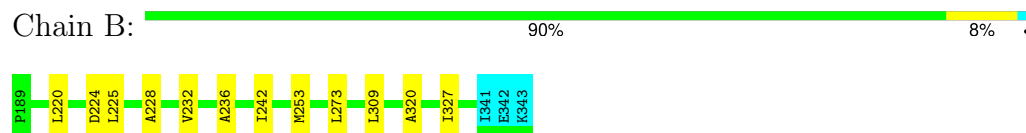


### 4.2.7 Score per residue for model 7 (medoid)

- Molecule 1: Anti-sigma-I factor RsgI9

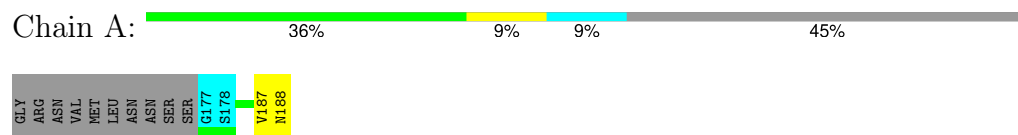


- Molecule 2: Anti-sigma-I factor RsgI9

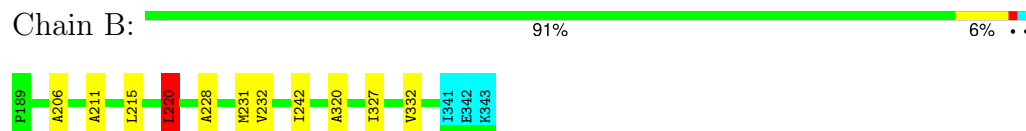


### 4.2.8 Score per residue for model 8

- Molecule 1: Anti-sigma-I factor RsgI9

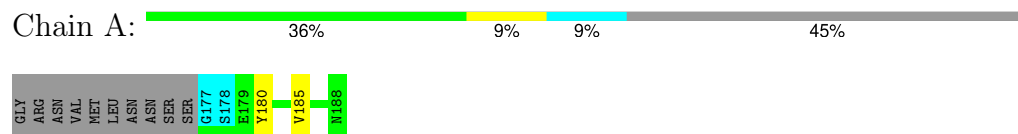


- Molecule 2: Anti-sigma-I factor RsgI9

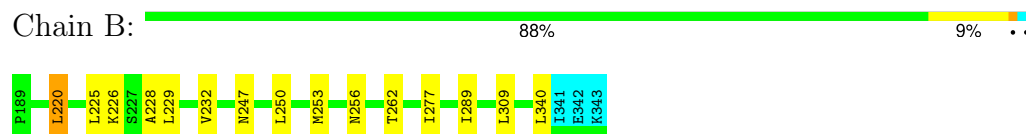


### 4.2.9 Score per residue for model 9

- Molecule 1: Anti-sigma-I factor RsgI9

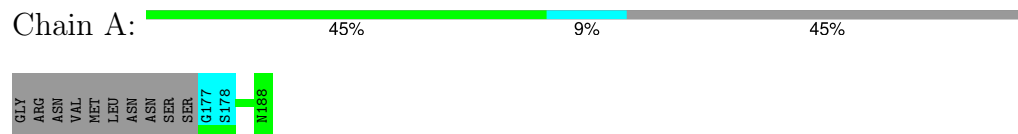


- Molecule 2: Anti-sigma-I factor RsgI9

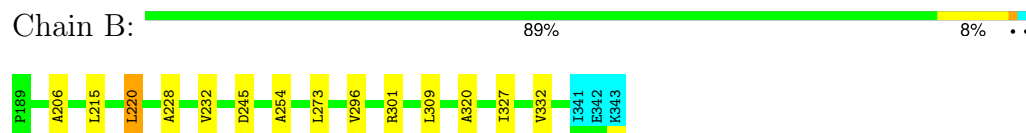


### 4.2.10 Score per residue for model 10

- Molecule 1: Anti-sigma-I factor RsgI9



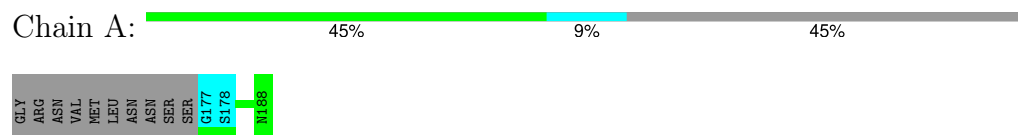
- Molecule 2: Anti-sigma-I factor RsgI9



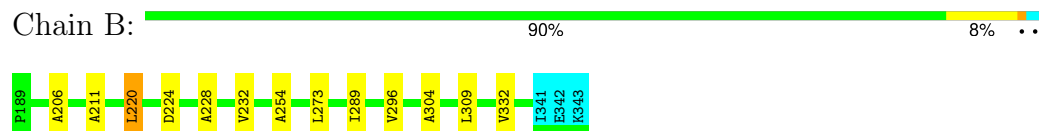


### 4.2.11 Score per residue for model 11

- Molecule 1: Anti-sigma-I factor RsgI9

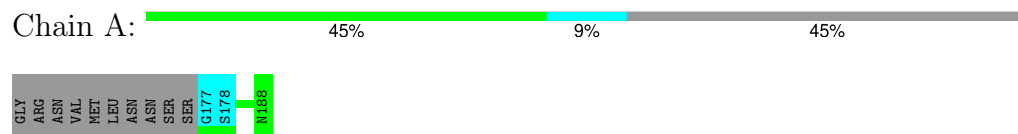


- Molecule 2: Anti-sigma-I factor RsgI9

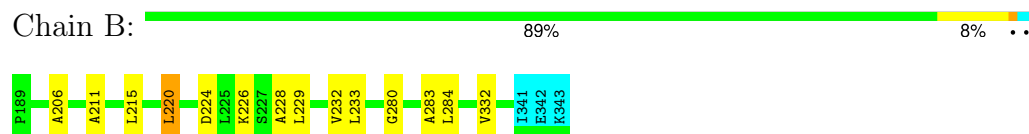


### 4.2.12 Score per residue for model 12

- Molecule 1: Anti-sigma-I factor RsgI9

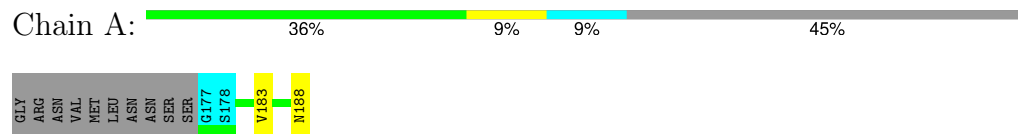


- Molecule 2: Anti-sigma-I factor RsgI9

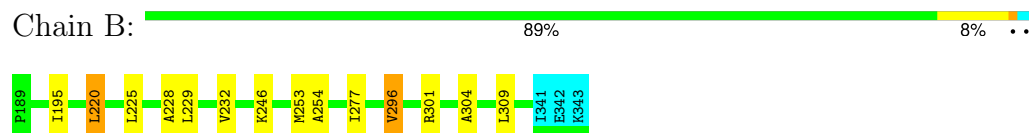


### 4.2.13 Score per residue for model 13

- Molecule 1: Anti-sigma-I factor RsgI9

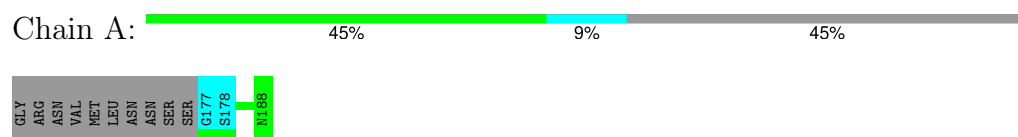


- Molecule 2: Anti-sigma-I factor RsgI9

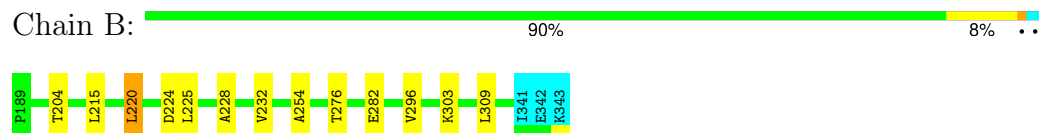


#### 4.2.14 Score per residue for model 14

- Molecule 1: Anti-sigma-I factor RsgI9

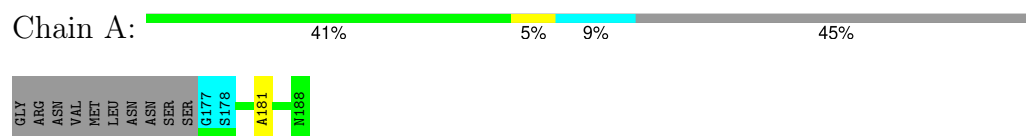


- Molecule 2: Anti-sigma-I factor RsgI9

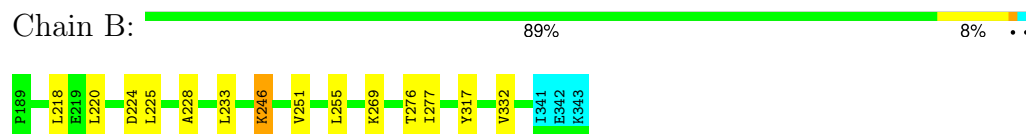


#### 4.2.15 Score per residue for model 15

- Molecule 1: Anti-sigma-I factor RsgI9

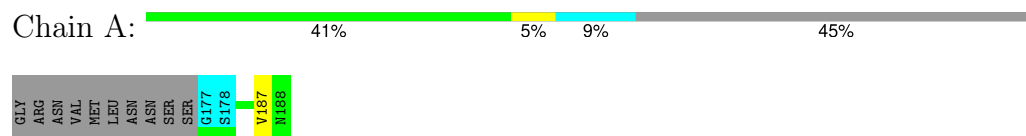


- Molecule 2: Anti-sigma-I factor RsgI9

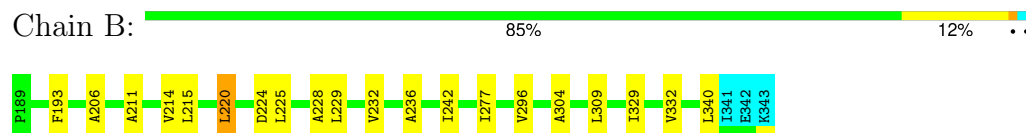


#### 4.2.16 Score per residue for model 16

- Molecule 1: Anti-sigma-I factor RsgI9

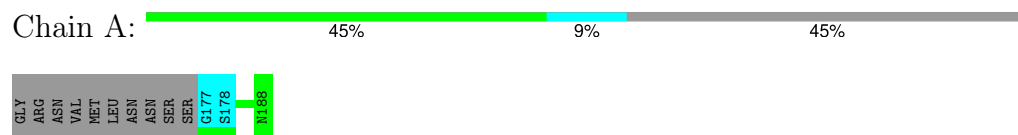


- Molecule 2: Anti-sigma-I factor RsgI9

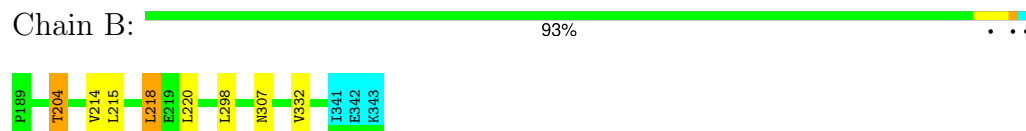


### 4.2.17 Score per residue for model 17

- Molecule 1: Anti-sigma-I factor RsgI9

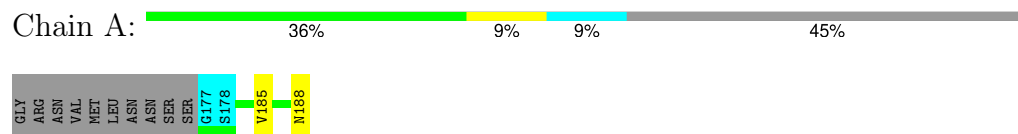


- Molecule 2: Anti-sigma-I factor RsgI9

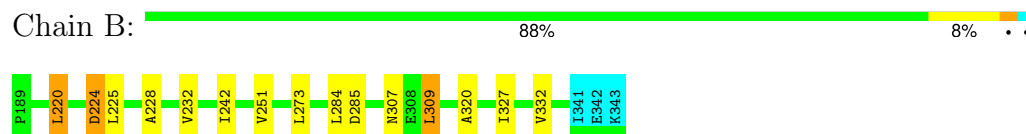


### 4.2.18 Score per residue for model 18

- Molecule 1: Anti-sigma-I factor RsgI9

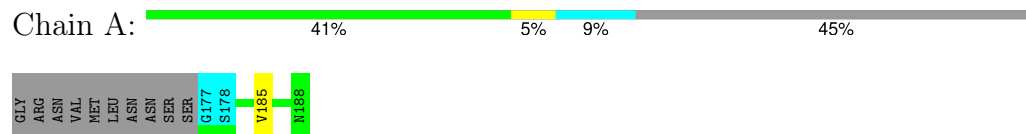


- Molecule 2: Anti-sigma-I factor RsgI9

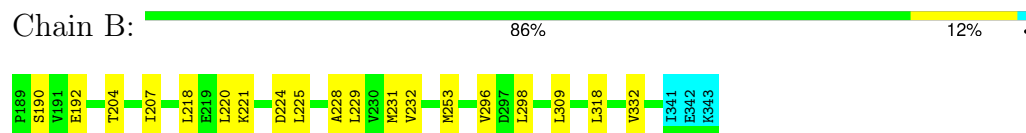


### 4.2.19 Score per residue for model 19

- Molecule 1: Anti-sigma-I factor RsgI9

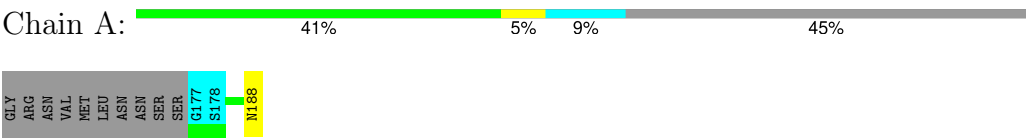


- Molecule 2: Anti-sigma-I factor RsgI9

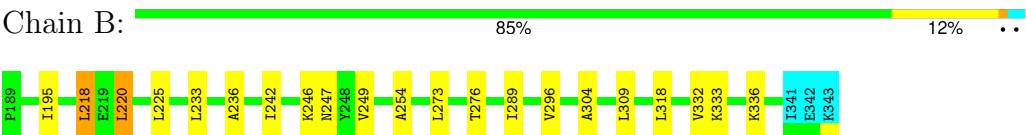


4.2.20 Score per residue for model 20

- Molecule 1: Anti-sigma-I factor RsgI9



- Molecule 2: Anti-sigma-I factor RsgI9



## 5 Refinement protocol and experimental data overview

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

Of the 200 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

| Software name           | Classification        | Version |
|-------------------------|-----------------------|---------|
| X-PLOR NIH              | structure calculation | 3.6     |
| MOLMOL                  | refinement            |         |
| TALOS-N                 | geometry optimization |         |
| PROCHECK / PROCHECK-NMR | refinement            |         |

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

| Chemical shift file(s)                       | working_cs.cif |
|--|----------------|
| Number of chemical shift lists               | 1              |
| Total number of shifts                       | 1910           |
| Number of shifts mapped to atoms             | 1844           |
| Number of unparsed shifts                    | 0              |
| Number of shifts with mapping errors         | 66             |
| Number of shifts with mapping warnings       | 0              |
| Assignment completeness (well-defined parts) | 81%            |

## 6 Model quality

### 6.1 Standard geometry

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 6.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes |
|-----|-------|-------|----------|----------|---------|
| 1   | A     | 82    | 71       | 71       | 1±1     |
| 2   | B     | 1208  | 1233     | 1231     | 6±3     |
| All | All   | 25800 | 26080    | 26040    | 127     |

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 2.

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

| Atom-1          | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|-----------------|------------------|----------|-------------|--------|-------|
|                 |                  |          |             | Worst  | Total |
| 2:B:320:ALA:HB1 | 2:B:327:ILE:HD12 | 0.76     | 1.55        | 18     | 6     |
| 2:B:206:ALA:HB2 | 2:B:215:LEU:HD21 | 0.76     | 1.58        | 16     | 2     |
| 2:B:236:ALA:HB3 | 2:B:242:ILE:HD12 | 0.69     | 1.64        | 7      | 4     |
| 2:B:225:LEU:CD2 | 2:B:276:THR:HG21 | 0.67     | 2.20        | 20     | 1     |
| 1:A:181:ALA:HB2 | 2:B:255:LEU:HD23 | 0.64     | 1.70        | 15     | 1     |
| 2:B:304:ALA:HB1 | 2:B:309:LEU:O    | 0.63     | 1.93        | 16     | 6     |
| 2:B:206:ALA:HB1 | 2:B:211:ALA:HB3  | 0.62     | 1.70        | 16     | 5     |
| 2:B:254:ALA:HB2 | 2:B:296:VAL:HG13 | 0.62     | 1.72        | 13     | 1     |
| 2:B:193:PHE:CE2 | 2:B:228:ALA:HB1  | 0.60     | 2.31        | 16     | 1     |
| 2:B:266:ARG:O   | 2:B:270:ILE:HG23 | 0.60     | 1.97        | 3      | 1     |
| 2:B:190:SER:O   | 2:B:207:ILE:HD12 | 0.56     | 2.01        | 19     | 1     |
| 2:B:228:ALA:O   | 2:B:232:VAL:HG22 | 0.55     | 2.01        | 7      | 2     |
| 2:B:254:ALA:HB2 | 2:B:296:VAL:HB   | 0.55     | 1.78        | 20     | 2     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 2:B:206:ALA:HB2  | 2:B:215:LEU:HD12 | 0.54     | 1.79        | 2      | 2     |
| 1:A:180:TYR:OH   | 2:B:262:THR:HG23 | 0.54     | 2.03        | 1      | 3     |
| 2:B:206:ALA:HB2  | 2:B:215:LEU:CD2  | 0.54     | 2.32        | 10     | 2     |
| 2:B:224:ASP:O    | 2:B:228:ALA:HB3  | 0.54     | 2.02        | 7      | 6     |
| 2:B:192:GLU:N    | 2:B:207:ILE:HD11 | 0.54     | 2.18        | 19     | 1     |
| 2:B:247:ASN:CB   | 2:B:289:ILE:HD13 | 0.53     | 2.34        | 9      | 1     |
| 1:A:185:VAL:HG21 | 2:B:229:LEU:HD21 | 0.52     | 1.81        | 19     | 2     |
| 2:B:206:ALA:HB1  | 2:B:211:ALA:CB   | 0.51     | 2.35        | 8      | 6     |
| 2:B:247:ASN:HB2  | 2:B:289:ILE:HD13 | 0.51     | 1.81        | 9      | 2     |
| 2:B:220:LEU:HD12 | 2:B:220:LEU:O    | 0.51     | 2.06        | 2      | 4     |
| 2:B:225:LEU:HD23 | 2:B:276:THR:HG21 | 0.51     | 1.83        | 15     | 2     |
| 2:B:204:THR:OG1  | 2:B:215:LEU:HD11 | 0.50     | 2.06        | 14     | 2     |
| 2:B:320:ALA:CB   | 2:B:327:ILE:HD12 | 0.48     | 2.38        | 1      | 1     |
| 2:B:228:ALA:O    | 2:B:232:VAL:HG23 | 0.48     | 2.09        | 14     | 11    |
| 2:B:195:ILE:HD11 | 2:B:225:LEU:HD13 | 0.48     | 1.85        | 20     | 1     |
| 2:B:233:LEU:HD21 | 2:B:249:VAL:HG21 | 0.48     | 1.84        | 20     | 1     |
| 2:B:229:LEU:HD21 | 2:B:277:ILE:HD11 | 0.47     | 1.86        | 2      | 1     |
| 2:B:224:ASP:O    | 2:B:228:ALA:HB2  | 0.47     | 2.10        | 16     | 1     |
| 2:B:229:LEU:HD11 | 2:B:277:ILE:HD12 | 0.47     | 1.86        | 13     | 1     |
| 2:B:236:ALA:CB   | 2:B:242:ILE:HD12 | 0.47     | 2.39        | 1      | 4     |
| 2:B:228:ALA:O    | 2:B:232:VAL:HG13 | 0.47     | 2.08        | 4      | 3     |
| 1:A:187:VAL:HG22 | 2:B:242:ILE:HD11 | 0.47     | 1.87        | 16     | 1     |
| 2:B:254:ALA:HB2  | 2:B:296:VAL:CG2  | 0.47     | 2.39        | 10     | 1     |
| 2:B:233:LEU:HD22 | 2:B:284:LEU:HD13 | 0.46     | 1.87        | 4      | 1     |
| 2:B:224:ASP:OD1  | 2:B:228:ALA:HB2  | 0.46     | 2.09        | 4      | 1     |
| 2:B:225:LEU:HD23 | 2:B:276:THR:CG2  | 0.45     | 2.41        | 15     | 1     |
| 1:A:185:VAL:HG12 | 2:B:251:VAL:HG22 | 0.45     | 1.88        | 18     | 1     |
| 1:A:182:TYR:CE1  | 2:B:254:ALA:HB3  | 0.45     | 2.46        | 1      | 1     |
| 2:B:211:ALA:O    | 2:B:214:VAL:HG22 | 0.45     | 2.11        | 16     | 1     |
| 2:B:254:ALA:HB2  | 2:B:296:VAL:HG23 | 0.45     | 1.87        | 14     | 3     |
| 2:B:229:LEU:O    | 2:B:233:LEU:HD13 | 0.45     | 2.12        | 12     | 1     |
| 2:B:256:ASN:O    | 2:B:262:THR:HG21 | 0.44     | 2.12        | 9      | 1     |
| 1:A:187:VAL:HG21 | 2:B:242:ILE:HD11 | 0.44     | 1.89        | 2      | 3     |
| 2:B:229:LEU:HG   | 2:B:277:ILE:HD11 | 0.44     | 1.89        | 16     | 1     |
| 2:B:262:THR:HG22 | 2:B:266:ARG:CZ   | 0.43     | 2.43        | 2      | 1     |
| 1:A:181:ALA:HB1  | 2:B:255:LEU:HD23 | 0.43     | 1.90        | 1      | 1     |
| 2:B:236:ALA:HB1  | 2:B:241:TYR:CE1  | 0.43     | 2.48        | 4      | 1     |
| 2:B:220:LEU:HD13 | 2:B:227:SER:OG   | 0.43     | 2.13        | 4      | 1     |
| 2:B:309:LEU:HD21 | 2:B:329:ILE:HD13 | 0.43     | 1.90        | 16     | 1     |
| 2:B:251:VAL:HG11 | 2:B:277:ILE:HD13 | 0.43     | 1.91        | 15     | 1     |
| 1:A:188:ASN:OXT  | 2:B:242:ILE:HD13 | 0.42     | 2.14        | 18     | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 2:B:253:MET:SD   | 2:B:273:LEU:HD23 | 0.42     | 2.55        | 7      | 1     |
| 2:B:327:ILE:CG2  | 2:B:332:VAL:HG23 | 0.42     | 2.44        | 1      | 1     |
| 2:B:218:LEU:HD13 | 2:B:231:MET:SD   | 0.42     | 2.55        | 19     | 1     |
| 2:B:218:LEU:O    | 2:B:218:LEU:HD23 | 0.42     | 2.14        | 20     | 1     |
| 2:B:280:GLY:O    | 2:B:283:ALA:HB3  | 0.41     | 2.15        | 12     | 1     |
| 2:B:340:LEU:HD12 | 2:B:340:LEU:N    | 0.41     | 2.30        | 4      | 1     |
| 2:B:253:MET:O    | 2:B:296:VAL:HG22 | 0.41     | 2.15        | 19     | 1     |
| 2:B:215:LEU:HD12 | 2:B:215:LEU:O    | 0.41     | 2.16        | 10     | 1     |
| 2:B:332:VAL:HG22 | 2:B:340:LEU:HD21 | 0.41     | 1.93        | 4      | 1     |
| 1:A:183:VAL:HG21 | 2:B:195:ILE:HD12 | 0.41     | 1.93        | 13     | 1     |
| 2:B:242:ILE:HG23 | 2:B:247:ASN:ND2  | 0.40     | 2.31        | 6      | 1     |
| 2:B:307:ASN:ND2  | 2:B:309:LEU:HD21 | 0.40     | 2.32        | 18     | 1     |
| 2:B:214:VAL:O    | 2:B:218:LEU:HD21 | 0.40     | 2.17        | 17     | 1     |

## 6.3 Torsion angles ⓘ

### 6.3.1 Protein backbone ⓘ

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

| Mol | Chain | Analysed        | Favoured      | Allowed    | Outliers   | Percentiles |     |
|-----|-------|-----------------|---------------|------------|------------|-------------|-----|
| 1   | A     | 9/22 (41%)      | 9±0 (100±0%)  | 0±0 (0±0%) | 0±0 (0±0%) | 100         | 100 |
| 2   | B     | 151/155 (97%)   | 147±1 (97±1%) | 3±1 (2±1%) | 1±1 (1±0%) | 21          | 71  |
| All | All   | 3200/3540 (90%) | 3113 (97%)    | 66 (2%)    | 21 (1%)    | 21          | 71  |

All 3 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 2   | B     | 220 | LEU  | 16             |
| 2   | B     | 245 | ASP  | 3              |
| 2   | B     | 246 | LYS  | 2              |



### 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     | 9/19 (47%)      | 9±0 (97±5%)   | 0±0 (3±5%) | 40          | 88 |
| 2   | B     | 139/142 (98%)   | 133±2 (96±1%) | 6±2 (4±1%) | 26          | 79 |
| All | All   | 2960/3220 (92%) | 2834 (96%)    | 126 (4%)   | 27          | 80 |

All 38 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) |
|-----|-------|-----|------|----------------|
| 2   | B     | 220 | LEU  | 19             |
| 2   | B     | 332 | VAL  | 14             |
| 2   | B     | 225 | LEU  | 9              |
| 2   | B     | 309 | LEU  | 8              |
| 2   | B     | 224 | ASP  | 7              |
| 2   | B     | 273 | LEU  | 6              |
| 1   | A     | 188 | ASN  | 5              |
| 2   | B     | 218 | LEU  | 4              |
| 2   | B     | 226 | LYS  | 3              |
| 2   | B     | 253 | MET  | 3              |
| 2   | B     | 282 | GLU  | 3              |
| 2   | B     | 284 | LEU  | 3              |
| 2   | B     | 301 | ARG  | 3              |
| 2   | B     | 269 | LYS  | 3              |
| 2   | B     | 204 | THR  | 3              |
| 2   | B     | 200 | LYS  | 2              |
| 2   | B     | 242 | ILE  | 2              |
| 2   | B     | 250 | LEU  | 2              |
| 2   | B     | 233 | LEU  | 2              |
| 2   | B     | 231 | MET  | 2              |
| 2   | B     | 340 | LEU  | 2              |
| 2   | B     | 296 | VAL  | 2              |
| 2   | B     | 246 | LYS  | 2              |
| 2   | B     | 298 | LEU  | 2              |
| 2   | B     | 318 | LEU  | 2              |
| 2   | B     | 313 | ARG  | 1              |
| 2   | B     | 199 | HIS  | 1              |
| 2   | B     | 327 | ILE  | 1              |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 2   | B     | 277 | ILE  | 1              |
| 2   | B     | 289 | ILE  | 1              |
| 2   | B     | 215 | LEU  | 1              |
| 2   | B     | 303 | LYS  | 1              |
| 2   | B     | 317 | TYR  | 1              |
| 2   | B     | 307 | ASN  | 1              |
| 2   | B     | 285 | ASP  | 1              |
| 2   | B     | 221 | LYS  | 1              |
| 2   | B     | 333 | LYS  | 1              |
| 2   | B     | 336 | 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

The completeness of assignment taking into account all chemical shift lists is 81% for the well-defined parts and 81% for the entire structure.

### 7.1 Chemical shift list 1

File name: working\_cs.cif

Chemical shift list name: *starch\_output*

#### 7.1.1 Bookkeeping

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

|   |      |
|---|------|
| Total number of shifts                  | 1910 |
| Number of shifts mapped to atoms        | 1844 |
| Number of unparsed shifts               | 0    |
| Number of shifts with mapping errors    | 66   |
| Number of shifts with mapping warnings  | 0    |
| Number of shift outliers (ShiftChecker) | 5    |

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- No matching atom found in the structure. All 66 occurrences are reported below.

| List ID | Chain | Res | Type | Atom | Shift Data |             |           |
|---------|-------|-----|------|------|------------|-------------|-----------|
|         |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 1       | A     | 169 | ASN  | N    | 120.96     | .           | .         |
| 1       | A     | 169 | ASN  | H    | 8.65       | .           | .         |
| 1       | A     | 169 | ASN  | CA   | 53.0       | .           | .         |
| 1       | A     | 169 | ASN  | C    | 175.1      | .           | .         |
| 1       | A     | 169 | ASN  | CB   | 38.22      | .           | .         |
| 1       | A     | 169 | ASN  | HA   | 4.77       | .           | .         |
| 1       | A     | 169 | ASN  | HB2  | 2.82       | .           | .         |
| 1       | A     | 170 | VAL  | N    | 120.93     | .           | .         |
| 1       | A     | 170 | VAL  | H    | 8.19       | .           | .         |
| 1       | A     | 170 | VAL  | CA   | 62.4       | .           | .         |
| 1       | A     | 170 | VAL  | C    | 175.95     | .           | .         |
| 1       | A     | 170 | VAL  | CB   | 32.51      | .           | .         |
| 1       | A     | 170 | VAL  | CG1  | 21.01      | .           | .         |
| 1       | A     | 170 | VAL  | CG2  | 20.34      | .           | .         |

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| List ID | Chain | Res | Type | Atom | Shift Data |             |           |
|---------|-------|-----|------|------|------------|-------------|-----------|
|         |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 1       | A     | 170 | VAL  | HA   | 4.1        | .           | .         |
| 1       | A     | 170 | VAL  | HB   | 2.09       | .           | .         |
| 1       | A     | 170 | VAL  | HG11 | 0.92       | .           | .         |
| 1       | A     | 170 | VAL  | HG12 | 0.92       | .           | .         |
| 1       | A     | 170 | VAL  | HG13 | 0.92       | .           | .         |
| 1       | A     | 170 | VAL  | HG21 | 0.91       | .           | .         |
| 1       | A     | 170 | VAL  | HG22 | 0.91       | .           | .         |
| 1       | A     | 170 | VAL  | HG23 | 0.91       | .           | .         |
| 1       | A     | 171 | MET  | N    | 123.62     | .           | .         |
| 1       | A     | 171 | MET  | H    | 8.39       | .           | .         |
| 1       | A     | 171 | MET  | CA   | 55.33      | .           | .         |
| 1       | A     | 171 | MET  | CB   | 32.51      | .           | .         |
| 1       | A     | 171 | MET  | CG   | 17.41      | .           | .         |
| 1       | A     | 171 | MET  | CE   | 52.11      | .           | .         |
| 1       | A     | 171 | MET  | HA   | 4.45       | .           | .         |
| 1       | A     | 171 | MET  | HB2  | 2.05       | .           | .         |
| 1       | A     | 171 | MET  | HG2  | 2.6        | .           | .         |
| 1       | A     | 171 | MET  | HE1  | 0.917      | .           | .         |
| 1       | A     | 171 | MET  | HE2  | 0.917      | .           | .         |
| 1       | A     | 171 | MET  | HE3  | 0.917      | .           | .         |
| 1       | A     | 172 | LEU  | N    | 125.13     | .           | .         |
| 1       | A     | 172 | LEU  | H    | 8.48       | .           | .         |
| 1       | A     | 172 | LEU  | CA   | 55.08      | .           | .         |
| 1       | A     | 172 | LEU  | CB   | 42.34      | .           | .         |
| 1       | A     | 172 | LEU  | CG   | 26.69      | .           | .         |
| 1       | A     | 172 | LEU  | CD1  | 24.77      | .           | .         |
| 1       | A     | 172 | LEU  | CD2  | 23.18      | .           | .         |
| 1       | A     | 172 | LEU  | HA   | 4.34       | .           | .         |
| 1       | A     | 172 | LEU  | HB2  | 1.63       | .           | .         |
| 1       | A     | 172 | LEU  | HG   | 1.47       | .           | .         |
| 1       | A     | 172 | LEU  | HD11 | 0.83       | .           | .         |
| 1       | A     | 172 | LEU  | HD12 | 0.83       | .           | .         |
| 1       | A     | 172 | LEU  | HD13 | 0.83       | .           | .         |
| 1       | A     | 172 | LEU  | HD21 | 0.79       | .           | .         |
| 1       | A     | 172 | LEU  | HD22 | 0.79       | .           | .         |
| 1       | A     | 172 | LEU  | HD23 | 0.79       | .           | .         |
| 1       | A     | 173 | ASN  | N    | 119.33     | .           | .         |
| 1       | A     | 173 | ASN  | H    | 8.41       | .           | .         |
| 1       | A     | 173 | ASN  | CA   | 53.19      | .           | .         |
| 1       | A     | 173 | ASN  | C    | 174.91     | .           | .         |
| 1       | A     | 173 | ASN  | CB   | 38.68      | .           | .         |

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| List ID | Chain | Res | Type | Atom | Shift Data |             |           |
|---------|-------|-----|------|------|------------|-------------|-----------|
|         |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 1       | A     | 173 | ASN  | HA   | 4.68       | .           | .         |
| 1       | A     | 173 | ASN  | HB2  | 2.81       | .           | .         |
| 1       | A     | 174 | ASN  | N    | 116.37     | .           | .         |
| 1       | A     | 174 | ASN  | H    | 8.39       | .           | .         |
| 1       | A     | 174 | ASN  | CB   | 63.76      | .           | .         |
| 1       | A     | 176 | SER  | N    | 118.51     | .           | .         |
| 1       | A     | 176 | SER  | H    | 8.59       | .           | .         |
| 1       | A     | 176 | SER  | CA   | 59.25      | .           | .         |
| 1       | A     | 176 | SER  | CB   | 63.65      | .           | .         |
| 1       | A     | 176 | SER  | HA   | 4.46       | .           | .         |
| 1       | A     | 176 | SER  | HB2  | 3.96       | .           | .         |

### 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           |
|------------------------|----------|---------------------------------|----------------------------|
| $^{13}\text{C}_\alpha$ | 173      | $-0.08 \pm 0.15$                | None needed ( $< 0.5$ ppm) |
| $^{13}\text{C}_\beta$  | 166      | $0.28 \pm 0.11$                 | None needed ( $< 0.5$ ppm) |
| $^{13}\text{C}'$       | 137      | $-0.01 \pm 0.15$                | None needed ( $< 0.5$ ppm) |
| $^{15}\text{N}$        | 172      | $0.40 \pm 0.25$                 | 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 81%, i.e. 1792 atoms were assigned a chemical shift out of a possible 2223. 0 out of 32 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total           | $^1\text{H}$   | $^{13}\text{C}$ | $^{15}\text{N}$ |
|-----------|-----------------|----------------|-----------------|-----------------|
| Backbone  | 778/813 (96%)   | 326/328 (99%)  | 292/324 (90%)   | 160/161 (99%)   |
| Sidechain | 974/1323 (74%)  | 607/853 (71%)  | 362/426 (85%)   | 5/44 (11%)      |
| Aromatic  | 40/87 (46%)     | 20/41 (49%)    | 20/44 (45%)     | 0/2 (0%)        |
| Overall   | 1792/2223 (81%) | 953/1222 (78%) | 674/794 (85%)   | 165/207 (80%)   |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 81%, i.e. 1844 atoms were assigned a chemical shift out of a possible 2285. 0 out of 32 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total           | <sup>1</sup> H | <sup>13</sup> C | <sup>15</sup> N |
|-----------|-----------------|----------------|-----------------|-----------------|
| Backbone  | 803/839 (96%)   | 337/339 (99%)  | 301/334 (90%)   | 165/166 (99%)   |
| Sidechain | 1001/1359 (74%) | 623/876 (71%)  | 373/438 (85%)   | 5/45 (11%)      |
| Aromatic  | 40/87 (46%)     | 20/41 (49%)    | 20/44 (45%)     | 0/2 (0%)        |
| Overall   | 1844/2285 (81%) | 980/1256 (78%) | 694/816 (85%)   | 170/213 (80%)   |

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

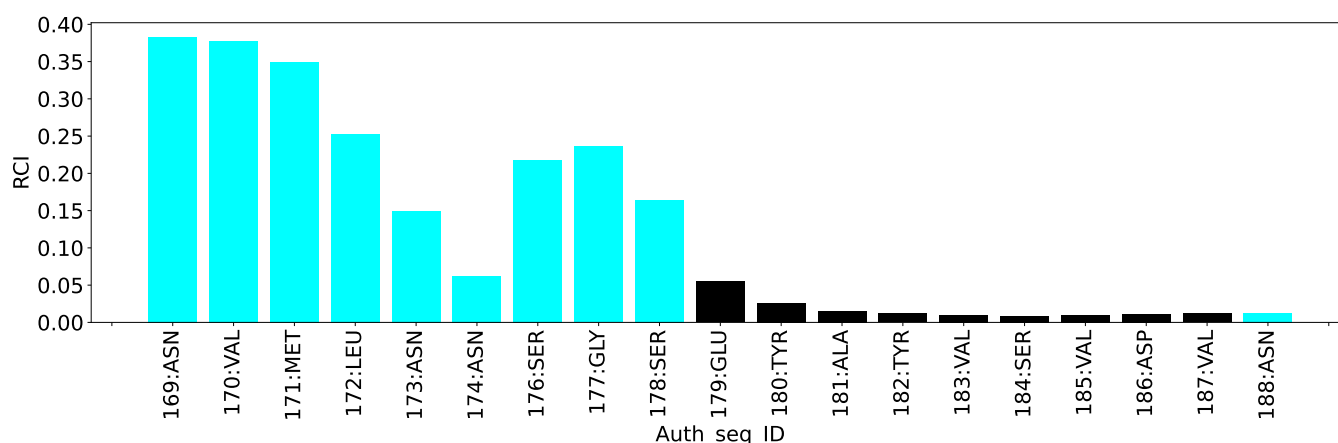
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

| List Id | Chain | Res | Type | Atom | Shift, ppm | Expected range, ppm | Z-score |
|---------|-------|-----|------|------|------------|---------------------|---------|
| 1       | A     | 171 | MET  | CE   | 52.11      | 8.39 – 25.85        | 20.0    |
| 1       | A     | 174 | ASN  | CB   | 63.76      | 30.50 – 46.89       | 15.3    |
| 1       | A     | 171 | MET  | CG   | 17.41      | 25.46 – 38.60       | -11.1   |
| 1       | B     | 298 | LEU  | CG   | 37.88      | 21.37 – 32.19       | 10.3    |
| 1       | B     | 189 | PRO  | HA   | 1.26       | 2.78 – 6.00         | -9.7    |

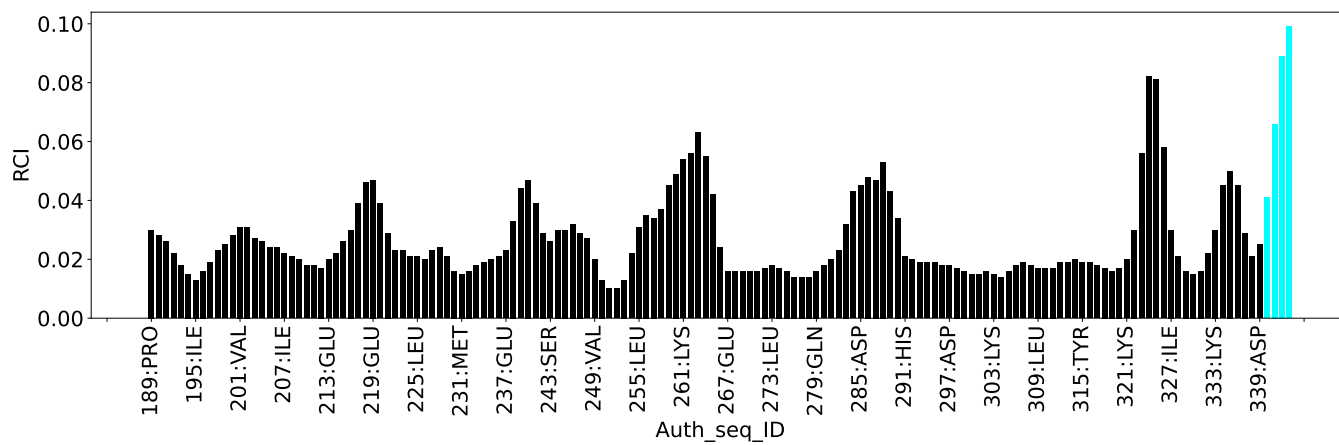
### 7.1.5 Random Coil Index (RCI) plots [i](#)

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:



Random coil index (RCI) for chain B:



## 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                                | 1668  |
| Intra-residue ( $ i-j =0$ )                              | 438   |
| Sequential ( $ i-j =1$ )                                 | 463   |
| Medium range ( $ i-j >1$ and $ i-j <5$ )                 | 260   |
| Long range ( $ i-j \geq 5$ )                             | 408   |
| Inter-chain  | 99    |
| Hydrogen bond restraints                                 | 0     |
| Disulfide bond restraints                                | 0     |
| Total dihedral-angle restraints                          | 301   |
| Number of unmapped restraints                            | 0     |
| Number of restraints per residue                         | 11.1  |
| Number of long range restraints per residue <sup>1</sup> | 2.3   |

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

### 8.2 Residual restraint violations

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)  | 16.6                                   | 0.2     |
| 0.2-0.5 (Medium) | 10.0                                   | 0.46    |
| >0.5 (Large)     | None                                   | None    |



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

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

| Bins (°)           | Average number of violations per model | Max (°) |
|--------------------|--|---------|
| 1.0-10.0 (Small)   | 14.9                                   | 4.97    |
| 10.0-20.0 (Medium) | None                                   | None    |
| >20.0 (Large)      | None                                   | None    |

## 9 Distance violation analysis ⓘ

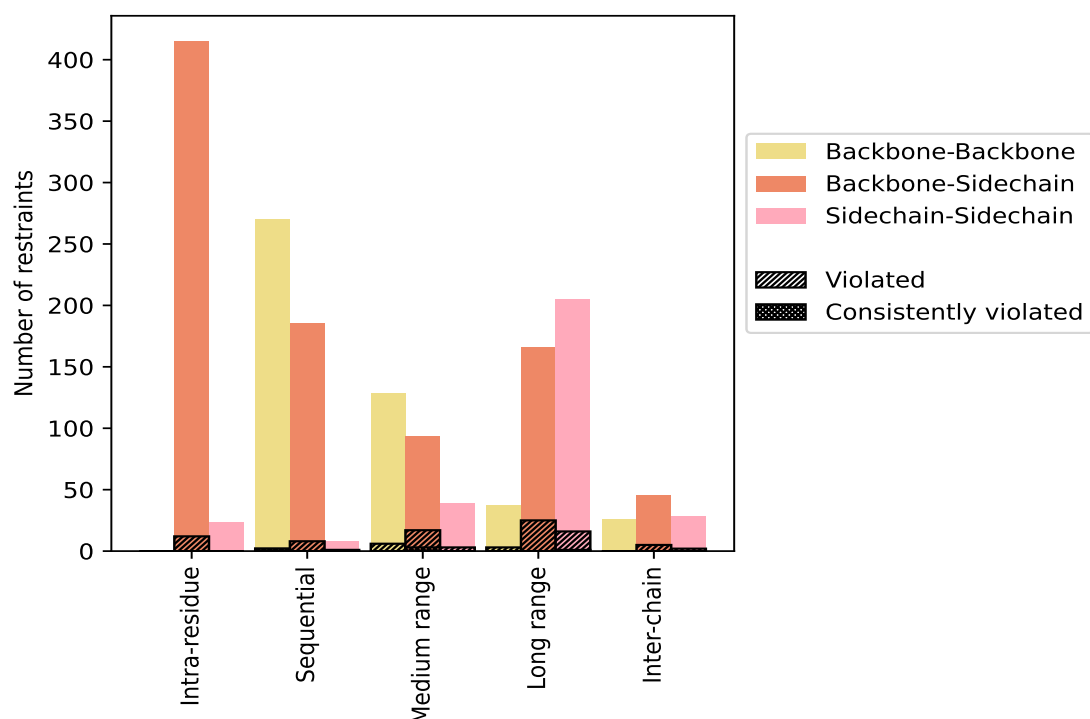
### 9.1 Summary of distance violations ⓘ

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>438</b>  | <b>26.3</b>    | <b>12</b>             | <b>2.7</b>     | <b>0.7</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  | 415         | 24.9           | 12                    | 2.9            | 0.7            | 0                                  | 0.0            | 0.0            |
| Sidechain-Sidechain   | 23          | 1.4            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| <b>Sequential (<math> i-j =1</math>)</b>                                    | <b>463</b>  | <b>27.8</b>    | <b>11</b>             | <b>2.4</b>     | <b>0.7</b>     | <b>2</b>                           | <b>0.4</b>     | <b>0.1</b>     |
| Backbone-Backbone   | 270         | 16.2           | 2                     | 0.7            | 0.1            | 2                                  | 0.7            | 0.1            |
| Backbone-Sidechain  | 185         | 11.1           | 8                     | 4.3            | 0.5            | 0                                  | 0.0            | 0.0            |
| Sidechain-Sidechain   | 8           | 0.5            | 1                     | 12.5           | 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>260</b>  | <b>15.6</b>    | <b>26</b>             | <b>10.0</b>    | <b>1.6</b>     | <b>3</b>                           | <b>1.2</b>     | <b>0.2</b>     |
| Backbone-Backbone   | 128         | 7.7            | 6                     | 4.7            | 0.4            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain  | 93          | 5.6            | 17                    | 18.3           | 1.0            | 3                                  | 3.2            | 0.2            |
| Sidechain-Sidechain   | 39          | 2.3            | 3                     | 7.7            | 0.2            | 0                                  | 0.0            | 0.0            |
| <b>Long range (<math> i-j \geq 5</math>)</b>                                | <b>408</b>  | <b>24.5</b>    | <b>44</b>             | <b>10.8</b>    | <b>2.6</b>     | <b>1</b>                           | <b>0.2</b>     | <b>0.1</b>     |
| Backbone-Backbone   | 37          | 2.2            | 3                     | 8.1            | 0.2            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain  | 166         | 10.0           | 25                    | 15.1           | 1.5            | 0                                  | 0.0            | 0.0            |
| Sidechain-Sidechain   | 205         | 12.3           | 16                    | 7.8            | 1.0            | 1                                  | 0.5            | 0.1            |
| <b>Inter-chain</b>  | <b>99</b>   | <b>5.9</b>     | <b>7</b>              | <b>7.1</b>     | <b>0.4</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| Backbone-Backbone   | 26          | 1.6            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain  | 45          | 2.7            | 5                     | 11.1           | 0.3            | 0                                  | 0.0            | 0.0            |
| Sidechain-Sidechain   | 28          | 1.7            | 2                     | 7.1            | 0.1            | 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>1668</b> | <b>100.0</b>   | <b>100</b>            | <b>6.0</b>     | <b>6.0</b>     | <b>6</b>                           | <b>0.4</b>     | <b>0.4</b>     |
| Backbone-Backbone   | 461         | 27.6           | 11                    | 2.4            | 0.7            | 2                                  | 0.4            | 0.1            |
| Backbone-Sidechain  | 904         | 54.2           | 67                    | 7.4            | 4.0            | 3                                  | 0.3            | 0.2            |
| Sidechain-Sidechain   | 303         | 18.2           | 22                    | 7.3            | 1.3            | 1                                  | 0.3            | 0.1            |

<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                    | 6               | 10              | 8               | 2               | 27    | 0.17     | 0.34    | 0.07                | 0.14       |
| 2        | 3                    | 5               | 10              | 10              | 1               | 29    | 0.18     | 0.36    | 0.07                | 0.16       |
| 3        | 1                    | 6               | 11              | 9               | 0               | 27    | 0.2      | 0.44    | 0.1                 | 0.14       |
| 4        | 0                    | 5               | 10              | 13              | 1               | 29    | 0.2      | 0.34    | 0.07                | 0.2        |
| 5        | 2                    | 4               | 11              | 8               | 0               | 25    | 0.21     | 0.38    | 0.08                | 0.19       |
| 6        | 5                    | 5               | 12              | 6               | 0               | 28    | 0.19     | 0.37    | 0.07                | 0.17       |
| 7        | 2                    | 7               | 11              | 8               | 0               | 28    | 0.2      | 0.41    | 0.08                | 0.17       |
| 8        | 5                    | 4               | 15              | 11              | 0               | 35    | 0.19     | 0.39    | 0.08                | 0.16       |
| 9        | 0                    | 3               | 11              | 10              | 2               | 26    | 0.18     | 0.39    | 0.07                | 0.16       |
| 10       | 3                    | 3               | 9               | 9               | 3               | 27    | 0.18     | 0.46    | 0.09                | 0.13       |

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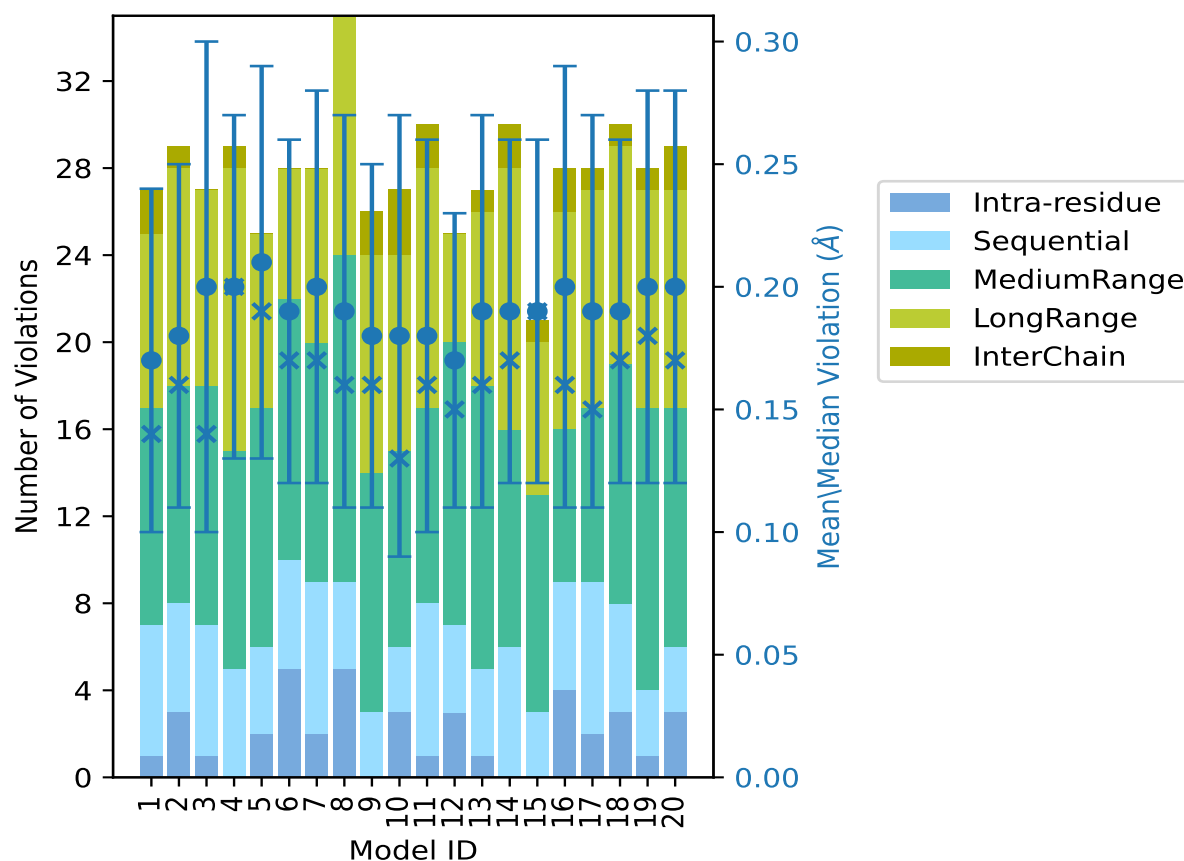
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| Model ID | Number of violations |                 |                 |                 |                 |       | Mean (Å) | Max (Å) | SD <sup>6</sup> (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
|          | IR <sup>1</sup>      | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total |          |         |                     |            |
| 11       | 1                    | 7               | 9               | 11              | 2               | 30    | 0.18     | 0.37    | 0.08                | 0.16       |
| 12       | 3                    | 4               | 13              | 5               | 0               | 25    | 0.17     | 0.34    | 0.06                | 0.15       |
| 13       | 1                    | 4               | 13              | 8               | 1               | 27    | 0.19     | 0.38    | 0.08                | 0.16       |
| 14       | 0                    | 6               | 10              | 12              | 2               | 30    | 0.19     | 0.37    | 0.07                | 0.17       |
| 15       | 0                    | 3               | 10              | 7               | 1               | 21    | 0.19     | 0.39    | 0.07                | 0.19       |
| 16       | 4                    | 5               | 7               | 10              | 2               | 28    | 0.2      | 0.46    | 0.09                | 0.16       |
| 17       | 2                    | 7               | 8               | 10              | 1               | 28    | 0.19     | 0.38    | 0.08                | 0.15       |
| 18       | 3                    | 5               | 11              | 10              | 1               | 30    | 0.19     | 0.38    | 0.07                | 0.17       |
| 19       | 1                    | 3               | 13              | 10              | 1               | 28    | 0.2      | 0.44    | 0.08                | 0.18       |
| 20       | 3                    | 3               | 11              | 10              | 2               | 29    | 0.2      | 0.37    | 0.08                | 0.17       |

<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

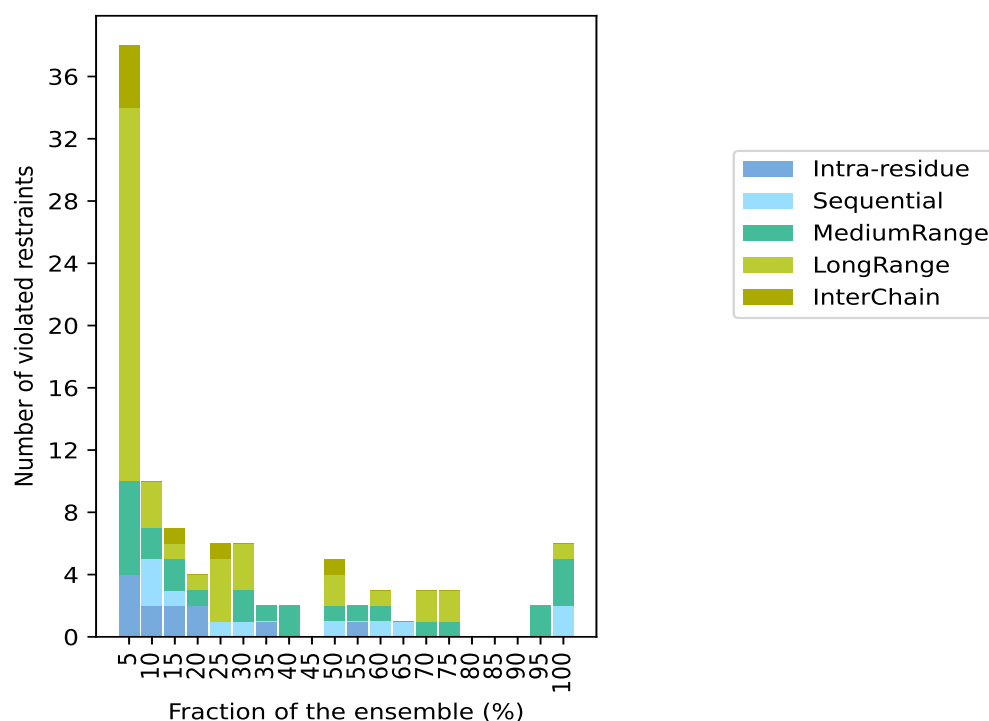
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1568(IR:426, SQ:452, MR:234, LR:364, IC:92) restraints are 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                             | 0               | 6               | 24              | 4               | 38    | 1                        | 5.0   |
| 2                             | 3               | 2               | 3               | 0               | 10    | 2                        | 10.0  |
| 2                             | 1               | 2               | 1               | 1               | 7     | 3                        | 15.0  |
| 2                             | 0               | 1               | 1               | 0               | 4     | 4                        | 20.0  |
| 0                             | 1               | 0               | 4               | 1               | 6     | 5                        | 25.0  |
| 0                             | 1               | 2               | 3               | 0               | 6     | 6                        | 30.0  |
| 1                             | 0               | 1               | 0               | 0               | 2     | 7                        | 35.0  |
| 0                             | 0               | 2               | 0               | 0               | 2     | 8                        | 40.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 9                        | 45.0  |
| 0                             | 1               | 1               | 2               | 1               | 5     | 10                       | 50.0  |
| 1                             | 0               | 1               | 0               | 0               | 2     | 11                       | 55.0  |
| 0                             | 1               | 1               | 1               | 0               | 3     | 12                       | 60.0  |
| 0                             | 1               | 0               | 0               | 0               | 1     | 13                       | 65.0  |
| 0                             | 0               | 1               | 2               | 0               | 3     | 14                       | 70.0  |
| 0                             | 0               | 1               | 2               | 0               | 3     | 15                       | 75.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 16                       | 80.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 17                       | 85.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 18                       | 90.0  |
| 0                             | 0               | 2               | 0               | 0               | 2     | 19                       | 95.0  |
| 0                             | 2               | 3               | 1               | 0               | 6     | 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

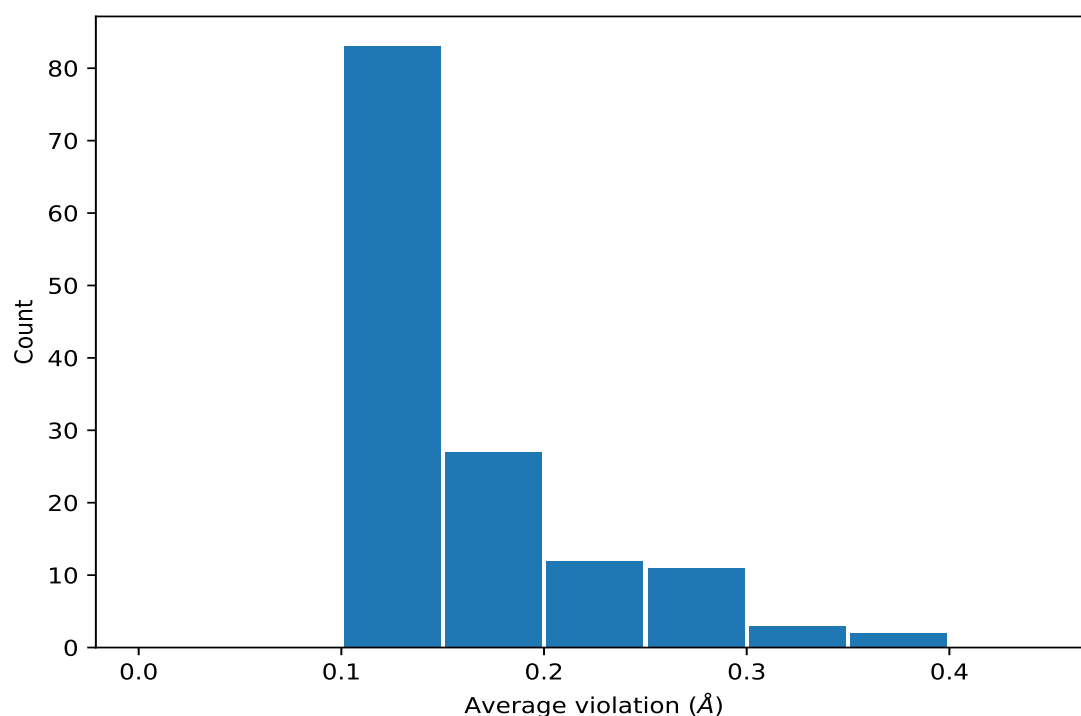
### 9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



## 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) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,853)  | 2:243:B:SER:H   | 2:244:B:ASP:H   | 20                  | 0.38     | 0.04                | 0.38       |
| (1,166)  | 2:281:B:ILE:H   | 2:279:B:GLN:HB2 | 20                  | 0.27     | 0.04                | 0.27       |
| (1,166)  | 2:281:B:ILE:H   | 2:279:B:GLN:HB3 | 20                  | 0.27     | 0.04                | 0.27       |
| (1,77)   | 2:331:B:GLU:H   | 2:333:B:LYS:HB2 | 20                  | 0.26     | 0.06                | 0.26       |
| (1,77)   | 2:331:B:GLU:H   | 2:333:B:LYS:HB3 | 20                  | 0.26     | 0.06                | 0.26       |
| (1,514)  | 2:238:B:SER:H   | 2:234:B:GLU:HB2 | 20                  | 0.26     | 0.03                | 0.26       |
| (1,514)  | 2:238:B:SER:H   | 2:234:B:GLU:HB3 | 20                  | 0.26     | 0.03                | 0.26       |
| (1,1234) | 2:255:B:LEU:HG  | 2:273:B:LEU:HB2 | 20                  | 0.19     | 0.05                | 0.18       |
| (1,1234) | 2:255:B:LEU:HG  | 2:273:B:LEU:HB3 | 20                  | 0.19     | 0.05                | 0.18       |
| (1,359)  | 2:342:B:GLU:H   | 2:343:B:LYS:H   | 20                  | 0.18     | 0.06                | 0.18       |
| (1,235)  | 2:299:B:GLU:H   | 2:297:B:ASP:H   | 19                  | 0.26     | 0.05                | 0.28       |
| (1,607)  | 2:282:B:GLU:H   | 2:279:B:GLN:HB2 | 19                  | 0.25     | 0.07                | 0.26       |
| (1,607)  | 2:282:B:GLU:H   | 2:279:B:GLN:HB3 | 19                  | 0.25     | 0.07                | 0.26       |
| (1,895)  | 2:279:B:GLN:H   | 2:226:B:LYS:HB2 | 15                  | 0.19     | 0.07                | 0.19       |
| (1,895)  | 2:279:B:GLN:H   | 2:226:B:LYS:HB3 | 15                  | 0.19     | 0.07                | 0.19       |
| (1,1168) | 2:193:B:PHE:HD1 | 2:215:B:LEU:HB2 | 15                  | 0.19     | 0.04                | 0.18       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,1168) | 2:193:B:PHE:HD1  | 2:215:B:LEU:HB3  | 15                  | 0.19     | 0.04                | 0.18       |
| (1,1168) | 2:193:B:PHE:HD2  | 2:215:B:LEU:HB2  | 15                  | 0.19     | 0.04                | 0.18       |
| (1,1168) | 2:193:B:PHE:HD2  | 2:215:B:LEU:HB3  | 15                  | 0.19     | 0.04                | 0.18       |
| (1,700)  | 2:256:B:ASN:H    | 2:259:B:ASN:H    | 15                  | 0.15     | 0.02                | 0.15       |
| (1,1599) | 2:207:B:ILE:HA   | 2:215:B:LEU:HD11 | 14                  | 0.17     | 0.03                | 0.16       |
| (1,1599) | 2:207:B:ILE:HA   | 2:215:B:LEU:HD12 | 14                  | 0.17     | 0.03                | 0.16       |
| (1,1599) | 2:207:B:ILE:HA   | 2:215:B:LEU:HD13 | 14                  | 0.17     | 0.03                | 0.16       |
| (1,1599) | 2:207:B:ILE:HA   | 2:215:B:LEU:HD21 | 14                  | 0.17     | 0.03                | 0.16       |
| (1,1599) | 2:207:B:ILE:HA   | 2:215:B:LEU:HD22 | 14                  | 0.17     | 0.03                | 0.16       |
| (1,1599) | 2:207:B:ILE:HA   | 2:215:B:LEU:HD23 | 14                  | 0.17     | 0.03                | 0.16       |
| (1,428)  | 2:222:B:GLU:H    | 2:202:B:ILE:HA   | 14                  | 0.16     | 0.04                | 0.16       |
| (1,464)  | 2:271:B:ASP:H    | 2:267:B:GLU:H    | 14                  | 0.13     | 0.02                | 0.13       |
| (1,956)  | 2:327:B:ILE:HD11 | 2:328:B:THR:HA   | 13                  | 0.23     | 0.05                | 0.22       |
| (1,956)  | 2:327:B:ILE:HD12 | 2:328:B:THR:HA   | 13                  | 0.23     | 0.05                | 0.22       |
| (1,956)  | 2:327:B:ILE:HD13 | 2:328:B:THR:HA   | 13                  | 0.23     | 0.05                | 0.22       |
| (1,1036) | 2:329:B:ILE:HD11 | 2:332:B:VAL:HB   | 12                  | 0.15     | 0.04                | 0.15       |
| (1,1036) | 2:329:B:ILE:HD12 | 2:332:B:VAL:HB   | 12                  | 0.15     | 0.04                | 0.15       |
| (1,1036) | 2:329:B:ILE:HD13 | 2:332:B:VAL:HB   | 12                  | 0.15     | 0.04                | 0.15       |
| (1,791)  | 2:288:B:THR:H    | 2:289:B:ILE:HG21 | 12                  | 0.14     | 0.02                | 0.15       |
| (1,791)  | 2:288:B:THR:H    | 2:289:B:ILE:HG22 | 12                  | 0.14     | 0.02                | 0.15       |
| (1,791)  | 2:288:B:THR:H    | 2:289:B:ILE:HG23 | 12                  | 0.14     | 0.02                | 0.15       |
| (1,1062) | 2:213:B:GLU:HB2  | 2:239:B:LEU:HA   | 12                  | 0.14     | 0.03                | 0.14       |
| (1,1062) | 2:213:B:GLU:HB3  | 2:239:B:LEU:HA   | 12                  | 0.14     | 0.03                | 0.14       |
| (1,146)  | 2:283:B:ALA:H    | 2:281:B:ILE:HG12 | 11                  | 0.26     | 0.07                | 0.25       |
| (1,146)  | 2:283:B:ALA:H    | 2:281:B:ILE:HG13 | 11                  | 0.26     | 0.07                | 0.25       |
| (1,733)  | 2:218:B:LEU:H    | 2:218:B:LEU:HG   | 11                  | 0.21     | 0.1                 | 0.16       |
| (1,351)  | 2:246:B:LYS:H    | 2:244:B:ASP:H    | 10                  | 0.17     | 0.05                | 0.15       |
| (1,1618) | 2:224:B:ASP:HA   | 2:193:B:PHE:HZ   | 10                  | 0.16     | 0.04                | 0.16       |
| (1,1139) | 1:188:A:ASN:HA   | 2:333:B:LYS:HB2  | 10                  | 0.14     | 0.02                | 0.13       |
| (1,1139) | 1:188:A:ASN:HA   | 2:333:B:LYS:HB3  | 10                  | 0.14     | 0.02                | 0.13       |
| (1,11)   | 2:295:B:THR:H    | 2:294:B:VAL:HB   | 10                  | 0.13     | 0.01                | 0.13       |
| (1,1347) | 2:244:B:ASP:HA   | 2:286:B:ASN:HB2  | 10                  | 0.12     | 0.02                | 0.11       |
| (1,1347) | 2:244:B:ASP:HA   | 2:286:B:ASN:HB3  | 10                  | 0.12     | 0.02                | 0.11       |
| (1,587)  | 2:328:B:THR:H    | 2:332:B:VAL:HB   | 8                   | 0.14     | 0.03                | 0.12       |
| (1,1098) | 2:276:B:THR:HA   | 2:272:B:GLU:HB2  | 8                   | 0.12     | 0.02                | 0.12       |
| (1,1098) | 2:276:B:THR:HA   | 2:272:B:GLU:HB3  | 8                   | 0.12     | 0.02                | 0.12       |
| (1,1588) | 2:223:B:LYS:HG2  | 2:221:B:LYS:HA   | 7                   | 0.32     | 0.08                | 0.34       |
| (1,1588) | 2:223:B:LYS:HG3  | 2:221:B:LYS:HA   | 7                   | 0.32     | 0.08                | 0.34       |
| (1,82)   | 2:321:B:LYS:H    | 2:321:B:LYS:HG2  | 7                   | 0.11     | 0.0                 | 0.11       |
| (1,82)   | 2:321:B:LYS:H    | 2:321:B:LYS:HG3  | 7                   | 0.11     | 0.0                 | 0.11       |
| (1,107)  | 2:246:B:LYS:H    | 2:245:B:ASP:HB2  | 6                   | 0.2      | 0.07                | 0.23       |
| (1,107)  | 2:246:B:LYS:H    | 2:245:B:ASP:HB3  | 6                   | 0.2      | 0.07                | 0.23       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,963)  | 2:220:B:LEU:HD11 | 2:204:B:THR:HB   | 6                   | 0.17     | 0.05                | 0.18       |
| (1,963)  | 2:220:B:LEU:HD12 | 2:204:B:THR:HB   | 6                   | 0.17     | 0.05                | 0.18       |
| (1,963)  | 2:220:B:LEU:HD13 | 2:204:B:THR:HB   | 6                   | 0.17     | 0.05                | 0.18       |
| (1,963)  | 2:220:B:LEU:HD21 | 2:204:B:THR:HB   | 6                   | 0.17     | 0.05                | 0.18       |
| (1,963)  | 2:220:B:LEU:HD22 | 2:204:B:THR:HB   | 6                   | 0.17     | 0.05                | 0.18       |
| (1,963)  | 2:220:B:LEU:HD23 | 2:204:B:THR:HB   | 6                   | 0.17     | 0.05                | 0.18       |
| (1,1562) | 2:194:B:THR:HA   | 2:202:B:ILE:HG21 | 6                   | 0.15     | 0.03                | 0.15       |
| (1,1562) | 2:194:B:THR:HA   | 2:202:B:ILE:HG22 | 6                   | 0.15     | 0.03                | 0.15       |
| (1,1562) | 2:194:B:THR:HA   | 2:202:B:ILE:HG23 | 6                   | 0.15     | 0.03                | 0.15       |
| (1,1109) | 2:193:B:PHE:HD1  | 2:203:B:VAL:HB   | 6                   | 0.14     | 0.02                | 0.15       |
| (1,1109) | 2:193:B:PHE:HD2  | 2:203:B:VAL:HB   | 6                   | 0.14     | 0.02                | 0.15       |
| (1,21)   | 2:281:B:ILE:H    | 2:277:B:ILE:HG21 | 6                   | 0.14     | 0.02                | 0.14       |
| (1,21)   | 2:281:B:ILE:H    | 2:277:B:ILE:HG22 | 6                   | 0.14     | 0.02                | 0.14       |
| (1,21)   | 2:281:B:ILE:H    | 2:277:B:ILE:HG23 | 6                   | 0.14     | 0.02                | 0.14       |
| (1,827)  | 2:320:B:ALA:H    | 2:323:B:LYS:HB2  | 6                   | 0.12     | 0.01                | 0.12       |
| (1,827)  | 2:320:B:ALA:H    | 2:323:B:LYS:HB3  | 6                   | 0.12     | 0.01                | 0.12       |
| (1,447)  | 2:241:B:TYR:H    | 2:242:B:ILE:HB   | 5                   | 0.31     | 0.08                | 0.35       |
| (1,1455) | 2:247:B:ASN:HA   | 2:289:B:ILE:HD11 | 5                   | 0.18     | 0.05                | 0.2        |
| (1,1455) | 2:247:B:ASN:HA   | 2:289:B:ILE:HD12 | 5                   | 0.18     | 0.05                | 0.2        |
| (1,1455) | 2:247:B:ASN:HA   | 2:289:B:ILE:HD13 | 5                   | 0.18     | 0.05                | 0.2        |
| (1,1660) | 2:337:B:ILE:HA   | 1:186:A:ASP:HB2  | 5                   | 0.15     | 0.05                | 0.12       |
| (1,1660) | 2:337:B:ILE:HA   | 1:186:A:ASP:HB3  | 5                   | 0.15     | 0.05                | 0.12       |
| (1,52)   | 2:327:B:ILE:H    | 2:321:B:LYS:HG2  | 5                   | 0.14     | 0.02                | 0.14       |
| (1,52)   | 2:327:B:ILE:H    | 2:321:B:LYS:HG3  | 5                   | 0.14     | 0.02                | 0.14       |
| (1,996)  | 2:294:B:VAL:HG11 | 2:318:B:LEU:HB2  | 5                   | 0.13     | 0.01                | 0.13       |
| (1,996)  | 2:294:B:VAL:HG11 | 2:318:B:LEU:HB3  | 5                   | 0.13     | 0.01                | 0.13       |
| (1,996)  | 2:294:B:VAL:HG12 | 2:318:B:LEU:HB2  | 5                   | 0.13     | 0.01                | 0.13       |
| (1,996)  | 2:294:B:VAL:HG12 | 2:318:B:LEU:HB3  | 5                   | 0.13     | 0.01                | 0.13       |
| (1,996)  | 2:294:B:VAL:HG13 | 2:318:B:LEU:HB2  | 5                   | 0.13     | 0.01                | 0.13       |
| (1,996)  | 2:294:B:VAL:HG13 | 2:318:B:LEU:HB3  | 5                   | 0.13     | 0.01                | 0.13       |
| (1,996)  | 2:294:B:VAL:HG21 | 2:318:B:LEU:HB2  | 5                   | 0.13     | 0.01                | 0.13       |
| (1,996)  | 2:294:B:VAL:HG21 | 2:318:B:LEU:HB3  | 5                   | 0.13     | 0.01                | 0.13       |
| (1,996)  | 2:294:B:VAL:HG22 | 2:318:B:LEU:HB2  | 5                   | 0.13     | 0.01                | 0.13       |
| (1,996)  | 2:294:B:VAL:HG22 | 2:318:B:LEU:HB3  | 5                   | 0.13     | 0.01                | 0.13       |
| (1,996)  | 2:294:B:VAL:HG23 | 2:318:B:LEU:HB2  | 5                   | 0.13     | 0.01                | 0.13       |
| (1,996)  | 2:294:B:VAL:HG23 | 2:318:B:LEU:HB3  | 5                   | 0.13     | 0.01                | 0.13       |
| (1,1162) | 2:218:B:LEU:HG   | 2:193:B:PHE:HE1  | 5                   | 0.13     | 0.02                | 0.13       |
| (1,1162) | 2:218:B:LEU:HG   | 2:193:B:PHE:HE2  | 5                   | 0.13     | 0.02                | 0.13       |
| (1,1224) | 2:282:B:GLU:HG2  | 2:278:B:GLU:HA   | 4                   | 0.21     | 0.02                | 0.22       |
| (1,1224) | 2:282:B:GLU:HG3  | 2:278:B:GLU:HA   | 4                   | 0.21     | 0.02                | 0.22       |
| (1,889)  | 2:327:B:ILE:H    | 2:327:B:ILE:HD11 | 4                   | 0.15     | 0.07                | 0.12       |
| (1,889)  | 2:327:B:ILE:H    | 2:327:B:ILE:HD12 | 4                   | 0.15     | 0.07                | 0.12       |

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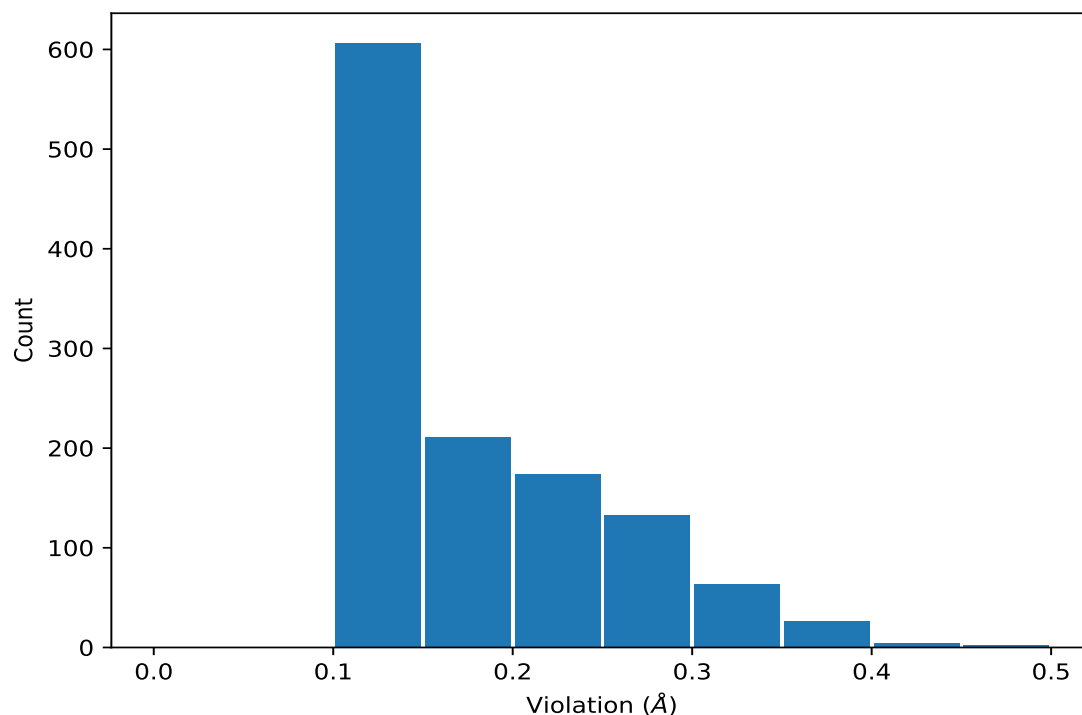
| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,889)  | 2:327:B:ILE:H    | 2:327:B:ILE:HD13 | 4                   | 0.15     | 0.07                | 0.12       |
| (1,1634) | 2:241:B:TYR:HA   | 2:210:B:ASP:HB2  | 4                   | 0.14     | 0.04                | 0.14       |
| (1,1634) | 2:241:B:TYR:HA   | 2:210:B:ASP:HB3  | 4                   | 0.14     | 0.04                | 0.14       |
| (1,445)  | 2:322:B:GLU:H    | 2:322:B:GLU:HG2  | 4                   | 0.13     | 0.0                 | 0.13       |
| (1,445)  | 2:322:B:GLU:H    | 2:322:B:GLU:HG3  | 4                   | 0.13     | 0.0                 | 0.13       |
| (1,779)  | 2:248:B:TYR:H    | 2:248:B:TYR:HE1  | 3                   | 0.23     | 0.05                | 0.21       |
| (1,779)  | 2:248:B:TYR:H    | 2:248:B:TYR:HE2  | 3                   | 0.23     | 0.05                | 0.21       |
| (1,980)  | 2:262:B:THR:HG21 | 2:255:B:LEU:HA   | 3                   | 0.14     | 0.01                | 0.14       |
| (1,980)  | 2:262:B:THR:HG22 | 2:255:B:LEU:HA   | 3                   | 0.14     | 0.01                | 0.14       |
| (1,980)  | 2:262:B:THR:HG23 | 2:255:B:LEU:HA   | 3                   | 0.14     | 0.01                | 0.14       |
| (1,865)  | 2:328:B:THR:H    | 2:328:B:THR:HB   | 3                   | 0.14     | 0.01                | 0.13       |
| (1,1548) | 2:337:B:ILE:HG21 | 1:186:A:ASP:HA   | 3                   | 0.12     | 0.01                | 0.12       |
| (1,1548) | 2:337:B:ILE:HG22 | 1:186:A:ASP:HA   | 3                   | 0.12     | 0.01                | 0.12       |
| (1,1548) | 2:337:B:ILE:HG23 | 1:186:A:ASP:HA   | 3                   | 0.12     | 0.01                | 0.12       |
| (1,831)  | 2:292:B:ARG:H    | 2:291:B:HIS:HD2  | 3                   | 0.12     | 0.0                 | 0.12       |
| (1,379)  | 2:327:B:ILE:H    | 2:325:B:MET:HA   | 3                   | 0.12     | 0.0                 | 0.12       |
| (1,1123) | 2:207:B:ILE:HD11 | 2:205:B:SER:HA   | 3                   | 0.11     | 0.0                 | 0.11       |
| (1,1123) | 2:207:B:ILE:HD12 | 2:205:B:SER:HA   | 3                   | 0.11     | 0.0                 | 0.11       |
| (1,1123) | 2:207:B:ILE:HD13 | 2:205:B:SER:HA   | 3                   | 0.11     | 0.0                 | 0.11       |
| (1,1144) | 2:266:B:ARG:HA   | 2:270:B:ILE:HB   | 2                   | 0.36     | 0.08                | 0.36       |
| (1,1211) | 2:327:B:ILE:HB   | 2:332:B:VAL:HB   | 2                   | 0.23     | 0.09                | 0.23       |
| (1,354)  | 2:283:B:ALA:H    | 2:284:B:LEU:HG   | 2                   | 0.22     | 0.02                | 0.22       |
| (1,952)  | 2:229:B:LEU:HD11 | 2:277:B:ILE:H    | 2                   | 0.14     | 0.02                | 0.14       |
| (1,952)  | 2:229:B:LEU:HD12 | 2:277:B:ILE:H    | 2                   | 0.14     | 0.02                | 0.14       |
| (1,952)  | 2:229:B:LEU:HD13 | 2:277:B:ILE:H    | 2                   | 0.14     | 0.02                | 0.14       |
| (1,952)  | 2:229:B:LEU:HD21 | 2:277:B:ILE:H    | 2                   | 0.14     | 0.02                | 0.14       |
| (1,952)  | 2:229:B:LEU:HD22 | 2:277:B:ILE:H    | 2                   | 0.14     | 0.02                | 0.14       |
| (1,952)  | 2:229:B:LEU:HD23 | 2:277:B:ILE:H    | 2                   | 0.14     | 0.02                | 0.14       |
| (1,571)  | 2:244:B:ASP:H    | 2:288:B:THR:HG21 | 2                   | 0.13     | 0.01                | 0.13       |
| (1,571)  | 2:244:B:ASP:H    | 2:288:B:THR:HG22 | 2                   | 0.13     | 0.01                | 0.13       |
| (1,571)  | 2:244:B:ASP:H    | 2:288:B:THR:HG23 | 2                   | 0.13     | 0.01                | 0.13       |
| (1,824)  | 2:229:B:LEU:H    | 2:229:B:LEU:HG   | 2                   | 0.12     | 0.02                | 0.12       |
| (1,888)  | 2:303:B:LYS:H    | 2:303:B:LYS:HE2  | 2                   | 0.12     | 0.02                | 0.12       |
| (1,888)  | 2:303:B:LYS:H    | 2:303:B:LYS:HE3  | 2                   | 0.12     | 0.02                | 0.12       |
| (1,1350) | 2:329:B:ILE:HB   | 2:328:B:THR:HB   | 2                   | 0.12     | 0.02                | 0.12       |
| (1,374)  | 2:328:B:THR:H    | 2:327:B:ILE:HB   | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,494)  | 2:283:B:ALA:H    | 2:279:B:GLN:HB2  | 2                   | 0.11     | 0.01                | 0.11       |
| (1,494)  | 2:283:B:ALA:H    | 2:279:B:GLN:HB3  | 2                   | 0.11     | 0.01                | 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) |
|----------|-----------------|----------------|----------|---------------|
| (1,853)  | 2:243:B:SER:H   | 2:244:B:ASP:H  | 10       | 0.46          |
| (1,853)  | 2:243:B:SER:H   | 2:244:B:ASP:H  | 16       | 0.46          |
| (1,1588) | 2:223:B:LYS:HG2 | 2:221:B:LYS:HA | 19       | 0.44          |
| (1,1588) | 2:223:B:LYS:HG3 | 2:221:B:LYS:HA | 19       | 0.44          |
| (1,1144) | 2:266:B:ARG:HA  | 2:270:B:ILE:HB | 3        | 0.44          |
| (1,853)  | 2:243:B:SER:H   | 2:244:B:ASP:H  | 7        | 0.41          |
| (1,853)  | 2:243:B:SER:H   | 2:244:B:ASP:H  | 3        | 0.39          |
| (1,853)  | 2:243:B:SER:H   | 2:244:B:ASP:H  | 8        | 0.39          |
| (1,853)  | 2:243:B:SER:H   | 2:244:B:ASP:H  | 9        | 0.39          |
| (1,853)  | 2:243:B:SER:H   | 2:244:B:ASP:H  | 15       | 0.39          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,853)  | 2:243:B:SER:H   | 2:244:B:ASP:H    | 5        | 0.38          |
| (1,853)  | 2:243:B:SER:H   | 2:244:B:ASP:H    | 13       | 0.38          |
| (1,853)  | 2:243:B:SER:H   | 2:244:B:ASP:H    | 17       | 0.38          |
| (1,853)  | 2:243:B:SER:H   | 2:244:B:ASP:H    | 18       | 0.38          |
| (1,853)  | 2:243:B:SER:H   | 2:244:B:ASP:H    | 19       | 0.38          |
| (1,447)  | 2:241:B:TYR:H   | 2:242:B:ILE:HB   | 17       | 0.38          |
| (1,853)  | 2:243:B:SER:H   | 2:244:B:ASP:H    | 6        | 0.37          |
| (1,853)  | 2:243:B:SER:H   | 2:244:B:ASP:H    | 11       | 0.37          |
| (1,733)  | 2:218:B:LEU:H   | 2:218:B:LEU:HG   | 20       | 0.37          |
| (1,607)  | 2:282:B:GLU:H   | 2:279:B:GLN:HB2  | 14       | 0.37          |
| (1,607)  | 2:282:B:GLU:H   | 2:279:B:GLN:HB3  | 14       | 0.37          |
| (1,447)  | 2:241:B:TYR:H   | 2:242:B:ILE:HB   | 14       | 0.37          |
| (1,146)  | 2:283:B:ALA:H   | 2:281:B:ILE:HG12 | 5        | 0.37          |
| (1,146)  | 2:283:B:ALA:H   | 2:281:B:ILE:HG13 | 5        | 0.37          |
| (1,1588) | 2:223:B:LYS:HG2 | 2:221:B:LYS:HA   | 8        | 0.36          |
| (1,1588) | 2:223:B:LYS:HG3 | 2:221:B:LYS:HA   | 8        | 0.36          |
| (1,1588) | 2:223:B:LYS:HG2 | 2:221:B:LYS:HA   | 18       | 0.36          |
| (1,1588) | 2:223:B:LYS:HG3 | 2:221:B:LYS:HA   | 18       | 0.36          |
| (1,853)  | 2:243:B:SER:H   | 2:244:B:ASP:H    | 2        | 0.36          |
| (1,853)  | 2:243:B:SER:H   | 2:244:B:ASP:H    | 14       | 0.36          |
| (1,853)  | 2:243:B:SER:H   | 2:244:B:ASP:H    | 20       | 0.36          |
| (1,77)   | 2:331:B:GLU:H   | 2:333:B:LYS:HB2  | 10       | 0.36          |
| (1,77)   | 2:331:B:GLU:H   | 2:333:B:LYS:HB3  | 10       | 0.36          |
| (1,447)  | 2:241:B:TYR:H   | 2:242:B:ILE:HB   | 11       | 0.35          |
| (1,146)  | 2:283:B:ALA:H   | 2:281:B:ILE:HG12 | 3        | 0.35          |
| (1,146)  | 2:283:B:ALA:H   | 2:281:B:ILE:HG13 | 3        | 0.35          |
| (1,146)  | 2:283:B:ALA:H   | 2:281:B:ILE:HG12 | 7        | 0.35          |
| (1,146)  | 2:283:B:ALA:H   | 2:281:B:ILE:HG13 | 7        | 0.35          |
| (1,1588) | 2:223:B:LYS:HG2 | 2:221:B:LYS:HA   | 2        | 0.34          |
| (1,1588) | 2:223:B:LYS:HG3 | 2:221:B:LYS:HA   | 2        | 0.34          |
| (1,895)  | 2:279:B:GLN:H   | 2:226:B:LYS:HB2  | 16       | 0.34          |
| (1,895)  | 2:279:B:GLN:H   | 2:226:B:LYS:HB3  | 16       | 0.34          |
| (1,853)  | 2:243:B:SER:H   | 2:244:B:ASP:H    | 1        | 0.34          |
| (1,853)  | 2:243:B:SER:H   | 2:244:B:ASP:H    | 12       | 0.34          |
| (1,733)  | 2:218:B:LEU:H   | 2:218:B:LEU:HG   | 3        | 0.34          |
| (1,733)  | 2:218:B:LEU:H   | 2:218:B:LEU:HG   | 8        | 0.34          |
| (1,514)  | 2:238:B:SER:H   | 2:234:B:GLU:HB2  | 4        | 0.34          |
| (1,514)  | 2:238:B:SER:H   | 2:234:B:GLU:HB3  | 4        | 0.34          |
| (1,235)  | 2:299:B:GLU:H   | 2:297:B:ASP:H    | 8        | 0.34          |
| (1,77)   | 2:331:B:GLU:H   | 2:333:B:LYS:HB2  | 19       | 0.34          |
| (1,77)   | 2:331:B:GLU:H   | 2:333:B:LYS:HB3  | 19       | 0.34          |
| (1,235)  | 2:299:B:GLU:H   | 2:297:B:ASP:H    | 4        | 0.33          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,77)   | 2:331:B:GLU:H   | 2:333:B:LYS:HB2 | 5        | 0.33          |
| (1,77)   | 2:331:B:GLU:H   | 2:333:B:LYS:HB3 | 5        | 0.33          |
| (1,1588) | 2:223:B:LYS:HG2 | 2:221:B:LYS:HA  | 4        | 0.32          |
| (1,1588) | 2:223:B:LYS:HG3 | 2:221:B:LYS:HA  | 4        | 0.32          |
| (1,1234) | 2:255:B:LEU:HG  | 2:273:B:LEU:HB2 | 4        | 0.32          |
| (1,1234) | 2:255:B:LEU:HG  | 2:273:B:LEU:HB3 | 4        | 0.32          |
| (1,1211) | 2:327:B:ILE:HB  | 2:332:B:VAL:HB  | 13       | 0.32          |
| (1,607)  | 2:282:B:GLU:H   | 2:279:B:GLN:HB2 | 3        | 0.32          |
| (1,607)  | 2:282:B:GLU:H   | 2:279:B:GLN:HB3 | 3        | 0.32          |
| (1,607)  | 2:282:B:GLU:H   | 2:279:B:GLN:HB2 | 5        | 0.32          |
| (1,607)  | 2:282:B:GLU:H   | 2:279:B:GLN:HB3 | 5        | 0.32          |
| (1,607)  | 2:282:B:GLU:H   | 2:279:B:GLN:HB2 | 10       | 0.32          |
| (1,607)  | 2:282:B:GLU:H   | 2:279:B:GLN:HB3 | 10       | 0.32          |
| (1,166)  | 2:281:B:ILE:H   | 2:279:B:GLN:HB2 | 9        | 0.32          |
| (1,166)  | 2:281:B:ILE:H   | 2:279:B:GLN:HB3 | 9        | 0.32          |
| (1,166)  | 2:281:B:ILE:H   | 2:279:B:GLN:HB2 | 11       | 0.32          |
| (1,166)  | 2:281:B:ILE:H   | 2:279:B:GLN:HB3 | 11       | 0.32          |
| (1,77)   | 2:331:B:GLU:H   | 2:333:B:LYS:HB2 | 3        | 0.32          |
| (1,77)   | 2:331:B:GLU:H   | 2:333:B:LYS:HB3 | 3        | 0.32          |
| (1,77)   | 2:331:B:GLU:H   | 2:333:B:LYS:HB2 | 13       | 0.32          |
| (1,77)   | 2:331:B:GLU:H   | 2:333:B:LYS:HB3 | 13       | 0.32          |
| (1,607)  | 2:282:B:GLU:H   | 2:279:B:GLN:HB2 | 1        | 0.31          |
| (1,607)  | 2:282:B:GLU:H   | 2:279:B:GLN:HB3 | 1        | 0.31          |
| (1,607)  | 2:282:B:GLU:H   | 2:279:B:GLN:HB2 | 7        | 0.31          |
| (1,607)  | 2:282:B:GLU:H   | 2:279:B:GLN:HB3 | 7        | 0.31          |
| (1,470)  | 2:343:B:LYS:H   | 2:343:B:LYS:HD2 | 16       | 0.31          |
| (1,470)  | 2:343:B:LYS:H   | 2:343:B:LYS:HD3 | 16       | 0.31          |
| (1,281)  | 2:343:B:LYS:H   | 2:343:B:LYS:HG2 | 16       | 0.31          |
| (1,281)  | 2:343:B:LYS:H   | 2:343:B:LYS:HG3 | 16       | 0.31          |
| (1,235)  | 2:299:B:GLU:H   | 2:297:B:ASP:H   | 3        | 0.31          |
| (1,235)  | 2:299:B:GLU:H   | 2:297:B:ASP:H   | 13       | 0.31          |
| (1,166)  | 2:281:B:ILE:H   | 2:279:B:GLN:HB2 | 2        | 0.31          |
| (1,166)  | 2:281:B:ILE:H   | 2:279:B:GLN:HB3 | 2        | 0.31          |
| (1,166)  | 2:281:B:ILE:H   | 2:279:B:GLN:HB2 | 4        | 0.31          |
| (1,166)  | 2:281:B:ILE:H   | 2:279:B:GLN:HB3 | 4        | 0.31          |
| (1,166)  | 2:281:B:ILE:H   | 2:279:B:GLN:HB2 | 8        | 0.31          |
| (1,166)  | 2:281:B:ILE:H   | 2:279:B:GLN:HB3 | 8        | 0.31          |
| (1,166)  | 2:281:B:ILE:H   | 2:279:B:GLN:HB2 | 19       | 0.31          |
| (1,166)  | 2:281:B:ILE:H   | 2:279:B:GLN:HB3 | 19       | 0.31          |
| (1,166)  | 2:281:B:ILE:H   | 2:279:B:GLN:HB2 | 20       | 0.31          |
| (1,166)  | 2:281:B:ILE:H   | 2:279:B:GLN:HB3 | 20       | 0.31          |
| (1,77)   | 2:331:B:GLU:H   | 2:333:B:LYS:HB2 | 6        | 0.31          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,77)   | 2:331:B:GLU:H    | 2:333:B:LYS:HB3  | 6        | 0.31          |
| (1,77)   | 2:331:B:GLU:H    | 2:333:B:LYS:HB2  | 20       | 0.31          |
| (1,77)   | 2:331:B:GLU:H    | 2:333:B:LYS:HB3  | 20       | 0.31          |
| (1,956)  | 2:327:B:ILE:HD11 | 2:328:B:THR:HA   | 20       | 0.3           |
| (1,956)  | 2:327:B:ILE:HD12 | 2:328:B:THR:HA   | 20       | 0.3           |
| (1,956)  | 2:327:B:ILE:HD13 | 2:328:B:THR:HA   | 20       | 0.3           |
| (1,895)  | 2:279:B:GLN:H    | 2:226:B:LYS:HB2  | 10       | 0.3           |
| (1,895)  | 2:279:B:GLN:H    | 2:226:B:LYS:HB3  | 10       | 0.3           |
| (1,779)  | 2:248:B:TYR:H    | 2:248:B:TYR:HE1  | 20       | 0.3           |
| (1,779)  | 2:248:B:TYR:H    | 2:248:B:TYR:HE2  | 20       | 0.3           |
| (1,514)  | 2:238:B:SER:H    | 2:234:B:GLU:HB2  | 11       | 0.3           |
| (1,514)  | 2:238:B:SER:H    | 2:234:B:GLU:HB3  | 11       | 0.3           |
| (1,447)  | 2:241:B:TYR:H    | 2:242:B:ILE:HB   | 5        | 0.3           |
| (1,166)  | 2:281:B:ILE:H    | 2:279:B:GLN:HB2  | 14       | 0.3           |
| (1,166)  | 2:281:B:ILE:H    | 2:279:B:GLN:HB3  | 14       | 0.3           |
| (1,146)  | 2:283:B:ALA:H    | 2:281:B:ILE:HG12 | 16       | 0.3           |
| (1,146)  | 2:283:B:ALA:H    | 2:281:B:ILE:HG13 | 16       | 0.3           |
| (1,1234) | 2:255:B:LEU:HG   | 2:273:B:LEU:HB2  | 2        | 0.29          |
| (1,1234) | 2:255:B:LEU:HG   | 2:273:B:LEU:HB3  | 2        | 0.29          |
| (1,956)  | 2:327:B:ILE:HD11 | 2:328:B:THR:HA   | 19       | 0.29          |
| (1,956)  | 2:327:B:ILE:HD12 | 2:328:B:THR:HA   | 19       | 0.29          |
| (1,956)  | 2:327:B:ILE:HD13 | 2:328:B:THR:HA   | 19       | 0.29          |
| (1,607)  | 2:282:B:GLU:H    | 2:279:B:GLN:HB2  | 16       | 0.29          |
| (1,607)  | 2:282:B:GLU:H    | 2:279:B:GLN:HB3  | 16       | 0.29          |
| (1,514)  | 2:238:B:SER:H    | 2:234:B:GLU:HB2  | 5        | 0.29          |
| (1,514)  | 2:238:B:SER:H    | 2:234:B:GLU:HB3  | 5        | 0.29          |
| (1,235)  | 2:299:B:GLU:H    | 2:297:B:ASP:H    | 6        | 0.29          |
| (1,235)  | 2:299:B:GLU:H    | 2:297:B:ASP:H    | 10       | 0.29          |
| (1,77)   | 2:331:B:GLU:H    | 2:333:B:LYS:HB2  | 1        | 0.29          |
| (1,77)   | 2:331:B:GLU:H    | 2:333:B:LYS:HB3  | 1        | 0.29          |
| (1,77)   | 2:331:B:GLU:H    | 2:333:B:LYS:HB2  | 15       | 0.29          |
| (1,77)   | 2:331:B:GLU:H    | 2:333:B:LYS:HB3  | 15       | 0.29          |
| (1,1588) | 2:223:B:LYS:HG2  | 2:221:B:LYS:HA   | 5        | 0.28          |
| (1,1588) | 2:223:B:LYS:HG3  | 2:221:B:LYS:HA   | 5        | 0.28          |
| (1,1144) | 2:266:B:ARG:HA   | 2:270:B:ILE:HB   | 17       | 0.28          |
| (1,956)  | 2:327:B:ILE:HD11 | 2:328:B:THR:HA   | 3        | 0.28          |
| (1,956)  | 2:327:B:ILE:HD12 | 2:328:B:THR:HA   | 3        | 0.28          |
| (1,956)  | 2:327:B:ILE:HD13 | 2:328:B:THR:HA   | 3        | 0.28          |
| (1,956)  | 2:327:B:ILE:HD11 | 2:328:B:THR:HA   | 4        | 0.28          |
| (1,956)  | 2:327:B:ILE:HD12 | 2:328:B:THR:HA   | 4        | 0.28          |
| (1,956)  | 2:327:B:ILE:HD13 | 2:328:B:THR:HA   | 4        | 0.28          |
| (1,889)  | 2:327:B:ILE:H    | 2:327:B:ILE:HD11 | 6        | 0.28          |

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| Key     | Atom-1        | Atom-2           | Model ID | Violation (Å) |
|---------|---------------|------------------|----------|---------------|
| (1,889) | 2:327:B:ILE:H | 2:327:B:ILE:HD12 | 6        | 0.28          |
| (1,889) | 2:327:B:ILE:H | 2:327:B:ILE:HD13 | 6        | 0.28          |
| (1,607) | 2:282:B:GLU:H | 2:279:B:GLN:HB2  | 6        | 0.28          |
| (1,607) | 2:282:B:GLU:H | 2:279:B:GLN:HB3  | 6        | 0.28          |
| (1,514) | 2:238:B:SER:H | 2:234:B:GLU:HB2  | 3        | 0.28          |
| (1,514) | 2:238:B:SER:H | 2:234:B:GLU:HB3  | 3        | 0.28          |
| (1,514) | 2:238:B:SER:H | 2:234:B:GLU:HB2  | 8        | 0.28          |
| (1,514) | 2:238:B:SER:H | 2:234:B:GLU:HB3  | 8        | 0.28          |
| (1,514) | 2:238:B:SER:H | 2:234:B:GLU:HB2  | 17       | 0.28          |
| (1,514) | 2:238:B:SER:H | 2:234:B:GLU:HB3  | 17       | 0.28          |
| (1,514) | 2:238:B:SER:H | 2:234:B:GLU:HB2  | 20       | 0.28          |
| (1,514) | 2:238:B:SER:H | 2:234:B:GLU:HB3  | 20       | 0.28          |
| (1,235) | 2:299:B:GLU:H | 2:297:B:ASP:H    | 7        | 0.28          |
| (1,235) | 2:299:B:GLU:H | 2:297:B:ASP:H    | 9        | 0.28          |
| (1,235) | 2:299:B:GLU:H | 2:297:B:ASP:H    | 14       | 0.28          |
| (1,235) | 2:299:B:GLU:H | 2:297:B:ASP:H    | 20       | 0.28          |
| (1,166) | 2:281:B:ILE:H | 2:279:B:GLN:HB2  | 13       | 0.28          |
| (1,166) | 2:281:B:ILE:H | 2:279:B:GLN:HB3  | 13       | 0.28          |
| (1,166) | 2:281:B:ILE:H | 2:279:B:GLN:HB2  | 17       | 0.28          |
| (1,166) | 2:281:B:ILE:H | 2:279:B:GLN:HB3  | 17       | 0.28          |
| (1,77)  | 2:331:B:GLU:H | 2:333:B:LYS:HB2  | 7        | 0.28          |
| (1,77)  | 2:331:B:GLU:H | 2:333:B:LYS:HB3  | 7        | 0.28          |
| (1,607) | 2:282:B:GLU:H | 2:279:B:GLN:HB2  | 18       | 0.27          |
| (1,607) | 2:282:B:GLU:H | 2:279:B:GLN:HB3  | 18       | 0.27          |
| (1,514) | 2:238:B:SER:H | 2:234:B:GLU:HB2  | 16       | 0.27          |
| (1,514) | 2:238:B:SER:H | 2:234:B:GLU:HB3  | 16       | 0.27          |
| (1,359) | 2:342:B:GLU:H | 2:343:B:LYS:H    | 1        | 0.27          |
| (1,107) | 2:246:B:LYS:H | 2:245:B:ASP:HB2  | 7        | 0.27          |
| (1,107) | 2:246:B:LYS:H | 2:245:B:ASP:HB3  | 7        | 0.27          |
| (1,607) | 2:282:B:GLU:H | 2:279:B:GLN:HB2  | 15       | 0.26          |
| (1,607) | 2:282:B:GLU:H | 2:279:B:GLN:HB3  | 15       | 0.26          |
| (1,514) | 2:238:B:SER:H | 2:234:B:GLU:HB2  | 6        | 0.26          |
| (1,514) | 2:238:B:SER:H | 2:234:B:GLU:HB3  | 6        | 0.26          |
| (1,514) | 2:238:B:SER:H | 2:234:B:GLU:HB2  | 13       | 0.26          |
| (1,514) | 2:238:B:SER:H | 2:234:B:GLU:HB3  | 13       | 0.26          |
| (1,514) | 2:238:B:SER:H | 2:234:B:GLU:HB2  | 19       | 0.26          |
| (1,514) | 2:238:B:SER:H | 2:234:B:GLU:HB3  | 19       | 0.26          |
| (1,166) | 2:281:B:ILE:H | 2:279:B:GLN:HB2  | 3        | 0.26          |
| (1,166) | 2:281:B:ILE:H | 2:279:B:GLN:HB3  | 3        | 0.26          |
| (1,166) | 2:281:B:ILE:H | 2:279:B:GLN:HB2  | 7        | 0.26          |
| (1,166) | 2:281:B:ILE:H | 2:279:B:GLN:HB3  | 7        | 0.26          |
| (1,107) | 2:246:B:LYS:H | 2:245:B:ASP:HB2  | 8        | 0.26          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,107)  | 2:246:B:LYS:H    | 2:245:B:ASP:HB3  | 8        | 0.26          |
| (1,1660) | 2:337:B:ILE:HA   | 1:186:A:ASP:HB2  | 14       | 0.25          |
| (1,1660) | 2:337:B:ILE:HA   | 1:186:A:ASP:HB3  | 14       | 0.25          |
| (1,1533) | 2:262:B:THR:HA   | 2:255:B:LEU:HD11 | 2        | 0.25          |
| (1,1533) | 2:262:B:THR:HA   | 2:255:B:LEU:HD12 | 2        | 0.25          |
| (1,1533) | 2:262:B:THR:HA   | 2:255:B:LEU:HD13 | 2        | 0.25          |
| (1,1533) | 2:262:B:THR:HA   | 2:255:B:LEU:HD21 | 2        | 0.25          |
| (1,1533) | 2:262:B:THR:HA   | 2:255:B:LEU:HD22 | 2        | 0.25          |
| (1,1533) | 2:262:B:THR:HA   | 2:255:B:LEU:HD23 | 2        | 0.25          |
| (1,1455) | 2:247:B:ASN:HA   | 2:289:B:ILE:HD11 | 19       | 0.25          |
| (1,1455) | 2:247:B:ASN:HA   | 2:289:B:ILE:HD12 | 19       | 0.25          |
| (1,1455) | 2:247:B:ASN:HA   | 2:289:B:ILE:HD13 | 19       | 0.25          |
| (1,1234) | 2:255:B:LEU:HG   | 2:273:B:LEU:HB2  | 12       | 0.25          |
| (1,1234) | 2:255:B:LEU:HG   | 2:273:B:LEU:HB3  | 12       | 0.25          |
| (1,1234) | 2:255:B:LEU:HG   | 2:273:B:LEU:HB2  | 20       | 0.25          |
| (1,1234) | 2:255:B:LEU:HG   | 2:273:B:LEU:HB3  | 20       | 0.25          |
| (1,1168) | 2:193:B:PHE:HD1  | 2:215:B:LEU:HB2  | 20       | 0.25          |
| (1,1168) | 2:193:B:PHE:HD1  | 2:215:B:LEU:HB3  | 20       | 0.25          |
| (1,1168) | 2:193:B:PHE:HD2  | 2:215:B:LEU:HB2  | 20       | 0.25          |
| (1,1168) | 2:193:B:PHE:HD2  | 2:215:B:LEU:HB3  | 20       | 0.25          |
| (1,956)  | 2:327:B:ILE:HD11 | 2:328:B:THR:HA   | 7        | 0.25          |
| (1,956)  | 2:327:B:ILE:HD12 | 2:328:B:THR:HA   | 7        | 0.25          |
| (1,956)  | 2:327:B:ILE:HD13 | 2:328:B:THR:HA   | 7        | 0.25          |
| (1,895)  | 2:279:B:GLN:H    | 2:226:B:LYS:HB2  | 9        | 0.25          |
| (1,895)  | 2:279:B:GLN:H    | 2:226:B:LYS:HB3  | 9        | 0.25          |
| (1,853)  | 2:243:B:SER:H    | 2:244:B:ASP:H    | 4        | 0.25          |
| (1,733)  | 2:218:B:LEU:H    | 2:218:B:LEU:HG   | 2        | 0.25          |
| (1,733)  | 2:218:B:LEU:H    | 2:218:B:LEU:HG   | 19       | 0.25          |
| (1,607)  | 2:282:B:GLU:H    | 2:279:B:GLN:HB2  | 4        | 0.25          |
| (1,607)  | 2:282:B:GLU:H    | 2:279:B:GLN:HB3  | 4        | 0.25          |
| (1,607)  | 2:282:B:GLU:H    | 2:279:B:GLN:HB2  | 12       | 0.25          |
| (1,607)  | 2:282:B:GLU:H    | 2:279:B:GLN:HB3  | 12       | 0.25          |
| (1,514)  | 2:238:B:SER:H    | 2:234:B:GLU:HB2  | 2        | 0.25          |
| (1,514)  | 2:238:B:SER:H    | 2:234:B:GLU:HB3  | 2        | 0.25          |
| (1,359)  | 2:342:B:GLU:H    | 2:343:B:LYS:H    | 4        | 0.25          |
| (1,359)  | 2:342:B:GLU:H    | 2:343:B:LYS:H    | 7        | 0.25          |
| (1,351)  | 2:246:B:LYS:H    | 2:244:B:ASP:H    | 6        | 0.25          |
| (1,235)  | 2:299:B:GLU:H    | 2:297:B:ASP:H    | 12       | 0.25          |
| (1,166)  | 2:281:B:ILE:H    | 2:279:B:GLN:HB2  | 16       | 0.25          |
| (1,166)  | 2:281:B:ILE:H    | 2:279:B:GLN:HB3  | 16       | 0.25          |
| (1,166)  | 2:281:B:ILE:H    | 2:279:B:GLN:HB2  | 18       | 0.25          |
| (1,166)  | 2:281:B:ILE:H    | 2:279:B:GLN:HB3  | 18       | 0.25          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,146)  | 2:283:B:ALA:H   | 2:281:B:ILE:HG12 | 15       | 0.25          |
| (1,146)  | 2:283:B:ALA:H   | 2:281:B:ILE:HG13 | 15       | 0.25          |
| (1,146)  | 2:283:B:ALA:H   | 2:281:B:ILE:HG12 | 18       | 0.25          |
| (1,146)  | 2:283:B:ALA:H   | 2:281:B:ILE:HG13 | 18       | 0.25          |
| (1,107)  | 2:246:B:LYS:H   | 2:245:B:ASP:HB2  | 17       | 0.25          |
| (1,107)  | 2:246:B:LYS:H   | 2:245:B:ASP:HB3  | 17       | 0.25          |
| (1,77)   | 2:331:B:GLU:H   | 2:333:B:LYS:HB2  | 12       | 0.25          |
| (1,77)   | 2:331:B:GLU:H   | 2:333:B:LYS:HB3  | 12       | 0.25          |
| (1,77)   | 2:331:B:GLU:H   | 2:333:B:LYS:HB2  | 17       | 0.25          |
| (1,77)   | 2:331:B:GLU:H   | 2:333:B:LYS:HB3  | 17       | 0.25          |
| (1,1234) | 2:255:B:LEU:HG  | 2:273:B:LEU:HB2  | 10       | 0.24          |
| (1,1234) | 2:255:B:LEU:HG  | 2:273:B:LEU:HB3  | 10       | 0.24          |
| (1,1224) | 2:282:B:GLU:HG2 | 2:278:B:GLU:HA   | 9        | 0.24          |
| (1,1224) | 2:282:B:GLU:HG3 | 2:278:B:GLU:HA   | 9        | 0.24          |
| (1,1168) | 2:193:B:PHE:HD1 | 2:215:B:LEU:HB2  | 15       | 0.24          |
| (1,1168) | 2:193:B:PHE:HD1 | 2:215:B:LEU:HB3  | 15       | 0.24          |
| (1,1168) | 2:193:B:PHE:HD2 | 2:215:B:LEU:HB2  | 15       | 0.24          |
| (1,1168) | 2:193:B:PHE:HD2 | 2:215:B:LEU:HB3  | 15       | 0.24          |
| (1,895)  | 2:279:B:GLN:H   | 2:226:B:LYS:HB2  | 4        | 0.24          |
| (1,895)  | 2:279:B:GLN:H   | 2:226:B:LYS:HB3  | 4        | 0.24          |
| (1,514)  | 2:238:B:SER:H   | 2:234:B:GLU:HB2  | 15       | 0.24          |
| (1,514)  | 2:238:B:SER:H   | 2:234:B:GLU:HB3  | 15       | 0.24          |
| (1,514)  | 2:238:B:SER:H   | 2:234:B:GLU:HB2  | 18       | 0.24          |
| (1,514)  | 2:238:B:SER:H   | 2:234:B:GLU:HB3  | 18       | 0.24          |
| (1,428)  | 2:222:B:GLU:H   | 2:202:B:ILE:HA   | 9        | 0.24          |
| (1,359)  | 2:342:B:GLU:H   | 2:343:B:LYS:H    | 5        | 0.24          |
| (1,359)  | 2:342:B:GLU:H   | 2:343:B:LYS:H    | 8        | 0.24          |
| (1,359)  | 2:342:B:GLU:H   | 2:343:B:LYS:H    | 18       | 0.24          |
| (1,351)  | 2:246:B:LYS:H   | 2:244:B:ASP:H    | 11       | 0.24          |
| (1,146)  | 2:283:B:ALA:H   | 2:281:B:ILE:HG12 | 1        | 0.24          |
| (1,146)  | 2:283:B:ALA:H   | 2:281:B:ILE:HG13 | 1        | 0.24          |
| (1,146)  | 2:283:B:ALA:H   | 2:281:B:ILE:HG12 | 14       | 0.24          |
| (1,146)  | 2:283:B:ALA:H   | 2:281:B:ILE:HG13 | 14       | 0.24          |
| (1,77)   | 2:331:B:GLU:H   | 2:333:B:LYS:HB2  | 4        | 0.24          |
| (1,77)   | 2:331:B:GLU:H   | 2:333:B:LYS:HB3  | 4        | 0.24          |
| (1,1618) | 2:224:B:ASP:HA  | 2:193:B:PHE:HZ   | 13       | 0.23          |
| (1,1234) | 2:255:B:LEU:HG  | 2:273:B:LEU:HB2  | 8        | 0.23          |
| (1,1234) | 2:255:B:LEU:HG  | 2:273:B:LEU:HB3  | 8        | 0.23          |
| (1,1224) | 2:282:B:GLU:HG2 | 2:278:B:GLU:HA   | 19       | 0.23          |
| (1,1224) | 2:282:B:GLU:HG3 | 2:278:B:GLU:HA   | 19       | 0.23          |
| (1,1168) | 2:193:B:PHE:HD1 | 2:215:B:LEU:HB2  | 6        | 0.23          |
| (1,1168) | 2:193:B:PHE:HD1 | 2:215:B:LEU:HB3  | 6        | 0.23          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1168) | 2:193:B:PHE:HD2  | 2:215:B:LEU:HB2  | 6        | 0.23          |
| (1,1168) | 2:193:B:PHE:HD2  | 2:215:B:LEU:HB3  | 6        | 0.23          |
| (1,1168) | 2:193:B:PHE:HD1  | 2:215:B:LEU:HB2  | 19       | 0.23          |
| (1,1168) | 2:193:B:PHE:HD1  | 2:215:B:LEU:HB3  | 19       | 0.23          |
| (1,1168) | 2:193:B:PHE:HD2  | 2:215:B:LEU:HB2  | 19       | 0.23          |
| (1,1168) | 2:193:B:PHE:HD2  | 2:215:B:LEU:HB3  | 19       | 0.23          |
| (1,1036) | 2:329:B:ILE:HD11 | 2:332:B:VAL:HB   | 4        | 0.23          |
| (1,1036) | 2:329:B:ILE:HD12 | 2:332:B:VAL:HB   | 4        | 0.23          |
| (1,1036) | 2:329:B:ILE:HD13 | 2:332:B:VAL:HB   | 4        | 0.23          |
| (1,963)  | 2:220:B:LEU:HD11 | 2:204:B:THR:HB   | 4        | 0.23          |
| (1,963)  | 2:220:B:LEU:HD12 | 2:204:B:THR:HB   | 4        | 0.23          |
| (1,963)  | 2:220:B:LEU:HD13 | 2:204:B:THR:HB   | 4        | 0.23          |
| (1,963)  | 2:220:B:LEU:HD21 | 2:204:B:THR:HB   | 4        | 0.23          |
| (1,963)  | 2:220:B:LEU:HD22 | 2:204:B:THR:HB   | 4        | 0.23          |
| (1,963)  | 2:220:B:LEU:HD23 | 2:204:B:THR:HB   | 4        | 0.23          |
| (1,956)  | 2:327:B:ILE:HD11 | 2:328:B:THR:HA   | 8        | 0.23          |
| (1,956)  | 2:327:B:ILE:HD12 | 2:328:B:THR:HA   | 8        | 0.23          |
| (1,956)  | 2:327:B:ILE:HD13 | 2:328:B:THR:HA   | 8        | 0.23          |
| (1,895)  | 2:279:B:GLN:H    | 2:226:B:LYS:HB2  | 18       | 0.23          |
| (1,895)  | 2:279:B:GLN:H    | 2:226:B:LYS:HB3  | 18       | 0.23          |
| (1,428)  | 2:222:B:GLU:H    | 2:202:B:ILE:HA   | 17       | 0.23          |
| (1,359)  | 2:342:B:GLU:H    | 2:343:B:LYS:H    | 11       | 0.23          |
| (1,354)  | 2:283:B:ALA:H    | 2:284:B:LEU:HG   | 14       | 0.23          |
| (1,235)  | 2:299:B:GLU:H    | 2:297:B:ASP:H    | 2        | 0.23          |
| (1,235)  | 2:299:B:GLU:H    | 2:297:B:ASP:H    | 15       | 0.23          |
| (1,1599) | 2:207:B:ILE:HA   | 2:215:B:LEU:HD11 | 7        | 0.22          |
| (1,1599) | 2:207:B:ILE:HA   | 2:215:B:LEU:HD12 | 7        | 0.22          |
| (1,1599) | 2:207:B:ILE:HA   | 2:215:B:LEU:HD13 | 7        | 0.22          |
| (1,1599) | 2:207:B:ILE:HA   | 2:215:B:LEU:HD21 | 7        | 0.22          |
| (1,1599) | 2:207:B:ILE:HA   | 2:215:B:LEU:HD22 | 7        | 0.22          |
| (1,1599) | 2:207:B:ILE:HA   | 2:215:B:LEU:HD23 | 7        | 0.22          |
| (1,1099) | 2:198:B:LYS:HA   | 2:200:B:LYS:HE2  | 12       | 0.22          |
| (1,1099) | 2:198:B:LYS:HA   | 2:200:B:LYS:HE3  | 12       | 0.22          |
| (1,956)  | 2:327:B:ILE:HD11 | 2:328:B:THR:HA   | 2        | 0.22          |
| (1,956)  | 2:327:B:ILE:HD12 | 2:328:B:THR:HA   | 2        | 0.22          |
| (1,956)  | 2:327:B:ILE:HD13 | 2:328:B:THR:HA   | 2        | 0.22          |
| (1,956)  | 2:327:B:ILE:HD11 | 2:328:B:THR:HA   | 5        | 0.22          |
| (1,956)  | 2:327:B:ILE:HD12 | 2:328:B:THR:HA   | 5        | 0.22          |
| (1,956)  | 2:327:B:ILE:HD13 | 2:328:B:THR:HA   | 5        | 0.22          |
| (1,956)  | 2:327:B:ILE:HD11 | 2:328:B:THR:HA   | 10       | 0.22          |
| (1,956)  | 2:327:B:ILE:HD12 | 2:328:B:THR:HA   | 10       | 0.22          |
| (1,956)  | 2:327:B:ILE:HD13 | 2:328:B:THR:HA   | 10       | 0.22          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,956)  | 2:327:B:ILE:HD11 | 2:328:B:THR:HA   | 16       | 0.22          |
| (1,956)  | 2:327:B:ILE:HD12 | 2:328:B:THR:HA   | 16       | 0.22          |
| (1,956)  | 2:327:B:ILE:HD13 | 2:328:B:THR:HA   | 16       | 0.22          |
| (1,956)  | 2:327:B:ILE:HD11 | 2:328:B:THR:HA   | 18       | 0.22          |
| (1,956)  | 2:327:B:ILE:HD12 | 2:328:B:THR:HA   | 18       | 0.22          |
| (1,956)  | 2:327:B:ILE:HD13 | 2:328:B:THR:HA   | 18       | 0.22          |
| (1,607)  | 2:282:B:GLU:H    | 2:279:B:GLN:HB2  | 8        | 0.22          |
| (1,607)  | 2:282:B:GLU:H    | 2:279:B:GLN:HB3  | 8        | 0.22          |
| (1,587)  | 2:328:B:THR:H    | 2:332:B:VAL:HB   | 4        | 0.22          |
| (1,514)  | 2:238:B:SER:H    | 2:234:B:GLU:HB2  | 1        | 0.22          |
| (1,514)  | 2:238:B:SER:H    | 2:234:B:GLU:HB3  | 1        | 0.22          |
| (1,514)  | 2:238:B:SER:H    | 2:234:B:GLU:HB2  | 7        | 0.22          |
| (1,514)  | 2:238:B:SER:H    | 2:234:B:GLU:HB3  | 7        | 0.22          |
| (1,514)  | 2:238:B:SER:H    | 2:234:B:GLU:HB2  | 9        | 0.22          |
| (1,514)  | 2:238:B:SER:H    | 2:234:B:GLU:HB3  | 9        | 0.22          |
| (1,514)  | 2:238:B:SER:H    | 2:234:B:GLU:HB2  | 10       | 0.22          |
| (1,514)  | 2:238:B:SER:H    | 2:234:B:GLU:HB3  | 10       | 0.22          |
| (1,514)  | 2:238:B:SER:H    | 2:234:B:GLU:HB2  | 14       | 0.22          |
| (1,514)  | 2:238:B:SER:H    | 2:234:B:GLU:HB3  | 14       | 0.22          |
| (1,359)  | 2:342:B:GLU:H    | 2:343:B:LYS:H    | 6        | 0.22          |
| (1,359)  | 2:342:B:GLU:H    | 2:343:B:LYS:H    | 15       | 0.22          |
| (1,359)  | 2:342:B:GLU:H    | 2:343:B:LYS:H    | 16       | 0.22          |
| (1,351)  | 2:246:B:LYS:H    | 2:244:B:ASP:H    | 5        | 0.22          |
| (1,235)  | 2:299:B:GLU:H    | 2:297:B:ASP:H    | 1        | 0.22          |
| (1,235)  | 2:299:B:GLU:H    | 2:297:B:ASP:H    | 11       | 0.22          |
| (1,235)  | 2:299:B:GLU:H    | 2:297:B:ASP:H    | 18       | 0.22          |
| (1,166)  | 2:281:B:ILE:H    | 2:279:B:GLN:HB2  | 1        | 0.22          |
| (1,166)  | 2:281:B:ILE:H    | 2:279:B:GLN:HB3  | 1        | 0.22          |
| (1,166)  | 2:281:B:ILE:H    | 2:279:B:GLN:HB2  | 10       | 0.22          |
| (1,166)  | 2:281:B:ILE:H    | 2:279:B:GLN:HB3  | 10       | 0.22          |
| (1,166)  | 2:281:B:ILE:H    | 2:279:B:GLN:HB2  | 12       | 0.22          |
| (1,166)  | 2:281:B:ILE:H    | 2:279:B:GLN:HB3  | 12       | 0.22          |
| (1,77)   | 2:331:B:GLU:H    | 2:333:B:LYS:HB2  | 2        | 0.22          |
| (1,77)   | 2:331:B:GLU:H    | 2:333:B:LYS:HB3  | 2        | 0.22          |
| (1,77)   | 2:331:B:GLU:H    | 2:333:B:LYS:HB2  | 9        | 0.22          |
| (1,77)   | 2:331:B:GLU:H    | 2:333:B:LYS:HB3  | 9        | 0.22          |
| (1,77)   | 2:331:B:GLU:H    | 2:333:B:LYS:HB2  | 11       | 0.22          |
| (1,77)   | 2:331:B:GLU:H    | 2:333:B:LYS:HB3  | 11       | 0.22          |
| (1,1599) | 2:207:B:ILE:HA   | 2:215:B:LEU:HD11 | 13       | 0.21          |
| (1,1599) | 2:207:B:ILE:HA   | 2:215:B:LEU:HD12 | 13       | 0.21          |
| (1,1599) | 2:207:B:ILE:HA   | 2:215:B:LEU:HD13 | 13       | 0.21          |
| (1,1599) | 2:207:B:ILE:HA   | 2:215:B:LEU:HD21 | 13       | 0.21          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1599) | 2:207:B:ILE:HA   | 2:215:B:LEU:HD22 | 13       | 0.21          |
| (1,1599) | 2:207:B:ILE:HA   | 2:215:B:LEU:HD23 | 13       | 0.21          |
| (1,1599) | 2:207:B:ILE:HA   | 2:215:B:LEU:HD11 | 16       | 0.21          |
| (1,1599) | 2:207:B:ILE:HA   | 2:215:B:LEU:HD12 | 16       | 0.21          |
| (1,1599) | 2:207:B:ILE:HA   | 2:215:B:LEU:HD13 | 16       | 0.21          |
| (1,1599) | 2:207:B:ILE:HA   | 2:215:B:LEU:HD21 | 16       | 0.21          |
| (1,1599) | 2:207:B:ILE:HA   | 2:215:B:LEU:HD22 | 16       | 0.21          |
| (1,1599) | 2:207:B:ILE:HA   | 2:215:B:LEU:HD23 | 16       | 0.21          |
| (1,1455) | 2:247:B:ASN:HA   | 2:289:B:ILE:HD11 | 12       | 0.21          |
| (1,1455) | 2:247:B:ASN:HA   | 2:289:B:ILE:HD12 | 12       | 0.21          |
| (1,1455) | 2:247:B:ASN:HA   | 2:289:B:ILE:HD13 | 12       | 0.21          |
| (1,1168) | 2:193:B:PHE:HD1  | 2:215:B:LEU:HB2  | 7        | 0.21          |
| (1,1168) | 2:193:B:PHE:HD1  | 2:215:B:LEU:HB3  | 7        | 0.21          |
| (1,1168) | 2:193:B:PHE:HD2  | 2:215:B:LEU:HB2  | 7        | 0.21          |
| (1,1168) | 2:193:B:PHE:HD2  | 2:215:B:LEU:HB3  | 7        | 0.21          |
| (1,963)  | 2:220:B:LEU:HD11 | 2:204:B:THR:HB   | 20       | 0.21          |
| (1,963)  | 2:220:B:LEU:HD12 | 2:204:B:THR:HB   | 20       | 0.21          |
| (1,963)  | 2:220:B:LEU:HD13 | 2:204:B:THR:HB   | 20       | 0.21          |
| (1,963)  | 2:220:B:LEU:HD21 | 2:204:B:THR:HB   | 20       | 0.21          |
| (1,963)  | 2:220:B:LEU:HD22 | 2:204:B:THR:HB   | 20       | 0.21          |
| (1,963)  | 2:220:B:LEU:HD23 | 2:204:B:THR:HB   | 20       | 0.21          |
| (1,895)  | 2:279:B:GLN:H    | 2:226:B:LYS:HB2  | 7        | 0.21          |
| (1,895)  | 2:279:B:GLN:H    | 2:226:B:LYS:HB3  | 7        | 0.21          |
| (1,779)  | 2:248:B:TYR:H    | 2:248:B:TYR:HE1  | 17       | 0.21          |
| (1,779)  | 2:248:B:TYR:H    | 2:248:B:TYR:HE2  | 17       | 0.21          |
| (1,607)  | 2:282:B:GLU:H    | 2:279:B:GLN:HB2  | 19       | 0.21          |
| (1,607)  | 2:282:B:GLU:H    | 2:279:B:GLN:HB3  | 19       | 0.21          |
| (1,514)  | 2:238:B:SER:H    | 2:234:B:GLU:HB2  | 12       | 0.21          |
| (1,514)  | 2:238:B:SER:H    | 2:234:B:GLU:HB3  | 12       | 0.21          |
| (1,428)  | 2:222:B:GLU:H    | 2:202:B:ILE:HA   | 20       | 0.21          |
| (1,166)  | 2:281:B:ILE:H    | 2:279:B:GLN:HB2  | 6        | 0.21          |
| (1,166)  | 2:281:B:ILE:H    | 2:279:B:GLN:HB3  | 6        | 0.21          |
| (1,166)  | 2:281:B:ILE:H    | 2:279:B:GLN:HB2  | 15       | 0.21          |
| (1,166)  | 2:281:B:ILE:H    | 2:279:B:GLN:HB3  | 15       | 0.21          |
| (1,107)  | 2:246:B:LYS:H    | 2:245:B:ASP:HB2  | 11       | 0.21          |
| (1,107)  | 2:246:B:LYS:H    | 2:245:B:ASP:HB3  | 11       | 0.21          |
| (1,1618) | 2:224:B:ASP:HA   | 2:193:B:PHE:HZ   | 8        | 0.2           |
| (1,1455) | 2:247:B:ASN:HA   | 2:289:B:ILE:HD11 | 13       | 0.2           |
| (1,1455) | 2:247:B:ASN:HA   | 2:289:B:ILE:HD12 | 13       | 0.2           |
| (1,1455) | 2:247:B:ASN:HA   | 2:289:B:ILE:HD13 | 13       | 0.2           |
| (1,1224) | 2:282:B:GLU:HG2  | 2:278:B:GLU:HA   | 13       | 0.2           |
| (1,1224) | 2:282:B:GLU:HG3  | 2:278:B:GLU:HA   | 13       | 0.2           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,963)  | 2:220:B:LEU:HD11 | 2:204:B:THR:HB   | 19       | 0.2           |
| (1,963)  | 2:220:B:LEU:HD12 | 2:204:B:THR:HB   | 19       | 0.2           |
| (1,963)  | 2:220:B:LEU:HD13 | 2:204:B:THR:HB   | 19       | 0.2           |
| (1,963)  | 2:220:B:LEU:HD21 | 2:204:B:THR:HB   | 19       | 0.2           |
| (1,963)  | 2:220:B:LEU:HD22 | 2:204:B:THR:HB   | 19       | 0.2           |
| (1,963)  | 2:220:B:LEU:HD23 | 2:204:B:THR:HB   | 19       | 0.2           |
| (1,781)  | 2:237:B:GLU:H    | 2:242:B:ILE:HB   | 4        | 0.2           |
| (1,354)  | 2:283:B:ALA:H    | 2:284:B:LEU:HG   | 1        | 0.2           |
| (1,166)  | 2:281:B:ILE:H    | 2:279:B:GLN:HB2  | 5        | 0.2           |
| (1,166)  | 2:281:B:ILE:H    | 2:279:B:GLN:HB3  | 5        | 0.2           |
| (1,146)  | 2:283:B:ALA:H    | 2:281:B:ILE:HG12 | 10       | 0.2           |
| (1,146)  | 2:283:B:ALA:H    | 2:281:B:ILE:HG13 | 10       | 0.2           |
| (1,77)   | 2:331:B:GLU:H    | 2:333:B:LYS:HB2  | 16       | 0.2           |
| (1,77)   | 2:331:B:GLU:H    | 2:333:B:LYS:HB3  | 16       | 0.2           |
| (1,77)   | 2:331:B:GLU:H    | 2:333:B:LYS:HB2  | 18       | 0.2           |
| (1,77)   | 2:331:B:GLU:H    | 2:333:B:LYS:HB3  | 18       | 0.2           |
| (1,1599) | 2:207:B:ILE:HA   | 2:215:B:LEU:HD11 | 5        | 0.19          |
| (1,1599) | 2:207:B:ILE:HA   | 2:215:B:LEU:HD12 | 5        | 0.19          |
| (1,1599) | 2:207:B:ILE:HA   | 2:215:B:LEU:HD13 | 5        | 0.19          |
| (1,1599) | 2:207:B:ILE:HA   | 2:215:B:LEU:HD21 | 5        | 0.19          |
| (1,1599) | 2:207:B:ILE:HA   | 2:215:B:LEU:HD22 | 5        | 0.19          |
| (1,1599) | 2:207:B:ILE:HA   | 2:215:B:LEU:HD23 | 5        | 0.19          |
| (1,1599) | 2:207:B:ILE:HA   | 2:215:B:LEU:HD11 | 15       | 0.19          |
| (1,1599) | 2:207:B:ILE:HA   | 2:215:B:LEU:HD12 | 15       | 0.19          |
| (1,1599) | 2:207:B:ILE:HA   | 2:215:B:LEU:HD13 | 15       | 0.19          |
| (1,1599) | 2:207:B:ILE:HA   | 2:215:B:LEU:HD21 | 15       | 0.19          |
| (1,1599) | 2:207:B:ILE:HA   | 2:215:B:LEU:HD22 | 15       | 0.19          |
| (1,1599) | 2:207:B:ILE:HA   | 2:215:B:LEU:HD23 | 15       | 0.19          |
| (1,1599) | 2:207:B:ILE:HA   | 2:215:B:LEU:HD11 | 18       | 0.19          |
| (1,1599) | 2:207:B:ILE:HA   | 2:215:B:LEU:HD12 | 18       | 0.19          |
| (1,1599) | 2:207:B:ILE:HA   | 2:215:B:LEU:HD13 | 18       | 0.19          |
| (1,1599) | 2:207:B:ILE:HA   | 2:215:B:LEU:HD21 | 18       | 0.19          |
| (1,1599) | 2:207:B:ILE:HA   | 2:215:B:LEU:HD22 | 18       | 0.19          |
| (1,1599) | 2:207:B:ILE:HA   | 2:215:B:LEU:HD23 | 18       | 0.19          |
| (1,1562) | 2:194:B:THR:HA   | 2:202:B:ILE:HG21 | 18       | 0.19          |
| (1,1562) | 2:194:B:THR:HA   | 2:202:B:ILE:HG22 | 18       | 0.19          |
| (1,1562) | 2:194:B:THR:HA   | 2:202:B:ILE:HG23 | 18       | 0.19          |
| (1,1408) | 2:275:B:GLU:HG2  | 2:278:B:GLU:HA   | 9        | 0.19          |
| (1,1408) | 2:275:B:GLU:HG3  | 2:278:B:GLU:HA   | 9        | 0.19          |
| (1,1234) | 2:255:B:LEU:HG   | 2:273:B:LEU:HB2  | 1        | 0.19          |
| (1,1234) | 2:255:B:LEU:HG   | 2:273:B:LEU:HB3  | 1        | 0.19          |
| (1,1234) | 2:255:B:LEU:HG   | 2:273:B:LEU:HB2  | 5        | 0.19          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1234) | 2:255:B:LEU:HG   | 2:273:B:LEU:HB3 | 5        | 0.19          |
| (1,1234) | 2:255:B:LEU:HG   | 2:273:B:LEU:HB2 | 6        | 0.19          |
| (1,1234) | 2:255:B:LEU:HG   | 2:273:B:LEU:HB3 | 6        | 0.19          |
| (1,1234) | 2:255:B:LEU:HG   | 2:273:B:LEU:HB2 | 13       | 0.19          |
| (1,1234) | 2:255:B:LEU:HG   | 2:273:B:LEU:HB3 | 13       | 0.19          |
| (1,1168) | 2:193:B:PHE:HD1  | 2:215:B:LEU:HB2 | 13       | 0.19          |
| (1,1168) | 2:193:B:PHE:HD1  | 2:215:B:LEU:HB3 | 13       | 0.19          |
| (1,1168) | 2:193:B:PHE:HD2  | 2:215:B:LEU:HB2 | 13       | 0.19          |
| (1,1168) | 2:193:B:PHE:HD2  | 2:215:B:LEU:HB3 | 13       | 0.19          |
| (1,1168) | 2:193:B:PHE:HD1  | 2:215:B:LEU:HB2 | 17       | 0.19          |
| (1,1168) | 2:193:B:PHE:HD1  | 2:215:B:LEU:HB3 | 17       | 0.19          |
| (1,1168) | 2:193:B:PHE:HD2  | 2:215:B:LEU:HB2 | 17       | 0.19          |
| (1,1168) | 2:193:B:PHE:HD2  | 2:215:B:LEU:HB3 | 17       | 0.19          |
| (1,1139) | 1:188:A:ASN:HA   | 2:333:B:LYS:HB2 | 14       | 0.19          |
| (1,1139) | 1:188:A:ASN:HA   | 2:333:B:LYS:HB3 | 14       | 0.19          |
| (1,1062) | 2:213:B:GLU:HB2  | 2:239:B:LEU:HA  | 11       | 0.19          |
| (1,1062) | 2:213:B:GLU:HB3  | 2:239:B:LEU:HA  | 11       | 0.19          |
| (1,1036) | 2:329:B:ILE:HD11 | 2:332:B:VAL:HB  | 2        | 0.19          |
| (1,1036) | 2:329:B:ILE:HD12 | 2:332:B:VAL:HB  | 2        | 0.19          |
| (1,1036) | 2:329:B:ILE:HD13 | 2:332:B:VAL:HB  | 2        | 0.19          |
| (1,1036) | 2:329:B:ILE:HD11 | 2:332:B:VAL:HB  | 20       | 0.19          |
| (1,1036) | 2:329:B:ILE:HD12 | 2:332:B:VAL:HB  | 20       | 0.19          |
| (1,1036) | 2:329:B:ILE:HD13 | 2:332:B:VAL:HB  | 20       | 0.19          |
| (1,895)  | 2:279:B:GLN:H    | 2:226:B:LYS:HB2 | 14       | 0.19          |
| (1,895)  | 2:279:B:GLN:H    | 2:226:B:LYS:HB3 | 14       | 0.19          |
| (1,895)  | 2:279:B:GLN:H    | 2:226:B:LYS:HB2 | 19       | 0.19          |
| (1,895)  | 2:279:B:GLN:H    | 2:226:B:LYS:HB3 | 19       | 0.19          |
| (1,428)  | 2:222:B:GLU:H    | 2:202:B:ILE:HA  | 15       | 0.19          |
| (1,351)  | 2:246:B:LYS:H    | 2:244:B:ASP:H   | 2        | 0.19          |
| (1,235)  | 2:299:B:GLU:H    | 2:297:B:ASP:H   | 16       | 0.19          |
| (1,1634) | 2:241:B:TYR:HA   | 2:210:B:ASP:HB2 | 14       | 0.18          |
| (1,1634) | 2:241:B:TYR:HA   | 2:210:B:ASP:HB3 | 14       | 0.18          |
| (1,1234) | 2:255:B:LEU:HG   | 2:273:B:LEU:HB2 | 17       | 0.18          |
| (1,1234) | 2:255:B:LEU:HG   | 2:273:B:LEU:HB3 | 17       | 0.18          |
| (1,1224) | 2:282:B:GLU:HG2  | 2:278:B:GLU:HA  | 8        | 0.18          |
| (1,1224) | 2:282:B:GLU:HG3  | 2:278:B:GLU:HA  | 8        | 0.18          |
| (1,1168) | 2:193:B:PHE:HD1  | 2:215:B:LEU:HB2 | 3        | 0.18          |
| (1,1168) | 2:193:B:PHE:HD1  | 2:215:B:LEU:HB3 | 3        | 0.18          |
| (1,1168) | 2:193:B:PHE:HD2  | 2:215:B:LEU:HB2 | 3        | 0.18          |
| (1,1168) | 2:193:B:PHE:HD2  | 2:215:B:LEU:HB3 | 3        | 0.18          |
| (1,1168) | 2:193:B:PHE:HD1  | 2:215:B:LEU:HB2 | 14       | 0.18          |
| (1,1168) | 2:193:B:PHE:HD1  | 2:215:B:LEU:HB3 | 14       | 0.18          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1168) | 2:193:B:PHE:HD2 | 2:215:B:LEU:HB2  | 14       | 0.18          |
| (1,1168) | 2:193:B:PHE:HD2 | 2:215:B:LEU:HB3  | 14       | 0.18          |
| (1,1109) | 2:193:B:PHE:HD1 | 2:203:B:VAL:HB   | 9        | 0.18          |
| (1,1109) | 2:193:B:PHE:HD2 | 2:203:B:VAL:HB   | 9        | 0.18          |
| (1,700)  | 2:256:B:ASN:H   | 2:259:B:ASN:H    | 11       | 0.18          |
| (1,700)  | 2:256:B:ASN:H   | 2:259:B:ASN:H    | 19       | 0.18          |
| (1,607)  | 2:282:B:GLU:H   | 2:279:B:GLN:HB2  | 9        | 0.18          |
| (1,607)  | 2:282:B:GLU:H   | 2:279:B:GLN:HB3  | 9        | 0.18          |
| (1,607)  | 2:282:B:GLU:H   | 2:279:B:GLN:HB2  | 11       | 0.18          |
| (1,607)  | 2:282:B:GLU:H   | 2:279:B:GLN:HB3  | 11       | 0.18          |
| (1,428)  | 2:222:B:GLU:H   | 2:202:B:ILE:HA   | 1        | 0.18          |
| (1,428)  | 2:222:B:GLU:H   | 2:202:B:ILE:HA   | 7        | 0.18          |
| (1,235)  | 2:299:B:GLU:H   | 2:297:B:ASP:H    | 5        | 0.18          |
| (1,146)  | 2:283:B:ALA:H   | 2:281:B:ILE:HG12 | 6        | 0.18          |
| (1,146)  | 2:283:B:ALA:H   | 2:281:B:ILE:HG13 | 6        | 0.18          |
| (1,77)   | 2:331:B:GLU:H   | 2:333:B:LYS:HB2  | 8        | 0.18          |
| (1,77)   | 2:331:B:GLU:H   | 2:333:B:LYS:HB3  | 8        | 0.18          |
| (1,21)   | 2:281:B:ILE:H   | 2:277:B:ILE:HG21 | 14       | 0.18          |
| (1,21)   | 2:281:B:ILE:H   | 2:277:B:ILE:HG22 | 14       | 0.18          |
| (1,21)   | 2:281:B:ILE:H   | 2:277:B:ILE:HG23 | 14       | 0.18          |
| (1,1634) | 2:241:B:TYR:HA  | 2:210:B:ASP:HB2  | 4        | 0.17          |
| (1,1634) | 2:241:B:TYR:HA  | 2:210:B:ASP:HB3  | 4        | 0.17          |
| (1,1618) | 2:224:B:ASP:HA  | 2:193:B:PHE:HZ   | 2        | 0.17          |
| (1,1618) | 2:224:B:ASP:HA  | 2:193:B:PHE:HZ   | 14       | 0.17          |
| (1,1599) | 2:207:B:ILE:HA  | 2:215:B:LEU:HD11 | 20       | 0.17          |
| (1,1599) | 2:207:B:ILE:HA  | 2:215:B:LEU:HD12 | 20       | 0.17          |
| (1,1599) | 2:207:B:ILE:HA  | 2:215:B:LEU:HD13 | 20       | 0.17          |
| (1,1599) | 2:207:B:ILE:HA  | 2:215:B:LEU:HD21 | 20       | 0.17          |
| (1,1599) | 2:207:B:ILE:HA  | 2:215:B:LEU:HD22 | 20       | 0.17          |
| (1,1599) | 2:207:B:ILE:HA  | 2:215:B:LEU:HD23 | 20       | 0.17          |
| (1,1359) | 2:231:B:MET:HB2 | 2:218:B:LEU:HA   | 10       | 0.17          |
| (1,1359) | 2:231:B:MET:HB3 | 2:218:B:LEU:HA   | 10       | 0.17          |
| (1,1347) | 2:244:B:ASP:HA  | 2:286:B:ASN:HB2  | 16       | 0.17          |
| (1,1347) | 2:244:B:ASP:HA  | 2:286:B:ASN:HB3  | 16       | 0.17          |
| (1,1234) | 2:255:B:LEU:HG  | 2:273:B:LEU:HB2  | 9        | 0.17          |
| (1,1234) | 2:255:B:LEU:HG  | 2:273:B:LEU:HB3  | 9        | 0.17          |
| (1,1234) | 2:255:B:LEU:HG  | 2:273:B:LEU:HB2  | 18       | 0.17          |
| (1,1234) | 2:255:B:LEU:HG  | 2:273:B:LEU:HB3  | 18       | 0.17          |
| (1,1234) | 2:255:B:LEU:HG  | 2:273:B:LEU:HB2  | 19       | 0.17          |
| (1,1234) | 2:255:B:LEU:HG  | 2:273:B:LEU:HB3  | 19       | 0.17          |
| (1,1168) | 2:193:B:PHE:HD1 | 2:215:B:LEU:HB2  | 1        | 0.17          |
| (1,1168) | 2:193:B:PHE:HD1 | 2:215:B:LEU:HB3  | 1        | 0.17          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1168) | 2:193:B:PHE:HD2  | 2:215:B:LEU:HB2  | 1        | 0.17          |
| (1,1168) | 2:193:B:PHE:HD2  | 2:215:B:LEU:HB3  | 1        | 0.17          |
| (1,1168) | 2:193:B:PHE:HD1  | 2:215:B:LEU:HB2  | 18       | 0.17          |
| (1,1168) | 2:193:B:PHE:HD1  | 2:215:B:LEU:HB3  | 18       | 0.17          |
| (1,1168) | 2:193:B:PHE:HD2  | 2:215:B:LEU:HB2  | 18       | 0.17          |
| (1,1168) | 2:193:B:PHE:HD2  | 2:215:B:LEU:HB3  | 18       | 0.17          |
| (1,1062) | 2:213:B:GLU:HB2  | 2:239:B:LEU:HA   | 19       | 0.17          |
| (1,1062) | 2:213:B:GLU:HB3  | 2:239:B:LEU:HA   | 19       | 0.17          |
| (1,1036) | 2:329:B:ILE:HD11 | 2:332:B:VAL:HB   | 11       | 0.17          |
| (1,1036) | 2:329:B:ILE:HD12 | 2:332:B:VAL:HB   | 11       | 0.17          |
| (1,1036) | 2:329:B:ILE:HD13 | 2:332:B:VAL:HB   | 11       | 0.17          |
| (1,895)  | 2:279:B:GLN:H    | 2:226:B:LYS:HB2  | 20       | 0.17          |
| (1,895)  | 2:279:B:GLN:H    | 2:226:B:LYS:HB3  | 20       | 0.17          |
| (1,791)  | 2:288:B:THR:H    | 2:289:B:ILE:HG21 | 1        | 0.17          |
| (1,791)  | 2:288:B:THR:H    | 2:289:B:ILE:HG22 | 1        | 0.17          |
| (1,791)  | 2:288:B:THR:H    | 2:289:B:ILE:HG23 | 1        | 0.17          |
| (1,791)  | 2:288:B:THR:H    | 2:289:B:ILE:HG21 | 6        | 0.17          |
| (1,791)  | 2:288:B:THR:H    | 2:289:B:ILE:HG22 | 6        | 0.17          |
| (1,791)  | 2:288:B:THR:H    | 2:289:B:ILE:HG23 | 6        | 0.17          |
| (1,779)  | 2:248:B:TYR:H    | 2:248:B:TYR:HE1  | 6        | 0.17          |
| (1,779)  | 2:248:B:TYR:H    | 2:248:B:TYR:HE2  | 6        | 0.17          |
| (1,700)  | 2:256:B:ASN:H    | 2:259:B:ASN:H    | 9        | 0.17          |
| (1,700)  | 2:256:B:ASN:H    | 2:259:B:ASN:H    | 15       | 0.17          |
| (1,607)  | 2:282:B:GLU:H    | 2:279:B:GLN:HB2  | 2        | 0.17          |
| (1,607)  | 2:282:B:GLU:H    | 2:279:B:GLN:HB3  | 2        | 0.17          |
| (1,550)  | 2:201:B:VAL:H    | 2:222:B:GLU:H    | 11       | 0.17          |
| (1,541)  | 2:296:B:VAL:H    | 2:253:B:MET:HG2  | 18       | 0.17          |
| (1,541)  | 2:296:B:VAL:H    | 2:253:B:MET:HG3  | 18       | 0.17          |
| (1,464)  | 2:271:B:ASP:H    | 2:267:B:GLU:H    | 6        | 0.17          |
| (1,447)  | 2:241:B:TYR:H    | 2:242:B:ILE:HB   | 4        | 0.17          |
| (1,428)  | 2:222:B:GLU:H    | 2:202:B:ILE:HA   | 8        | 0.17          |
| (1,235)  | 2:299:B:GLU:H    | 2:297:B:ASP:H    | 19       | 0.17          |
| (1,227)  | 2:336:B:LYS:H    | 2:336:B:LYS:HD2  | 8        | 0.17          |
| (1,227)  | 2:336:B:LYS:H    | 2:336:B:LYS:HD3  | 8        | 0.17          |
| (1,77)   | 2:331:B:GLU:H    | 2:333:B:LYS:HB2  | 14       | 0.17          |
| (1,77)   | 2:331:B:GLU:H    | 2:333:B:LYS:HB3  | 14       | 0.17          |
| (1,52)   | 2:327:B:ILE:H    | 2:321:B:LYS:HG2  | 8        | 0.17          |
| (1,52)   | 2:327:B:ILE:H    | 2:321:B:LYS:HG3  | 8        | 0.17          |
| (1,1653) | 2:248:B:TYR:HE1  | 2:338:B:SER:HB2  | 17       | 0.16          |
| (1,1653) | 2:248:B:TYR:HE1  | 2:338:B:SER:HB3  | 17       | 0.16          |
| (1,1653) | 2:248:B:TYR:HE2  | 2:338:B:SER:HB2  | 17       | 0.16          |
| (1,1653) | 2:248:B:TYR:HE2  | 2:338:B:SER:HB3  | 17       | 0.16          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1618) | 2:224:B:ASP:HA   | 2:193:B:PHE:HZ   | 20       | 0.16          |
| (1,1599) | 2:207:B:ILE:HA   | 2:215:B:LEU:HD11 | 19       | 0.16          |
| (1,1599) | 2:207:B:ILE:HA   | 2:215:B:LEU:HD12 | 19       | 0.16          |
| (1,1599) | 2:207:B:ILE:HA   | 2:215:B:LEU:HD13 | 19       | 0.16          |
| (1,1599) | 2:207:B:ILE:HA   | 2:215:B:LEU:HD21 | 19       | 0.16          |
| (1,1599) | 2:207:B:ILE:HA   | 2:215:B:LEU:HD22 | 19       | 0.16          |
| (1,1599) | 2:207:B:ILE:HA   | 2:215:B:LEU:HD23 | 19       | 0.16          |
| (1,1588) | 2:223:B:LYS:HG2  | 2:221:B:LYS:HA   | 13       | 0.16          |
| (1,1588) | 2:223:B:LYS:HG3  | 2:221:B:LYS:HA   | 13       | 0.16          |
| (1,1562) | 2:194:B:THR:HA   | 2:202:B:ILE:HG21 | 8        | 0.16          |
| (1,1562) | 2:194:B:THR:HA   | 2:202:B:ILE:HG22 | 8        | 0.16          |
| (1,1562) | 2:194:B:THR:HA   | 2:202:B:ILE:HG23 | 8        | 0.16          |
| (1,1562) | 2:194:B:THR:HA   | 2:202:B:ILE:HG21 | 15       | 0.16          |
| (1,1562) | 2:194:B:THR:HA   | 2:202:B:ILE:HG22 | 15       | 0.16          |
| (1,1562) | 2:194:B:THR:HA   | 2:202:B:ILE:HG23 | 15       | 0.16          |
| (1,1234) | 2:255:B:LEU:HG   | 2:273:B:LEU:HB2  | 7        | 0.16          |
| (1,1234) | 2:255:B:LEU:HG   | 2:273:B:LEU:HB3  | 7        | 0.16          |
| (1,1139) | 1:188:A:ASN:HA   | 2:333:B:LYS:HB2  | 11       | 0.16          |
| (1,1139) | 1:188:A:ASN:HA   | 2:333:B:LYS:HB3  | 11       | 0.16          |
| (1,1109) | 2:193:B:PHE:HD1  | 2:203:B:VAL:HB   | 14       | 0.16          |
| (1,1109) | 2:193:B:PHE:HD2  | 2:203:B:VAL:HB   | 14       | 0.16          |
| (1,1062) | 2:213:B:GLU:HB2  | 2:239:B:LEU:HA   | 7        | 0.16          |
| (1,1062) | 2:213:B:GLU:HB3  | 2:239:B:LEU:HA   | 7        | 0.16          |
| (1,1062) | 2:213:B:GLU:HB2  | 2:239:B:LEU:HA   | 14       | 0.16          |
| (1,1062) | 2:213:B:GLU:HB3  | 2:239:B:LEU:HA   | 14       | 0.16          |
| (1,1036) | 2:329:B:ILE:HD11 | 2:332:B:VAL:HB   | 5        | 0.16          |
| (1,1036) | 2:329:B:ILE:HD12 | 2:332:B:VAL:HB   | 5        | 0.16          |
| (1,1036) | 2:329:B:ILE:HD13 | 2:332:B:VAL:HB   | 5        | 0.16          |
| (1,980)  | 2:262:B:THR:HG21 | 2:255:B:LEU:HA   | 20       | 0.16          |
| (1,980)  | 2:262:B:THR:HG22 | 2:255:B:LEU:HA   | 20       | 0.16          |
| (1,980)  | 2:262:B:THR:HG23 | 2:255:B:LEU:HA   | 20       | 0.16          |
| (1,956)  | 2:327:B:ILE:HD11 | 2:328:B:THR:HA   | 17       | 0.16          |
| (1,956)  | 2:327:B:ILE:HD12 | 2:328:B:THR:HA   | 17       | 0.16          |
| (1,956)  | 2:327:B:ILE:HD13 | 2:328:B:THR:HA   | 17       | 0.16          |
| (1,952)  | 2:229:B:LEU:HD11 | 2:277:B:ILE:H    | 18       | 0.16          |
| (1,952)  | 2:229:B:LEU:HD12 | 2:277:B:ILE:H    | 18       | 0.16          |
| (1,952)  | 2:229:B:LEU:HD13 | 2:277:B:ILE:H    | 18       | 0.16          |
| (1,952)  | 2:229:B:LEU:HD21 | 2:277:B:ILE:H    | 18       | 0.16          |
| (1,952)  | 2:229:B:LEU:HD22 | 2:277:B:ILE:H    | 18       | 0.16          |
| (1,952)  | 2:229:B:LEU:HD23 | 2:277:B:ILE:H    | 18       | 0.16          |
| (1,791)  | 2:288:B:THR:H    | 2:289:B:ILE:HG21 | 13       | 0.16          |
| (1,791)  | 2:288:B:THR:H    | 2:289:B:ILE:HG22 | 13       | 0.16          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,791)  | 2:288:B:THR:H   | 2:289:B:ILE:HG23 | 13       | 0.16          |
| (1,733)  | 2:218:B:LEU:H   | 2:218:B:LEU:HG   | 6        | 0.16          |
| (1,700)  | 2:256:B:ASN:H   | 2:259:B:ASN:H    | 4        | 0.16          |
| (1,700)  | 2:256:B:ASN:H   | 2:259:B:ASN:H    | 12       | 0.16          |
| (1,607)  | 2:282:B:GLU:H   | 2:279:B:GLN:HB2  | 20       | 0.16          |
| (1,607)  | 2:282:B:GLU:H   | 2:279:B:GLN:HB3  | 20       | 0.16          |
| (1,464)  | 2:271:B:ASP:H   | 2:267:B:GLU:H    | 5        | 0.16          |
| (1,464)  | 2:271:B:ASP:H   | 2:267:B:GLU:H    | 18       | 0.16          |
| (1,428)  | 2:222:B:GLU:H   | 2:202:B:ILE:HA   | 11       | 0.16          |
| (1,66)   | 2:231:B:MET:H   | 2:231:B:MET:HE1  | 18       | 0.16          |
| (1,66)   | 2:231:B:MET:H   | 2:231:B:MET:HE2  | 18       | 0.16          |
| (1,66)   | 2:231:B:MET:H   | 2:231:B:MET:HE3  | 18       | 0.16          |
| (1,52)   | 2:327:B:ILE:H   | 2:321:B:LYS:HG2  | 2        | 0.16          |
| (1,52)   | 2:327:B:ILE:H   | 2:321:B:LYS:HG3  | 2        | 0.16          |
| (1,21)   | 2:281:B:ILE:H   | 2:277:B:ILE:HG21 | 5        | 0.16          |
| (1,21)   | 2:281:B:ILE:H   | 2:277:B:ILE:HG22 | 5        | 0.16          |
| (1,21)   | 2:281:B:ILE:H   | 2:277:B:ILE:HG23 | 5        | 0.16          |
| (1,1618) | 2:224:B:ASP:HA  | 2:193:B:PHE:HZ   | 16       | 0.15          |
| (1,1599) | 2:207:B:ILE:HA  | 2:215:B:LEU:HD11 | 14       | 0.15          |
| (1,1599) | 2:207:B:ILE:HA  | 2:215:B:LEU:HD12 | 14       | 0.15          |
| (1,1599) | 2:207:B:ILE:HA  | 2:215:B:LEU:HD13 | 14       | 0.15          |
| (1,1599) | 2:207:B:ILE:HA  | 2:215:B:LEU:HD21 | 14       | 0.15          |
| (1,1599) | 2:207:B:ILE:HA  | 2:215:B:LEU:HD22 | 14       | 0.15          |
| (1,1599) | 2:207:B:ILE:HA  | 2:215:B:LEU:HD23 | 14       | 0.15          |
| (1,1599) | 2:207:B:ILE:HA  | 2:215:B:LEU:HD11 | 17       | 0.15          |
| (1,1599) | 2:207:B:ILE:HA  | 2:215:B:LEU:HD12 | 17       | 0.15          |
| (1,1599) | 2:207:B:ILE:HA  | 2:215:B:LEU:HD13 | 17       | 0.15          |
| (1,1599) | 2:207:B:ILE:HA  | 2:215:B:LEU:HD21 | 17       | 0.15          |
| (1,1599) | 2:207:B:ILE:HA  | 2:215:B:LEU:HD22 | 17       | 0.15          |
| (1,1599) | 2:207:B:ILE:HA  | 2:215:B:LEU:HD23 | 17       | 0.15          |
| (1,1347) | 2:244:B:ASP:HA  | 2:286:B:ASN:HB2  | 17       | 0.15          |
| (1,1347) | 2:244:B:ASP:HA  | 2:286:B:ASN:HB3  | 17       | 0.15          |
| (1,1234) | 2:255:B:LEU:HG  | 2:273:B:LEU:HB2  | 14       | 0.15          |
| (1,1234) | 2:255:B:LEU:HG  | 2:273:B:LEU:HB3  | 14       | 0.15          |
| (1,1234) | 2:255:B:LEU:HG  | 2:273:B:LEU:HB2  | 16       | 0.15          |
| (1,1234) | 2:255:B:LEU:HG  | 2:273:B:LEU:HB3  | 16       | 0.15          |
| (1,1168) | 2:193:B:PHE:HD1 | 2:215:B:LEU:HB2  | 5        | 0.15          |
| (1,1168) | 2:193:B:PHE:HD1 | 2:215:B:LEU:HB3  | 5        | 0.15          |
| (1,1168) | 2:193:B:PHE:HD2 | 2:215:B:LEU:HB2  | 5        | 0.15          |
| (1,1168) | 2:193:B:PHE:HD2 | 2:215:B:LEU:HB3  | 5        | 0.15          |
| (1,1168) | 2:193:B:PHE:HD1 | 2:215:B:LEU:HB2  | 9        | 0.15          |
| (1,1168) | 2:193:B:PHE:HD1 | 2:215:B:LEU:HB3  | 9        | 0.15          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1168) | 2:193:B:PHE:HD2  | 2:215:B:LEU:HB2  | 9        | 0.15          |
| (1,1168) | 2:193:B:PHE:HD2  | 2:215:B:LEU:HB3  | 9        | 0.15          |
| (1,1162) | 2:218:B:LEU:HG   | 2:193:B:PHE:HE1  | 9        | 0.15          |
| (1,1162) | 2:218:B:LEU:HG   | 2:193:B:PHE:HE2  | 9        | 0.15          |
| (1,1139) | 1:188:A:ASN:HA   | 2:333:B:LYS:HB2  | 19       | 0.15          |
| (1,1139) | 1:188:A:ASN:HA   | 2:333:B:LYS:HB3  | 19       | 0.15          |
| (1,1109) | 2:193:B:PHE:HD1  | 2:203:B:VAL:HB   | 16       | 0.15          |
| (1,1109) | 2:193:B:PHE:HD2  | 2:203:B:VAL:HB   | 16       | 0.15          |
| (1,1098) | 2:276:B:THR:HA   | 2:272:B:GLU:HB2  | 13       | 0.15          |
| (1,1098) | 2:276:B:THR:HA   | 2:272:B:GLU:HB3  | 13       | 0.15          |
| (1,1036) | 2:329:B:ILE:HD11 | 2:332:B:VAL:HB   | 12       | 0.15          |
| (1,1036) | 2:329:B:ILE:HD12 | 2:332:B:VAL:HB   | 12       | 0.15          |
| (1,1036) | 2:329:B:ILE:HD13 | 2:332:B:VAL:HB   | 12       | 0.15          |
| (1,1009) | 2:327:B:ILE:HG12 | 2:332:B:VAL:HB   | 14       | 0.15          |
| (1,1009) | 2:327:B:ILE:HG13 | 2:332:B:VAL:HB   | 14       | 0.15          |
| (1,996)  | 2:294:B:VAL:HG11 | 2:318:B:LEU:HB2  | 18       | 0.15          |
| (1,996)  | 2:294:B:VAL:HG11 | 2:318:B:LEU:HB3  | 18       | 0.15          |
| (1,996)  | 2:294:B:VAL:HG12 | 2:318:B:LEU:HB2  | 18       | 0.15          |
| (1,996)  | 2:294:B:VAL:HG12 | 2:318:B:LEU:HB3  | 18       | 0.15          |
| (1,996)  | 2:294:B:VAL:HG13 | 2:318:B:LEU:HB2  | 18       | 0.15          |
| (1,996)  | 2:294:B:VAL:HG13 | 2:318:B:LEU:HB3  | 18       | 0.15          |
| (1,996)  | 2:294:B:VAL:HG21 | 2:318:B:LEU:HB2  | 18       | 0.15          |
| (1,996)  | 2:294:B:VAL:HG21 | 2:318:B:LEU:HB3  | 18       | 0.15          |
| (1,996)  | 2:294:B:VAL:HG22 | 2:318:B:LEU:HB2  | 18       | 0.15          |
| (1,996)  | 2:294:B:VAL:HG22 | 2:318:B:LEU:HB3  | 18       | 0.15          |
| (1,996)  | 2:294:B:VAL:HG23 | 2:318:B:LEU:HB2  | 18       | 0.15          |
| (1,996)  | 2:294:B:VAL:HG23 | 2:318:B:LEU:HB3  | 18       | 0.15          |
| (1,963)  | 2:220:B:LEU:HD11 | 2:204:B:THR:HB   | 2        | 0.15          |
| (1,963)  | 2:220:B:LEU:HD12 | 2:204:B:THR:HB   | 2        | 0.15          |
| (1,963)  | 2:220:B:LEU:HD13 | 2:204:B:THR:HB   | 2        | 0.15          |
| (1,963)  | 2:220:B:LEU:HD21 | 2:204:B:THR:HB   | 2        | 0.15          |
| (1,963)  | 2:220:B:LEU:HD22 | 2:204:B:THR:HB   | 2        | 0.15          |
| (1,963)  | 2:220:B:LEU:HD23 | 2:204:B:THR:HB   | 2        | 0.15          |
| (1,932)  | 2:279:B:GLN:HG2  | 2:226:B:LYS:HA   | 17       | 0.15          |
| (1,932)  | 2:279:B:GLN:HG3  | 2:226:B:LYS:HA   | 17       | 0.15          |
| (1,865)  | 2:328:B:THR:H    | 2:328:B:THR:HB   | 13       | 0.15          |
| (1,824)  | 2:229:B:LEU:H    | 2:229:B:LEU:HG   | 16       | 0.15          |
| (1,791)  | 2:288:B:THR:H    | 2:289:B:ILE:HG21 | 2        | 0.15          |
| (1,791)  | 2:288:B:THR:H    | 2:289:B:ILE:HG22 | 2        | 0.15          |
| (1,791)  | 2:288:B:THR:H    | 2:289:B:ILE:HG23 | 2        | 0.15          |
| (1,791)  | 2:288:B:THR:H    | 2:289:B:ILE:HG21 | 3        | 0.15          |
| (1,791)  | 2:288:B:THR:H    | 2:289:B:ILE:HG22 | 3        | 0.15          |

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| Key      | Atom-1         | Atom-2           | Model ID | Violation (Å) |
|----------|----------------|------------------|----------|---------------|
| (1,791)  | 2:288:B:THR:H  | 2:289:B:ILE:HG23 | 3        | 0.15          |
| (1,791)  | 2:288:B:THR:H  | 2:289:B:ILE:HG21 | 14       | 0.15          |
| (1,791)  | 2:288:B:THR:H  | 2:289:B:ILE:HG22 | 14       | 0.15          |
| (1,791)  | 2:288:B:THR:H  | 2:289:B:ILE:HG23 | 14       | 0.15          |
| (1,791)  | 2:288:B:THR:H  | 2:289:B:ILE:HG21 | 18       | 0.15          |
| (1,791)  | 2:288:B:THR:H  | 2:289:B:ILE:HG22 | 18       | 0.15          |
| (1,791)  | 2:288:B:THR:H  | 2:289:B:ILE:HG23 | 18       | 0.15          |
| (1,700)  | 2:256:B:ASN:H  | 2:259:B:ASN:H    | 8        | 0.15          |
| (1,700)  | 2:256:B:ASN:H  | 2:259:B:ASN:H    | 14       | 0.15          |
| (1,700)  | 2:256:B:ASN:H  | 2:259:B:ASN:H    | 20       | 0.15          |
| (1,587)  | 2:328:B:THR:H  | 2:332:B:VAL:HB   | 13       | 0.15          |
| (1,587)  | 2:328:B:THR:H  | 2:332:B:VAL:HB   | 20       | 0.15          |
| (1,359)  | 2:342:B:GLU:H  | 2:343:B:LYS:H    | 12       | 0.15          |
| (1,351)  | 2:246:B:LYS:H  | 2:244:B:ASP:H    | 20       | 0.15          |
| (1,146)  | 2:283:B:ALA:H  | 2:281:B:ILE:HG12 | 12       | 0.15          |
| (1,146)  | 2:283:B:ALA:H  | 2:281:B:ILE:HG13 | 12       | 0.15          |
| (1,26)   | 2:206:B:ALA:H  | 2:215:B:LEU:HG   | 4        | 0.15          |
| (1,11)   | 2:295:B:THR:H  | 2:294:B:VAL:HB   | 3        | 0.15          |
| (1,11)   | 2:295:B:THR:H  | 2:294:B:VAL:HB   | 13       | 0.15          |
| (1,1660) | 2:337:B:ILE:HA | 1:186:A:ASP:HB2  | 10       | 0.14          |
| (1,1660) | 2:337:B:ILE:HA | 1:186:A:ASP:HB3  | 10       | 0.14          |
| (1,1599) | 2:207:B:ILE:HA | 2:215:B:LEU:HD11 | 3        | 0.14          |
| (1,1599) | 2:207:B:ILE:HA | 2:215:B:LEU:HD12 | 3        | 0.14          |
| (1,1599) | 2:207:B:ILE:HA | 2:215:B:LEU:HD13 | 3        | 0.14          |
| (1,1599) | 2:207:B:ILE:HA | 2:215:B:LEU:HD21 | 3        | 0.14          |
| (1,1599) | 2:207:B:ILE:HA | 2:215:B:LEU:HD22 | 3        | 0.14          |
| (1,1599) | 2:207:B:ILE:HA | 2:215:B:LEU:HD23 | 3        | 0.14          |
| (1,1599) | 2:207:B:ILE:HA | 2:215:B:LEU:HD11 | 6        | 0.14          |
| (1,1599) | 2:207:B:ILE:HA | 2:215:B:LEU:HD12 | 6        | 0.14          |
| (1,1599) | 2:207:B:ILE:HA | 2:215:B:LEU:HD13 | 6        | 0.14          |
| (1,1599) | 2:207:B:ILE:HA | 2:215:B:LEU:HD21 | 6        | 0.14          |
| (1,1599) | 2:207:B:ILE:HA | 2:215:B:LEU:HD22 | 6        | 0.14          |
| (1,1599) | 2:207:B:ILE:HA | 2:215:B:LEU:HD23 | 6        | 0.14          |
| (1,1599) | 2:207:B:ILE:HA | 2:215:B:LEU:HD11 | 9        | 0.14          |
| (1,1599) | 2:207:B:ILE:HA | 2:215:B:LEU:HD12 | 9        | 0.14          |
| (1,1599) | 2:207:B:ILE:HA | 2:215:B:LEU:HD13 | 9        | 0.14          |
| (1,1599) | 2:207:B:ILE:HA | 2:215:B:LEU:HD21 | 9        | 0.14          |
| (1,1599) | 2:207:B:ILE:HA | 2:215:B:LEU:HD22 | 9        | 0.14          |
| (1,1599) | 2:207:B:ILE:HA | 2:215:B:LEU:HD23 | 9        | 0.14          |
| (1,1562) | 2:194:B:THR:HA | 2:202:B:ILE:HG21 | 3        | 0.14          |
| (1,1562) | 2:194:B:THR:HA | 2:202:B:ILE:HG22 | 3        | 0.14          |
| (1,1562) | 2:194:B:THR:HA | 2:202:B:ILE:HG23 | 3        | 0.14          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1562) | 2:194:B:THR:HA   | 2:202:B:ILE:HG21 | 17       | 0.14          |
| (1,1562) | 2:194:B:THR:HA   | 2:202:B:ILE:HG22 | 17       | 0.14          |
| (1,1562) | 2:194:B:THR:HA   | 2:202:B:ILE:HG23 | 17       | 0.14          |
| (1,1548) | 2:337:B:ILE:HG21 | 1:186:A:ASP:HA   | 16       | 0.14          |
| (1,1548) | 2:337:B:ILE:HG22 | 1:186:A:ASP:HA   | 16       | 0.14          |
| (1,1548) | 2:337:B:ILE:HG23 | 1:186:A:ASP:HA   | 16       | 0.14          |
| (1,1350) | 2:329:B:ILE:HB   | 2:328:B:THR:HB   | 12       | 0.14          |
| (1,1211) | 2:327:B:ILE:HB   | 2:332:B:VAL:HB   | 6        | 0.14          |
| (1,1162) | 2:218:B:LEU:HG   | 2:193:B:PHE:HE1  | 16       | 0.14          |
| (1,1162) | 2:218:B:LEU:HG   | 2:193:B:PHE:HE2  | 16       | 0.14          |
| (1,1109) | 2:193:B:PHE:HD1  | 2:203:B:VAL:HB   | 3        | 0.14          |
| (1,1109) | 2:193:B:PHE:HD2  | 2:203:B:VAL:HB   | 3        | 0.14          |
| (1,1098) | 2:276:B:THR:HA   | 2:272:B:GLU:HB2  | 7        | 0.14          |
| (1,1098) | 2:276:B:THR:HA   | 2:272:B:GLU:HB3  | 7        | 0.14          |
| (1,1098) | 2:276:B:THR:HA   | 2:272:B:GLU:HB2  | 9        | 0.14          |
| (1,1098) | 2:276:B:THR:HA   | 2:272:B:GLU:HB3  | 9        | 0.14          |
| (1,1062) | 2:213:B:GLU:HB2  | 2:239:B:LEU:HA   | 3        | 0.14          |
| (1,1062) | 2:213:B:GLU:HB3  | 2:239:B:LEU:HA   | 3        | 0.14          |
| (1,1062) | 2:213:B:GLU:HB2  | 2:239:B:LEU:HA   | 8        | 0.14          |
| (1,1062) | 2:213:B:GLU:HB3  | 2:239:B:LEU:HA   | 8        | 0.14          |
| (1,1062) | 2:213:B:GLU:HB2  | 2:239:B:LEU:HA   | 20       | 0.14          |
| (1,1062) | 2:213:B:GLU:HB3  | 2:239:B:LEU:HA   | 20       | 0.14          |
| (1,1036) | 2:329:B:ILE:HD11 | 2:332:B:VAL:HB   | 8        | 0.14          |
| (1,1036) | 2:329:B:ILE:HD12 | 2:332:B:VAL:HB   | 8        | 0.14          |
| (1,1036) | 2:329:B:ILE:HD13 | 2:332:B:VAL:HB   | 8        | 0.14          |
| (1,1036) | 2:329:B:ILE:HD11 | 2:332:B:VAL:HB   | 16       | 0.14          |
| (1,1036) | 2:329:B:ILE:HD12 | 2:332:B:VAL:HB   | 16       | 0.14          |
| (1,1036) | 2:329:B:ILE:HD13 | 2:332:B:VAL:HB   | 16       | 0.14          |
| (1,1036) | 2:329:B:ILE:HD11 | 2:332:B:VAL:HB   | 18       | 0.14          |
| (1,1036) | 2:329:B:ILE:HD12 | 2:332:B:VAL:HB   | 18       | 0.14          |
| (1,1036) | 2:329:B:ILE:HD13 | 2:332:B:VAL:HB   | 18       | 0.14          |
| (1,980)  | 2:262:B:THR:HG21 | 2:255:B:LEU:HA   | 4        | 0.14          |
| (1,980)  | 2:262:B:THR:HG22 | 2:255:B:LEU:HA   | 4        | 0.14          |
| (1,980)  | 2:262:B:THR:HG23 | 2:255:B:LEU:HA   | 4        | 0.14          |
| (1,957)  | 2:192:B:GLU:HA   | 2:311:B:MET:HE1  | 19       | 0.14          |
| (1,957)  | 2:192:B:GLU:HA   | 2:311:B:MET:HE2  | 19       | 0.14          |
| (1,957)  | 2:192:B:GLU:HA   | 2:311:B:MET:HE3  | 19       | 0.14          |
| (1,895)  | 2:279:B:GLN:H    | 2:226:B:LYS:HB2  | 1        | 0.14          |
| (1,895)  | 2:279:B:GLN:H    | 2:226:B:LYS:HB3  | 1        | 0.14          |
| (1,888)  | 2:303:B:LYS:H    | 2:303:B:LYS:HE2  | 10       | 0.14          |
| (1,888)  | 2:303:B:LYS:H    | 2:303:B:LYS:HE3  | 10       | 0.14          |
| (1,835)  | 2:283:B:ALA:H    | 2:279:B:GLN:HG2  | 17       | 0.14          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,835)  | 2:283:B:ALA:H    | 2:279:B:GLN:HG3  | 17       | 0.14          |
| (1,827)  | 2:320:B:ALA:H    | 2:323:B:LYS:HB2  | 2        | 0.14          |
| (1,827)  | 2:320:B:ALA:H    | 2:323:B:LYS:HB3  | 2        | 0.14          |
| (1,700)  | 2:256:B:ASN:H    | 2:259:B:ASN:H    | 7        | 0.14          |
| (1,571)  | 2:244:B:ASP:H    | 2:288:B:THR:HG21 | 12       | 0.14          |
| (1,571)  | 2:244:B:ASP:H    | 2:288:B:THR:HG22 | 12       | 0.14          |
| (1,571)  | 2:244:B:ASP:H    | 2:288:B:THR:HG23 | 12       | 0.14          |
| (1,464)  | 2:271:B:ASP:H    | 2:267:B:GLU:H    | 8        | 0.14          |
| (1,464)  | 2:271:B:ASP:H    | 2:267:B:GLU:H    | 11       | 0.14          |
| (1,464)  | 2:271:B:ASP:H    | 2:267:B:GLU:H    | 12       | 0.14          |
| (1,445)  | 2:322:B:GLU:H    | 2:322:B:GLU:HG2  | 5        | 0.14          |
| (1,445)  | 2:322:B:GLU:H    | 2:322:B:GLU:HG3  | 5        | 0.14          |
| (1,428)  | 2:222:B:GLU:H    | 2:202:B:ILE:HA   | 4        | 0.14          |
| (1,428)  | 2:222:B:GLU:H    | 2:202:B:ILE:HA   | 14       | 0.14          |
| (1,359)  | 2:342:B:GLU:H    | 2:343:B:LYS:H    | 3        | 0.14          |
| (1,359)  | 2:342:B:GLU:H    | 2:343:B:LYS:H    | 14       | 0.14          |
| (1,359)  | 2:342:B:GLU:H    | 2:343:B:LYS:H    | 17       | 0.14          |
| (1,351)  | 2:246:B:LYS:H    | 2:244:B:ASP:H    | 19       | 0.14          |
| (1,52)   | 2:327:B:ILE:H    | 2:321:B:LYS:HG2  | 7        | 0.14          |
| (1,52)   | 2:327:B:ILE:H    | 2:321:B:LYS:HG3  | 7        | 0.14          |
| (1,21)   | 2:281:B:ILE:H    | 2:277:B:ILE:HG21 | 8        | 0.14          |
| (1,21)   | 2:281:B:ILE:H    | 2:277:B:ILE:HG22 | 8        | 0.14          |
| (1,21)   | 2:281:B:ILE:H    | 2:277:B:ILE:HG23 | 8        | 0.14          |
| (1,11)   | 2:295:B:THR:H    | 2:294:B:VAL:HB   | 6        | 0.14          |
| (1,1618) | 2:224:B:ASP:HA   | 2:193:B:PHE:HZ   | 11       | 0.13          |
| (1,1502) | 2:290:B:VAL:HB   | 2:248:B:TYR:HB2  | 5        | 0.13          |
| (1,1502) | 2:290:B:VAL:HB   | 2:248:B:TYR:HB3  | 5        | 0.13          |
| (1,1347) | 2:244:B:ASP:HA   | 2:286:B:ASN:HB2  | 14       | 0.13          |
| (1,1347) | 2:244:B:ASP:HA   | 2:286:B:ASN:HB3  | 14       | 0.13          |
| (1,1343) | 2:236:B:ALA:HB1  | 2:189:B:PRO:HD2  | 17       | 0.13          |
| (1,1343) | 2:236:B:ALA:HB1  | 2:189:B:PRO:HD3  | 17       | 0.13          |
| (1,1343) | 2:236:B:ALA:HB2  | 2:189:B:PRO:HD2  | 17       | 0.13          |
| (1,1343) | 2:236:B:ALA:HB2  | 2:189:B:PRO:HD3  | 17       | 0.13          |
| (1,1343) | 2:236:B:ALA:HB3  | 2:189:B:PRO:HD2  | 17       | 0.13          |
| (1,1343) | 2:236:B:ALA:HB3  | 2:189:B:PRO:HD3  | 17       | 0.13          |
| (1,1247) | 2:195:B:ILE:HG21 | 2:225:B:LEU:HA   | 7        | 0.13          |
| (1,1247) | 2:195:B:ILE:HG22 | 2:225:B:LEU:HA   | 7        | 0.13          |
| (1,1247) | 2:195:B:ILE:HG23 | 2:225:B:LEU:HA   | 7        | 0.13          |
| (1,1234) | 2:255:B:LEU:HG   | 2:273:B:LEU:HB2  | 3        | 0.13          |
| (1,1234) | 2:255:B:LEU:HG   | 2:273:B:LEU:HB3  | 3        | 0.13          |
| (1,1162) | 2:218:B:LEU:HG   | 2:193:B:PHE:HE1  | 2        | 0.13          |
| (1,1162) | 2:218:B:LEU:HG   | 2:193:B:PHE:HE2  | 2        | 0.13          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1139) | 1:188:A:ASN:HA   | 2:333:B:LYS:HB2 | 1        | 0.13          |
| (1,1139) | 1:188:A:ASN:HA   | 2:333:B:LYS:HB3 | 1        | 0.13          |
| (1,1139) | 1:188:A:ASN:HA   | 2:333:B:LYS:HB2 | 2        | 0.13          |
| (1,1139) | 1:188:A:ASN:HA   | 2:333:B:LYS:HB3 | 2        | 0.13          |
| (1,1139) | 1:188:A:ASN:HA   | 2:333:B:LYS:HB2 | 4        | 0.13          |
| (1,1139) | 1:188:A:ASN:HA   | 2:333:B:LYS:HB3 | 4        | 0.13          |
| (1,1109) | 2:193:B:PHE:HD1  | 2:203:B:VAL:HB  | 5        | 0.13          |
| (1,1109) | 2:193:B:PHE:HD2  | 2:203:B:VAL:HB  | 5        | 0.13          |
| (1,1062) | 2:213:B:GLU:HB2  | 2:239:B:LEU:HA  | 6        | 0.13          |
| (1,1062) | 2:213:B:GLU:HB3  | 2:239:B:LEU:HA  | 6        | 0.13          |
| (1,996)  | 2:294:B:VAL:HG11 | 2:318:B:LEU:HB2 | 2        | 0.13          |
| (1,996)  | 2:294:B:VAL:HG11 | 2:318:B:LEU:HB3 | 2        | 0.13          |
| (1,996)  | 2:294:B:VAL:HG12 | 2:318:B:LEU:HB2 | 2        | 0.13          |
| (1,996)  | 2:294:B:VAL:HG12 | 2:318:B:LEU:HB3 | 2        | 0.13          |
| (1,996)  | 2:294:B:VAL:HG13 | 2:318:B:LEU:HB2 | 2        | 0.13          |
| (1,996)  | 2:294:B:VAL:HG13 | 2:318:B:LEU:HB3 | 2        | 0.13          |
| (1,996)  | 2:294:B:VAL:HG21 | 2:318:B:LEU:HB2 | 2        | 0.13          |
| (1,996)  | 2:294:B:VAL:HG21 | 2:318:B:LEU:HB3 | 2        | 0.13          |
| (1,996)  | 2:294:B:VAL:HG22 | 2:318:B:LEU:HB2 | 2        | 0.13          |
| (1,996)  | 2:294:B:VAL:HG22 | 2:318:B:LEU:HB3 | 2        | 0.13          |
| (1,996)  | 2:294:B:VAL:HG23 | 2:318:B:LEU:HB2 | 2        | 0.13          |
| (1,996)  | 2:294:B:VAL:HG23 | 2:318:B:LEU:HB3 | 2        | 0.13          |
| (1,996)  | 2:294:B:VAL:HG11 | 2:318:B:LEU:HB2 | 4        | 0.13          |
| (1,996)  | 2:294:B:VAL:HG11 | 2:318:B:LEU:HB3 | 4        | 0.13          |
| (1,996)  | 2:294:B:VAL:HG12 | 2:318:B:LEU:HB2 | 4        | 0.13          |
| (1,996)  | 2:294:B:VAL:HG12 | 2:318:B:LEU:HB3 | 4        | 0.13          |
| (1,996)  | 2:294:B:VAL:HG13 | 2:318:B:LEU:HB2 | 4        | 0.13          |
| (1,996)  | 2:294:B:VAL:HG13 | 2:318:B:LEU:HB3 | 4        | 0.13          |
| (1,996)  | 2:294:B:VAL:HG21 | 2:318:B:LEU:HB2 | 4        | 0.13          |
| (1,996)  | 2:294:B:VAL:HG21 | 2:318:B:LEU:HB3 | 4        | 0.13          |
| (1,996)  | 2:294:B:VAL:HG22 | 2:318:B:LEU:HB2 | 4        | 0.13          |
| (1,996)  | 2:294:B:VAL:HG22 | 2:318:B:LEU:HB3 | 4        | 0.13          |
| (1,996)  | 2:294:B:VAL:HG23 | 2:318:B:LEU:HB2 | 4        | 0.13          |
| (1,996)  | 2:294:B:VAL:HG23 | 2:318:B:LEU:HB3 | 4        | 0.13          |
| (1,980)  | 2:262:B:THR:HG21 | 2:255:B:LEU:HA  | 16       | 0.13          |
| (1,980)  | 2:262:B:THR:HG22 | 2:255:B:LEU:HA  | 16       | 0.13          |
| (1,980)  | 2:262:B:THR:HG23 | 2:255:B:LEU:HA  | 16       | 0.13          |
| (1,956)  | 2:327:B:ILE:HD11 | 2:328:B:THR:HA  | 1        | 0.13          |
| (1,956)  | 2:327:B:ILE:HD12 | 2:328:B:THR:HA  | 1        | 0.13          |
| (1,956)  | 2:327:B:ILE:HD13 | 2:328:B:THR:HA  | 1        | 0.13          |
| (1,895)  | 2:279:B:GLN:H    | 2:226:B:LYS:HB2 | 3        | 0.13          |
| (1,895)  | 2:279:B:GLN:H    | 2:226:B:LYS:HB3 | 3        | 0.13          |

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| Key     | Atom-1        | Atom-2           | Model ID | Violation (Å) |
|---------|---------------|------------------|----------|---------------|
| (1,895) | 2:279:B:GLN:H | 2:226:B:LYS:HB2  | 15       | 0.13          |
| (1,895) | 2:279:B:GLN:H | 2:226:B:LYS:HB3  | 15       | 0.13          |
| (1,865) | 2:328:B:THR:H | 2:328:B:THR:HB   | 1        | 0.13          |
| (1,865) | 2:328:B:THR:H | 2:328:B:THR:HB   | 6        | 0.13          |
| (1,827) | 2:320:B:ALA:H | 2:323:B:LYS:HB2  | 6        | 0.13          |
| (1,827) | 2:320:B:ALA:H | 2:323:B:LYS:HB3  | 6        | 0.13          |
| (1,827) | 2:320:B:ALA:H | 2:323:B:LYS:HB2  | 7        | 0.13          |
| (1,827) | 2:320:B:ALA:H | 2:323:B:LYS:HB3  | 7        | 0.13          |
| (1,791) | 2:288:B:THR:H | 2:289:B:ILE:HG21 | 12       | 0.13          |
| (1,791) | 2:288:B:THR:H | 2:289:B:ILE:HG22 | 12       | 0.13          |
| (1,791) | 2:288:B:THR:H | 2:289:B:ILE:HG23 | 12       | 0.13          |
| (1,791) | 2:288:B:THR:H | 2:289:B:ILE:HG21 | 16       | 0.13          |
| (1,791) | 2:288:B:THR:H | 2:289:B:ILE:HG22 | 16       | 0.13          |
| (1,791) | 2:288:B:THR:H | 2:289:B:ILE:HG23 | 16       | 0.13          |
| (1,791) | 2:288:B:THR:H | 2:289:B:ILE:HG21 | 17       | 0.13          |
| (1,791) | 2:288:B:THR:H | 2:289:B:ILE:HG22 | 17       | 0.13          |
| (1,791) | 2:288:B:THR:H | 2:289:B:ILE:HG23 | 17       | 0.13          |
| (1,733) | 2:218:B:LEU:H | 2:218:B:LEU:HG   | 5        | 0.13          |
| (1,733) | 2:218:B:LEU:H | 2:218:B:LEU:HG   | 12       | 0.13          |
| (1,700) | 2:256:B:ASN:H | 2:259:B:ASN:H    | 6        | 0.13          |
| (1,700) | 2:256:B:ASN:H | 2:259:B:ASN:H    | 13       | 0.13          |
| (1,464) | 2:271:B:ASP:H | 2:267:B:GLU:H    | 4        | 0.13          |
| (1,464) | 2:271:B:ASP:H | 2:267:B:GLU:H    | 19       | 0.13          |
| (1,445) | 2:322:B:GLU:H | 2:322:B:GLU:HG2  | 7        | 0.13          |
| (1,445) | 2:322:B:GLU:H | 2:322:B:GLU:HG3  | 7        | 0.13          |
| (1,445) | 2:322:B:GLU:H | 2:322:B:GLU:HG2  | 8        | 0.13          |
| (1,445) | 2:322:B:GLU:H | 2:322:B:GLU:HG3  | 8        | 0.13          |
| (1,445) | 2:322:B:GLU:H | 2:322:B:GLU:HG2  | 17       | 0.13          |
| (1,445) | 2:322:B:GLU:H | 2:322:B:GLU:HG3  | 17       | 0.13          |
| (1,428) | 2:222:B:GLU:H | 2:202:B:ILE:HA   | 10       | 0.13          |
| (1,428) | 2:222:B:GLU:H | 2:202:B:ILE:HA   | 19       | 0.13          |
| (1,359) | 2:342:B:GLU:H | 2:343:B:LYS:H    | 13       | 0.13          |
| (1,359) | 2:342:B:GLU:H | 2:343:B:LYS:H    | 19       | 0.13          |
| (1,351) | 2:246:B:LYS:H | 2:244:B:ASP:H    | 13       | 0.13          |
| (1,52)  | 2:327:B:ILE:H | 2:321:B:LYS:HG2  | 10       | 0.13          |
| (1,52)  | 2:327:B:ILE:H | 2:321:B:LYS:HG3  | 10       | 0.13          |
| (1,21)  | 2:281:B:ILE:H | 2:277:B:ILE:HG21 | 10       | 0.13          |
| (1,21)  | 2:281:B:ILE:H | 2:277:B:ILE:HG22 | 10       | 0.13          |
| (1,21)  | 2:281:B:ILE:H | 2:277:B:ILE:HG23 | 10       | 0.13          |
| (1,19)  | 2:251:B:VAL:H | 2:293:B:THR:HG21 | 8        | 0.13          |
| (1,19)  | 2:251:B:VAL:H | 2:293:B:THR:HG22 | 8        | 0.13          |
| (1,19)  | 2:251:B:VAL:H | 2:293:B:THR:HG23 | 8        | 0.13          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,11)   | 2:295:B:THR:H    | 2:294:B:VAL:HB   | 7        | 0.13          |
| (1,11)   | 2:295:B:THR:H    | 2:294:B:VAL:HB   | 9        | 0.13          |
| (1,11)   | 2:295:B:THR:H    | 2:294:B:VAL:HB   | 11       | 0.13          |
| (1,11)   | 2:295:B:THR:H    | 2:294:B:VAL:HB   | 16       | 0.13          |
| (1,11)   | 2:295:B:THR:H    | 2:294:B:VAL:HB   | 17       | 0.13          |
| (1,1660) | 2:337:B:ILE:HA   | 1:186:A:ASP:HB2  | 1        | 0.12          |
| (1,1660) | 2:337:B:ILE:HA   | 1:186:A:ASP:HB3  | 1        | 0.12          |
| (1,1618) | 2:224:B:ASP:HA   | 2:193:B:PHE:HZ   | 3        | 0.12          |
| (1,1599) | 2:207:B:ILE:HA   | 2:215:B:LEU:HD11 | 10       | 0.12          |
| (1,1599) | 2:207:B:ILE:HA   | 2:215:B:LEU:HD12 | 10       | 0.12          |
| (1,1599) | 2:207:B:ILE:HA   | 2:215:B:LEU:HD13 | 10       | 0.12          |
| (1,1599) | 2:207:B:ILE:HA   | 2:215:B:LEU:HD21 | 10       | 0.12          |
| (1,1599) | 2:207:B:ILE:HA   | 2:215:B:LEU:HD22 | 10       | 0.12          |
| (1,1599) | 2:207:B:ILE:HA   | 2:215:B:LEU:HD23 | 10       | 0.12          |
| (1,1548) | 2:337:B:ILE:HG21 | 1:186:A:ASP:HA   | 10       | 0.12          |
| (1,1548) | 2:337:B:ILE:HG22 | 1:186:A:ASP:HA   | 10       | 0.12          |
| (1,1548) | 2:337:B:ILE:HG23 | 1:186:A:ASP:HA   | 10       | 0.12          |
| (1,1455) | 2:247:B:ASN:HA   | 2:289:B:ILE:HD11 | 8        | 0.12          |
| (1,1455) | 2:247:B:ASN:HA   | 2:289:B:ILE:HD12 | 8        | 0.12          |
| (1,1455) | 2:247:B:ASN:HA   | 2:289:B:ILE:HD13 | 8        | 0.12          |
| (1,1347) | 2:244:B:ASP:HA   | 2:286:B:ASN:HB2  | 11       | 0.12          |
| (1,1347) | 2:244:B:ASP:HA   | 2:286:B:ASN:HB3  | 11       | 0.12          |
| (1,1234) | 2:255:B:LEU:HG   | 2:273:B:LEU:HB2  | 15       | 0.12          |
| (1,1234) | 2:255:B:LEU:HG   | 2:273:B:LEU:HB3  | 15       | 0.12          |
| (1,1175) | 2:329:B:ILE:HD11 | 2:307:B:ASN:HA   | 8        | 0.12          |
| (1,1175) | 2:329:B:ILE:HD12 | 2:307:B:ASN:HA   | 8        | 0.12          |
| (1,1175) | 2:329:B:ILE:HD13 | 2:307:B:ASN:HA   | 8        | 0.12          |
| (1,1168) | 2:193:B:PHE:HD1  | 2:215:B:LEU:HB2  | 4        | 0.12          |
| (1,1168) | 2:193:B:PHE:HD1  | 2:215:B:LEU:HB3  | 4        | 0.12          |
| (1,1168) | 2:193:B:PHE:HD2  | 2:215:B:LEU:HB2  | 4        | 0.12          |
| (1,1168) | 2:193:B:PHE:HD2  | 2:215:B:LEU:HB3  | 4        | 0.12          |
| (1,1168) | 2:193:B:PHE:HD1  | 2:215:B:LEU:HB2  | 11       | 0.12          |
| (1,1168) | 2:193:B:PHE:HD1  | 2:215:B:LEU:HB3  | 11       | 0.12          |
| (1,1168) | 2:193:B:PHE:HD2  | 2:215:B:LEU:HB2  | 11       | 0.12          |
| (1,1168) | 2:193:B:PHE:HD2  | 2:215:B:LEU:HB3  | 11       | 0.12          |
| (1,1139) | 1:188:A:ASN:HA   | 2:333:B:LYS:HB2  | 10       | 0.12          |
| (1,1139) | 1:188:A:ASN:HA   | 2:333:B:LYS:HB3  | 10       | 0.12          |
| (1,1139) | 1:188:A:ASN:HA   | 2:333:B:LYS:HB2  | 16       | 0.12          |
| (1,1139) | 1:188:A:ASN:HA   | 2:333:B:LYS:HB3  | 16       | 0.12          |
| (1,1139) | 1:188:A:ASN:HA   | 2:333:B:LYS:HB2  | 20       | 0.12          |
| (1,1139) | 1:188:A:ASN:HA   | 2:333:B:LYS:HB3  | 20       | 0.12          |
| (1,1125) | 2:242:B:ILE:HG21 | 1:187:A:VAL:HA   | 9        | 0.12          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1125) | 2:242:B:ILE:HG22 | 1:187:A:VAL:HA  | 9        | 0.12          |
| (1,1125) | 2:242:B:ILE:HG23 | 1:187:A:VAL:HA  | 9        | 0.12          |
| (1,1123) | 2:207:B:ILE:HD11 | 2:205:B:SER:HA  | 10       | 0.12          |
| (1,1123) | 2:207:B:ILE:HD12 | 2:205:B:SER:HA  | 10       | 0.12          |
| (1,1123) | 2:207:B:ILE:HD13 | 2:205:B:SER:HA  | 10       | 0.12          |
| (1,1098) | 2:276:B:THR:HA   | 2:272:B:GLU:HB2 | 1        | 0.12          |
| (1,1098) | 2:276:B:THR:HA   | 2:272:B:GLU:HB3 | 1        | 0.12          |
| (1,1098) | 2:276:B:THR:HA   | 2:272:B:GLU:HB2 | 8        | 0.12          |
| (1,1098) | 2:276:B:THR:HA   | 2:272:B:GLU:HB3 | 8        | 0.12          |
| (1,1098) | 2:276:B:THR:HA   | 2:272:B:GLU:HB2 | 17       | 0.12          |
| (1,1098) | 2:276:B:THR:HA   | 2:272:B:GLU:HB3 | 17       | 0.12          |
| (1,1077) | 2:242:B:ILE:HB   | 2:237:B:GLU:HG2 | 17       | 0.12          |
| (1,1077) | 2:242:B:ILE:HB   | 2:237:B:GLU:HG3 | 17       | 0.12          |
| (1,1036) | 2:329:B:ILE:HD11 | 2:332:B:VAL:HB  | 17       | 0.12          |
| (1,1036) | 2:329:B:ILE:HD12 | 2:332:B:VAL:HB  | 17       | 0.12          |
| (1,1036) | 2:329:B:ILE:HD13 | 2:332:B:VAL:HB  | 17       | 0.12          |
| (1,996)  | 2:294:B:VAL:HG11 | 2:318:B:LEU:HB2 | 1        | 0.12          |
| (1,996)  | 2:294:B:VAL:HG11 | 2:318:B:LEU:HB3 | 1        | 0.12          |
| (1,996)  | 2:294:B:VAL:HG12 | 2:318:B:LEU:HB2 | 1        | 0.12          |
| (1,996)  | 2:294:B:VAL:HG12 | 2:318:B:LEU:HB3 | 1        | 0.12          |
| (1,996)  | 2:294:B:VAL:HG13 | 2:318:B:LEU:HB2 | 1        | 0.12          |
| (1,996)  | 2:294:B:VAL:HG13 | 2:318:B:LEU:HB3 | 1        | 0.12          |
| (1,996)  | 2:294:B:VAL:HG21 | 2:318:B:LEU:HB2 | 1        | 0.12          |
| (1,996)  | 2:294:B:VAL:HG21 | 2:318:B:LEU:HB3 | 1        | 0.12          |
| (1,996)  | 2:294:B:VAL:HG22 | 2:318:B:LEU:HB2 | 1        | 0.12          |
| (1,996)  | 2:294:B:VAL:HG22 | 2:318:B:LEU:HB3 | 1        | 0.12          |
| (1,996)  | 2:294:B:VAL:HG23 | 2:318:B:LEU:HB2 | 1        | 0.12          |
| (1,996)  | 2:294:B:VAL:HG23 | 2:318:B:LEU:HB3 | 1        | 0.12          |
| (1,963)  | 2:220:B:LEU:HD11 | 2:204:B:THR:HB  | 10       | 0.12          |
| (1,963)  | 2:220:B:LEU:HD12 | 2:204:B:THR:HB  | 10       | 0.12          |
| (1,963)  | 2:220:B:LEU:HD13 | 2:204:B:THR:HB  | 10       | 0.12          |
| (1,963)  | 2:220:B:LEU:HD21 | 2:204:B:THR:HB  | 10       | 0.12          |
| (1,963)  | 2:220:B:LEU:HD22 | 2:204:B:THR:HB  | 10       | 0.12          |
| (1,963)  | 2:220:B:LEU:HD23 | 2:204:B:THR:HB  | 10       | 0.12          |
| (1,952)  | 2:229:B:LEU:HD11 | 2:277:B:ILE:H   | 16       | 0.12          |
| (1,952)  | 2:229:B:LEU:HD12 | 2:277:B:ILE:H   | 16       | 0.12          |
| (1,952)  | 2:229:B:LEU:HD13 | 2:277:B:ILE:H   | 16       | 0.12          |
| (1,952)  | 2:229:B:LEU:HD21 | 2:277:B:ILE:H   | 16       | 0.12          |
| (1,952)  | 2:229:B:LEU:HD22 | 2:277:B:ILE:H   | 16       | 0.12          |
| (1,952)  | 2:229:B:LEU:HD23 | 2:277:B:ILE:H   | 16       | 0.12          |
| (1,895)  | 2:279:B:GLN:H    | 2:226:B:LYS:HB2 | 2        | 0.12          |
| (1,895)  | 2:279:B:GLN:H    | 2:226:B:LYS:HB3 | 2        | 0.12          |

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| Key     | Atom-1        | Atom-2           | Model ID | Violation (Å) |
|---------|---------------|------------------|----------|---------------|
| (1,895) | 2:279:B:GLN:H | 2:226:B:LYS:HB2  | 11       | 0.12          |
| (1,895) | 2:279:B:GLN:H | 2:226:B:LYS:HB3  | 11       | 0.12          |
| (1,889) | 2:327:B:ILE:H | 2:327:B:ILE:HD11 | 12       | 0.12          |
| (1,889) | 2:327:B:ILE:H | 2:327:B:ILE:HD12 | 12       | 0.12          |
| (1,889) | 2:327:B:ILE:H | 2:327:B:ILE:HD13 | 12       | 0.12          |
| (1,831) | 2:292:B:ARG:H | 2:291:B:HIS:HD2  | 6        | 0.12          |
| (1,831) | 2:292:B:ARG:H | 2:291:B:HIS:HD2  | 15       | 0.12          |
| (1,831) | 2:292:B:ARG:H | 2:291:B:HIS:HD2  | 18       | 0.12          |
| (1,827) | 2:320:B:ALA:H | 2:323:B:LYS:HB2  | 8        | 0.12          |
| (1,827) | 2:320:B:ALA:H | 2:323:B:LYS:HB3  | 8        | 0.12          |
| (1,791) | 2:288:B:THR:H | 2:289:B:ILE:HG21 | 4        | 0.12          |
| (1,791) | 2:288:B:THR:H | 2:289:B:ILE:HG22 | 4        | 0.12          |
| (1,791) | 2:288:B:THR:H | 2:289:B:ILE:HG23 | 4        | 0.12          |
| (1,700) | 2:256:B:ASN:H | 2:259:B:ASN:H    | 2        | 0.12          |
| (1,587) | 2:328:B:THR:H | 2:332:B:VAL:HB   | 6        | 0.12          |
| (1,587) | 2:328:B:THR:H | 2:332:B:VAL:HB   | 14       | 0.12          |
| (1,587) | 2:328:B:THR:H | 2:332:B:VAL:HB   | 19       | 0.12          |
| (1,571) | 2:244:B:ASP:H | 2:288:B:THR:HG21 | 1        | 0.12          |
| (1,571) | 2:244:B:ASP:H | 2:288:B:THR:HG22 | 1        | 0.12          |
| (1,571) | 2:244:B:ASP:H | 2:288:B:THR:HG23 | 1        | 0.12          |
| (1,494) | 2:283:B:ALA:H | 2:279:B:GLN:HB2  | 10       | 0.12          |
| (1,494) | 2:283:B:ALA:H | 2:279:B:GLN:HB3  | 10       | 0.12          |
| (1,464) | 2:271:B:ASP:H | 2:267:B:GLU:H    | 7        | 0.12          |
| (1,464) | 2:271:B:ASP:H | 2:267:B:GLU:H    | 9        | 0.12          |
| (1,464) | 2:271:B:ASP:H | 2:267:B:GLU:H    | 20       | 0.12          |
| (1,385) | 2:314:B:TYR:H | 2:304:B:ALA:HA   | 4        | 0.12          |
| (1,379) | 2:327:B:ILE:H | 2:325:B:MET:HA   | 3        | 0.12          |
| (1,379) | 2:327:B:ILE:H | 2:325:B:MET:HA   | 12       | 0.12          |
| (1,359) | 2:342:B:GLU:H | 2:343:B:LYS:H    | 2        | 0.12          |
| (1,359) | 2:342:B:GLU:H | 2:343:B:LYS:H    | 9        | 0.12          |
| (1,359) | 2:342:B:GLU:H | 2:343:B:LYS:H    | 20       | 0.12          |
| (1,351) | 2:246:B:LYS:H | 2:244:B:ASP:H    | 8        | 0.12          |
| (1,351) | 2:246:B:LYS:H | 2:244:B:ASP:H    | 17       | 0.12          |
| (1,90)  | 2:280:B:GLY:H | 2:226:B:LYS:HG2  | 5        | 0.12          |
| (1,90)  | 2:280:B:GLY:H | 2:226:B:LYS:HG3  | 5        | 0.12          |
| (1,82)  | 2:321:B:LYS:H | 2:321:B:LYS:HG2  | 7        | 0.12          |
| (1,82)  | 2:321:B:LYS:H | 2:321:B:LYS:HG3  | 7        | 0.12          |
| (1,82)  | 2:321:B:LYS:H | 2:321:B:LYS:HG2  | 8        | 0.12          |
| (1,82)  | 2:321:B:LYS:H | 2:321:B:LYS:HG3  | 8        | 0.12          |
| (1,82)  | 2:321:B:LYS:H | 2:321:B:LYS:HG2  | 10       | 0.12          |
| (1,82)  | 2:321:B:LYS:H | 2:321:B:LYS:HG3  | 10       | 0.12          |
| (1,21)  | 2:281:B:ILE:H | 2:277:B:ILE:HG21 | 18       | 0.12          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,21)   | 2:281:B:ILE:H    | 2:277:B:ILE:HG22 | 18       | 0.12          |
| (1,21)   | 2:281:B:ILE:H    | 2:277:B:ILE:HG23 | 18       | 0.12          |
| (1,11)   | 2:295:B:THR:H    | 2:294:B:VAL:HB   | 2        | 0.12          |
| (1,1660) | 2:337:B:ILE:HA   | 1:186:A:ASP:HB2  | 15       | 0.11          |
| (1,1660) | 2:337:B:ILE:HA   | 1:186:A:ASP:HB3  | 15       | 0.11          |
| (1,1660) | 2:337:B:ILE:HA   | 1:186:A:ASP:HB2  | 17       | 0.11          |
| (1,1660) | 2:337:B:ILE:HA   | 1:186:A:ASP:HB3  | 17       | 0.11          |
| (1,1634) | 2:241:B:TYR:HA   | 2:210:B:ASP:HB2  | 16       | 0.11          |
| (1,1634) | 2:241:B:TYR:HA   | 2:210:B:ASP:HB3  | 16       | 0.11          |
| (1,1618) | 2:224:B:ASP:HA   | 2:193:B:PHE:HZ   | 5        | 0.11          |
| (1,1618) | 2:224:B:ASP:HA   | 2:193:B:PHE:HZ   | 12       | 0.11          |
| (1,1548) | 2:337:B:ILE:HG21 | 1:186:A:ASP:HA   | 9        | 0.11          |
| (1,1548) | 2:337:B:ILE:HG22 | 1:186:A:ASP:HA   | 9        | 0.11          |
| (1,1548) | 2:337:B:ILE:HG23 | 1:186:A:ASP:HA   | 9        | 0.11          |
| (1,1539) | 2:281:B:ILE:HB   | 2:277:B:ILE:HG21 | 8        | 0.11          |
| (1,1539) | 2:281:B:ILE:HB   | 2:277:B:ILE:HG22 | 8        | 0.11          |
| (1,1539) | 2:281:B:ILE:HB   | 2:277:B:ILE:HG23 | 8        | 0.11          |
| (1,1455) | 2:247:B:ASN:HA   | 2:289:B:ILE:HD11 | 15       | 0.11          |
| (1,1455) | 2:247:B:ASN:HA   | 2:289:B:ILE:HD12 | 15       | 0.11          |
| (1,1455) | 2:247:B:ASN:HA   | 2:289:B:ILE:HD13 | 15       | 0.11          |
| (1,1403) | 2:337:B:ILE:HD11 | 2:250:B:LEU:HG   | 19       | 0.11          |
| (1,1403) | 2:337:B:ILE:HD12 | 2:250:B:LEU:HG   | 19       | 0.11          |
| (1,1403) | 2:337:B:ILE:HD13 | 2:250:B:LEU:HG   | 19       | 0.11          |
| (1,1350) | 2:329:B:ILE:HB   | 2:328:B:THR:HB   | 11       | 0.11          |
| (1,1347) | 2:244:B:ASP:HA   | 2:286:B:ASN:HB2  | 3        | 0.11          |
| (1,1347) | 2:244:B:ASP:HA   | 2:286:B:ASN:HB3  | 3        | 0.11          |
| (1,1347) | 2:244:B:ASP:HA   | 2:286:B:ASN:HB2  | 4        | 0.11          |
| (1,1347) | 2:244:B:ASP:HA   | 2:286:B:ASN:HB3  | 4        | 0.11          |
| (1,1347) | 2:244:B:ASP:HA   | 2:286:B:ASN:HB2  | 8        | 0.11          |
| (1,1347) | 2:244:B:ASP:HA   | 2:286:B:ASN:HB3  | 8        | 0.11          |
| (1,1347) | 2:244:B:ASP:HA   | 2:286:B:ASN:HB2  | 10       | 0.11          |
| (1,1347) | 2:244:B:ASP:HA   | 2:286:B:ASN:HB3  | 10       | 0.11          |
| (1,1306) | 2:229:B:LEU:HA   | 2:193:B:PHE:HZ   | 9        | 0.11          |
| (1,1291) | 2:314:B:TYR:HA   | 2:318:B:LEU:HA   | 3        | 0.11          |
| (1,1234) | 2:255:B:LEU:HG   | 2:273:B:LEU:HB2  | 11       | 0.11          |
| (1,1234) | 2:255:B:LEU:HG   | 2:273:B:LEU:HB3  | 11       | 0.11          |
| (1,1210) | 2:281:B:ILE:HD11 | 2:289:B:ILE:HG21 | 12       | 0.11          |
| (1,1210) | 2:281:B:ILE:HD11 | 2:289:B:ILE:HG22 | 12       | 0.11          |
| (1,1210) | 2:281:B:ILE:HD11 | 2:289:B:ILE:HG23 | 12       | 0.11          |
| (1,1210) | 2:281:B:ILE:HD12 | 2:289:B:ILE:HG21 | 12       | 0.11          |
| (1,1210) | 2:281:B:ILE:HD12 | 2:289:B:ILE:HG22 | 12       | 0.11          |
| (1,1210) | 2:281:B:ILE:HD12 | 2:289:B:ILE:HG23 | 12       | 0.11          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1210) | 2:281:B:ILE:HD13 | 2:289:B:ILE:HG21 | 12       | 0.11          |
| (1,1210) | 2:281:B:ILE:HD13 | 2:289:B:ILE:HG22 | 12       | 0.11          |
| (1,1210) | 2:281:B:ILE:HD13 | 2:289:B:ILE:HG23 | 12       | 0.11          |
| (1,1162) | 2:218:B:LEU:HG   | 2:193:B:PHE:HE1  | 14       | 0.11          |
| (1,1162) | 2:218:B:LEU:HG   | 2:193:B:PHE:HE2  | 14       | 0.11          |
| (1,1139) | 1:188:A:ASN:HA   | 2:333:B:LYS:HB2  | 18       | 0.11          |
| (1,1139) | 1:188:A:ASN:HA   | 2:333:B:LYS:HB3  | 18       | 0.11          |
| (1,1128) | 2:199:B:HIS:HB2  | 2:225:B:LEU:HB2  | 6        | 0.11          |
| (1,1128) | 2:199:B:HIS:HB2  | 2:225:B:LEU:HB3  | 6        | 0.11          |
| (1,1128) | 2:199:B:HIS:HB3  | 2:225:B:LEU:HB2  | 6        | 0.11          |
| (1,1128) | 2:199:B:HIS:HB3  | 2:225:B:LEU:HB3  | 6        | 0.11          |
| (1,1123) | 2:207:B:ILE:HD11 | 2:205:B:SER:HA   | 12       | 0.11          |
| (1,1123) | 2:207:B:ILE:HD12 | 2:205:B:SER:HA   | 12       | 0.11          |
| (1,1123) | 2:207:B:ILE:HD13 | 2:205:B:SER:HA   | 12       | 0.11          |
| (1,1123) | 2:207:B:ILE:HD11 | 2:205:B:SER:HA   | 19       | 0.11          |
| (1,1123) | 2:207:B:ILE:HD12 | 2:205:B:SER:HA   | 19       | 0.11          |
| (1,1123) | 2:207:B:ILE:HD13 | 2:205:B:SER:HA   | 19       | 0.11          |
| (1,1109) | 2:193:B:PHE:HD1  | 2:203:B:VAL:HB   | 18       | 0.11          |
| (1,1109) | 2:193:B:PHE:HD2  | 2:203:B:VAL:HB   | 18       | 0.11          |
| (1,1064) | 2:226:B:LYS:HE2  | 2:230:B:VAL:HG11 | 20       | 0.11          |
| (1,1064) | 2:226:B:LYS:HE2  | 2:230:B:VAL:HG12 | 20       | 0.11          |
| (1,1064) | 2:226:B:LYS:HE2  | 2:230:B:VAL:HG13 | 20       | 0.11          |
| (1,1064) | 2:226:B:LYS:HE2  | 2:230:B:VAL:HG21 | 20       | 0.11          |
| (1,1064) | 2:226:B:LYS:HE2  | 2:230:B:VAL:HG22 | 20       | 0.11          |
| (1,1064) | 2:226:B:LYS:HE2  | 2:230:B:VAL:HG23 | 20       | 0.11          |
| (1,1064) | 2:226:B:LYS:HE3  | 2:230:B:VAL:HG11 | 20       | 0.11          |
| (1,1064) | 2:226:B:LYS:HE3  | 2:230:B:VAL:HG12 | 20       | 0.11          |
| (1,1064) | 2:226:B:LYS:HE3  | 2:230:B:VAL:HG13 | 20       | 0.11          |
| (1,1064) | 2:226:B:LYS:HE3  | 2:230:B:VAL:HG21 | 20       | 0.11          |
| (1,1064) | 2:226:B:LYS:HE3  | 2:230:B:VAL:HG22 | 20       | 0.11          |
| (1,1064) | 2:226:B:LYS:HE3  | 2:230:B:VAL:HG23 | 20       | 0.11          |
| (1,1062) | 2:213:B:GLU:HB2  | 2:239:B:LEU:HA   | 1        | 0.11          |
| (1,1062) | 2:213:B:GLU:HB3  | 2:239:B:LEU:HA   | 1        | 0.11          |
| (1,1062) | 2:213:B:GLU:HB2  | 2:239:B:LEU:HA   | 9        | 0.11          |
| (1,1062) | 2:213:B:GLU:HB3  | 2:239:B:LEU:HA   | 9        | 0.11          |
| (1,1062) | 2:213:B:GLU:HB2  | 2:239:B:LEU:HA   | 10       | 0.11          |
| (1,1062) | 2:213:B:GLU:HB3  | 2:239:B:LEU:HA   | 10       | 0.11          |
| (1,1036) | 2:329:B:ILE:HD11 | 2:332:B:VAL:HB   | 3        | 0.11          |
| (1,1036) | 2:329:B:ILE:HD12 | 2:332:B:VAL:HB   | 3        | 0.11          |
| (1,1036) | 2:329:B:ILE:HD13 | 2:332:B:VAL:HB   | 3        | 0.11          |
| (1,996)  | 2:294:B:VAL:HG11 | 2:318:B:LEU:HB2  | 8        | 0.11          |
| (1,996)  | 2:294:B:VAL:HG11 | 2:318:B:LEU:HB3  | 8        | 0.11          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,996) | 2:294:B:VAL:HG12 | 2:318:B:LEU:HB2  | 8        | 0.11          |
| (1,996) | 2:294:B:VAL:HG12 | 2:318:B:LEU:HB3  | 8        | 0.11          |
| (1,996) | 2:294:B:VAL:HG13 | 2:318:B:LEU:HB2  | 8        | 0.11          |
| (1,996) | 2:294:B:VAL:HG13 | 2:318:B:LEU:HB3  | 8        | 0.11          |
| (1,996) | 2:294:B:VAL:HG21 | 2:318:B:LEU:HB2  | 8        | 0.11          |
| (1,996) | 2:294:B:VAL:HG21 | 2:318:B:LEU:HB3  | 8        | 0.11          |
| (1,996) | 2:294:B:VAL:HG22 | 2:318:B:LEU:HB2  | 8        | 0.11          |
| (1,996) | 2:294:B:VAL:HG22 | 2:318:B:LEU:HB3  | 8        | 0.11          |
| (1,996) | 2:294:B:VAL:HG23 | 2:318:B:LEU:HB2  | 8        | 0.11          |
| (1,996) | 2:294:B:VAL:HG23 | 2:318:B:LEU:HB3  | 8        | 0.11          |
| (1,963) | 2:220:B:LEU:HD11 | 2:204:B:THR:HB   | 9        | 0.11          |
| (1,963) | 2:220:B:LEU:HD12 | 2:204:B:THR:HB   | 9        | 0.11          |
| (1,963) | 2:220:B:LEU:HD13 | 2:204:B:THR:HB   | 9        | 0.11          |
| (1,963) | 2:220:B:LEU:HD21 | 2:204:B:THR:HB   | 9        | 0.11          |
| (1,963) | 2:220:B:LEU:HD22 | 2:204:B:THR:HB   | 9        | 0.11          |
| (1,963) | 2:220:B:LEU:HD23 | 2:204:B:THR:HB   | 9        | 0.11          |
| (1,889) | 2:327:B:ILE:H    | 2:327:B:ILE:HD11 | 8        | 0.11          |
| (1,889) | 2:327:B:ILE:H    | 2:327:B:ILE:HD12 | 8        | 0.11          |
| (1,889) | 2:327:B:ILE:H    | 2:327:B:ILE:HD13 | 8        | 0.11          |
| (1,888) | 2:303:B:LYS:H    | 2:303:B:LYS:HE2  | 11       | 0.11          |
| (1,888) | 2:303:B:LYS:H    | 2:303:B:LYS:HE3  | 11       | 0.11          |
| (1,827) | 2:320:B:ALA:H    | 2:323:B:LYS:HB2  | 9        | 0.11          |
| (1,827) | 2:320:B:ALA:H    | 2:323:B:LYS:HB3  | 9        | 0.11          |
| (1,827) | 2:320:B:ALA:H    | 2:323:B:LYS:HB2  | 12       | 0.11          |
| (1,827) | 2:320:B:ALA:H    | 2:323:B:LYS:HB3  | 12       | 0.11          |
| (1,791) | 2:288:B:THR:H    | 2:289:B:ILE:HG21 | 7        | 0.11          |
| (1,791) | 2:288:B:THR:H    | 2:289:B:ILE:HG22 | 7        | 0.11          |
| (1,791) | 2:288:B:THR:H    | 2:289:B:ILE:HG23 | 7        | 0.11          |
| (1,733) | 2:218:B:LEU:H    | 2:218:B:LEU:HG   | 16       | 0.11          |
| (1,733) | 2:218:B:LEU:H    | 2:218:B:LEU:HG   | 18       | 0.11          |
| (1,700) | 2:256:B:ASN:H    | 2:259:B:ASN:H    | 1        | 0.11          |
| (1,700) | 2:256:B:ASN:H    | 2:259:B:ASN:H    | 18       | 0.11          |
| (1,587) | 2:328:B:THR:H    | 2:332:B:VAL:HB   | 1        | 0.11          |
| (1,587) | 2:328:B:THR:H    | 2:332:B:VAL:HB   | 15       | 0.11          |
| (1,464) | 2:271:B:ASP:H    | 2:267:B:GLU:H    | 1        | 0.11          |
| (1,464) | 2:271:B:ASP:H    | 2:267:B:GLU:H    | 13       | 0.11          |
| (1,464) | 2:271:B:ASP:H    | 2:267:B:GLU:H    | 15       | 0.11          |
| (1,428) | 2:222:B:GLU:H    | 2:202:B:ILE:HA   | 13       | 0.11          |
| (1,379) | 2:327:B:ILE:H    | 2:325:B:MET:HA   | 15       | 0.11          |
| (1,374) | 2:328:B:THR:H    | 2:327:B:ILE:HB   | 7        | 0.11          |
| (1,374) | 2:328:B:THR:H    | 2:327:B:ILE:HB   | 11       | 0.11          |
| (1,359) | 2:342:B:GLU:H    | 2:343:B:LYS:H    | 10       | 0.11          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,82)   | 2:321:B:LYS:H    | 2:321:B:LYS:HG2  | 2        | 0.11          |
| (1,82)   | 2:321:B:LYS:H    | 2:321:B:LYS:HG3  | 2        | 0.11          |
| (1,82)   | 2:321:B:LYS:H    | 2:321:B:LYS:HG2  | 12       | 0.11          |
| (1,82)   | 2:321:B:LYS:H    | 2:321:B:LYS:HG3  | 12       | 0.11          |
| (1,82)   | 2:321:B:LYS:H    | 2:321:B:LYS:HG2  | 18       | 0.11          |
| (1,82)   | 2:321:B:LYS:H    | 2:321:B:LYS:HG3  | 18       | 0.11          |
| (1,82)   | 2:321:B:LYS:H    | 2:321:B:LYS:HG2  | 20       | 0.11          |
| (1,82)   | 2:321:B:LYS:H    | 2:321:B:LYS:HG3  | 20       | 0.11          |
| (1,52)   | 2:327:B:ILE:H    | 2:321:B:LYS:HG2  | 18       | 0.11          |
| (1,52)   | 2:327:B:ILE:H    | 2:321:B:LYS:HG3  | 18       | 0.11          |
| (1,21)   | 2:281:B:ILE:H    | 2:277:B:ILE:HG21 | 3        | 0.11          |
| (1,21)   | 2:281:B:ILE:H    | 2:277:B:ILE:HG22 | 3        | 0.11          |
| (1,21)   | 2:281:B:ILE:H    | 2:277:B:ILE:HG23 | 3        | 0.11          |
| (1,11)   | 2:295:B:THR:H    | 2:294:B:VAL:HB   | 14       | 0.11          |
| (1,1637) | 1:187:A:VAL:HB   | 2:233:B:LEU:HG   | 11       | 0.1           |
| (1,1634) | 2:241:B:TYR:HA   | 2:210:B:ASP:HB2  | 11       | 0.1           |
| (1,1634) | 2:241:B:TYR:HA   | 2:210:B:ASP:HB3  | 11       | 0.1           |
| (1,1613) | 2:329:B:ILE:HG21 | 2:309:B:LEU:HB2  | 11       | 0.1           |
| (1,1613) | 2:329:B:ILE:HG21 | 2:309:B:LEU:HB3  | 11       | 0.1           |
| (1,1613) | 2:329:B:ILE:HG22 | 2:309:B:LEU:HB2  | 11       | 0.1           |
| (1,1613) | 2:329:B:ILE:HG22 | 2:309:B:LEU:HB3  | 11       | 0.1           |
| (1,1613) | 2:329:B:ILE:HG23 | 2:309:B:LEU:HB2  | 11       | 0.1           |
| (1,1613) | 2:329:B:ILE:HG23 | 2:309:B:LEU:HB3  | 11       | 0.1           |
| (1,1580) | 2:273:B:LEU:HD11 | 1:180:A:TYR:HE1  | 20       | 0.1           |
| (1,1580) | 2:273:B:LEU:HD11 | 1:180:A:TYR:HE2  | 20       | 0.1           |
| (1,1580) | 2:273:B:LEU:HD12 | 1:180:A:TYR:HE1  | 20       | 0.1           |
| (1,1580) | 2:273:B:LEU:HD12 | 1:180:A:TYR:HE2  | 20       | 0.1           |
| (1,1580) | 2:273:B:LEU:HD13 | 1:180:A:TYR:HE1  | 20       | 0.1           |
| (1,1580) | 2:273:B:LEU:HD13 | 1:180:A:TYR:HE2  | 20       | 0.1           |
| (1,1580) | 2:273:B:LEU:HD21 | 1:180:A:TYR:HE1  | 20       | 0.1           |
| (1,1580) | 2:273:B:LEU:HD21 | 1:180:A:TYR:HE2  | 20       | 0.1           |
| (1,1580) | 2:273:B:LEU:HD22 | 1:180:A:TYR:HE1  | 20       | 0.1           |
| (1,1580) | 2:273:B:LEU:HD22 | 1:180:A:TYR:HE2  | 20       | 0.1           |
| (1,1580) | 2:273:B:LEU:HD23 | 1:180:A:TYR:HE1  | 20       | 0.1           |
| (1,1580) | 2:273:B:LEU:HD23 | 1:180:A:TYR:HE2  | 20       | 0.1           |
| (1,1562) | 2:194:B:THR:HA   | 2:202:B:ILE:HG21 | 4        | 0.1           |
| (1,1562) | 2:194:B:THR:HA   | 2:202:B:ILE:HG22 | 4        | 0.1           |
| (1,1562) | 2:194:B:THR:HA   | 2:202:B:ILE:HG23 | 4        | 0.1           |
| (1,1347) | 2:244:B:ASP:HA   | 2:286:B:ASN:HB2  | 1        | 0.1           |
| (1,1347) | 2:244:B:ASP:HA   | 2:286:B:ASN:HB3  | 1        | 0.1           |
| (1,1347) | 2:244:B:ASP:HA   | 2:286:B:ASN:HB2  | 20       | 0.1           |
| (1,1347) | 2:244:B:ASP:HA   | 2:286:B:ASN:HB3  | 20       | 0.1           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1340) | 2:225:B:LEU:HD11 | 1:183:A:VAL:HA   | 13       | 0.1           |
| (1,1340) | 2:225:B:LEU:HD12 | 1:183:A:VAL:HA   | 13       | 0.1           |
| (1,1340) | 2:225:B:LEU:HD13 | 1:183:A:VAL:HA   | 13       | 0.1           |
| (1,1340) | 2:225:B:LEU:HD21 | 1:183:A:VAL:HA   | 13       | 0.1           |
| (1,1340) | 2:225:B:LEU:HD22 | 1:183:A:VAL:HA   | 13       | 0.1           |
| (1,1340) | 2:225:B:LEU:HD23 | 1:183:A:VAL:HA   | 13       | 0.1           |
| (1,1162) | 2:218:B:LEU:HG   | 2:193:B:PHE:HE1  | 11       | 0.1           |
| (1,1162) | 2:218:B:LEU:HG   | 2:193:B:PHE:HE2  | 11       | 0.1           |
| (1,1098) | 2:276:B:THR:HA   | 2:272:B:GLU:HB2  | 14       | 0.1           |
| (1,1098) | 2:276:B:THR:HA   | 2:272:B:GLU:HB3  | 14       | 0.1           |
| (1,1098) | 2:276:B:THR:HA   | 2:272:B:GLU:HB2  | 19       | 0.1           |
| (1,1098) | 2:276:B:THR:HA   | 2:272:B:GLU:HB3  | 19       | 0.1           |
| (1,1062) | 2:213:B:GLU:HB2  | 2:239:B:LEU:HA   | 2        | 0.1           |
| (1,1062) | 2:213:B:GLU:HB3  | 2:239:B:LEU:HA   | 2        | 0.1           |
| (1,1036) | 2:329:B:ILE:HD11 | 2:332:B:VAL:HB   | 13       | 0.1           |
| (1,1036) | 2:329:B:ILE:HD12 | 2:332:B:VAL:HB   | 13       | 0.1           |
| (1,1036) | 2:329:B:ILE:HD13 | 2:332:B:VAL:HB   | 13       | 0.1           |
| (1,895)  | 2:279:B:GLN:H    | 2:226:B:LYS:HB2  | 5        | 0.1           |
| (1,895)  | 2:279:B:GLN:H    | 2:226:B:LYS:HB3  | 5        | 0.1           |
| (1,889)  | 2:327:B:ILE:H    | 2:327:B:ILE:HD11 | 2        | 0.1           |
| (1,889)  | 2:327:B:ILE:H    | 2:327:B:ILE:HD12 | 2        | 0.1           |
| (1,889)  | 2:327:B:ILE:H    | 2:327:B:ILE:HD13 | 2        | 0.1           |
| (1,824)  | 2:229:B:LEU:H    | 2:229:B:LEU:HG   | 6        | 0.1           |
| (1,782)  | 2:294:B:VAL:H    | 2:251:B:VAL:HB   | 13       | 0.1           |
| (1,733)  | 2:218:B:LEU:H    | 2:218:B:LEU:HG   | 10       | 0.1           |
| (1,607)  | 2:282:B:GLU:H    | 2:279:B:GLN:HB2  | 13       | 0.1           |
| (1,607)  | 2:282:B:GLU:H    | 2:279:B:GLN:HB3  | 13       | 0.1           |
| (1,494)  | 2:283:B:ALA:H    | 2:279:B:GLN:HB2  | 6        | 0.1           |
| (1,494)  | 2:283:B:ALA:H    | 2:279:B:GLN:HB3  | 6        | 0.1           |
| (1,428)  | 2:222:B:GLU:H    | 2:202:B:ILE:HA   | 2        | 0.1           |
| (1,351)  | 2:246:B:LYS:H    | 2:244:B:ASP:H    | 7        | 0.1           |
| (1,107)  | 2:246:B:LYS:H    | 2:245:B:ASP:HB2  | 1        | 0.1           |
| (1,107)  | 2:246:B:LYS:H    | 2:245:B:ASP:HB3  | 1        | 0.1           |
| (1,107)  | 2:246:B:LYS:H    | 2:245:B:ASP:HB2  | 3        | 0.1           |
| (1,107)  | 2:246:B:LYS:H    | 2:245:B:ASP:HB3  | 3        | 0.1           |



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

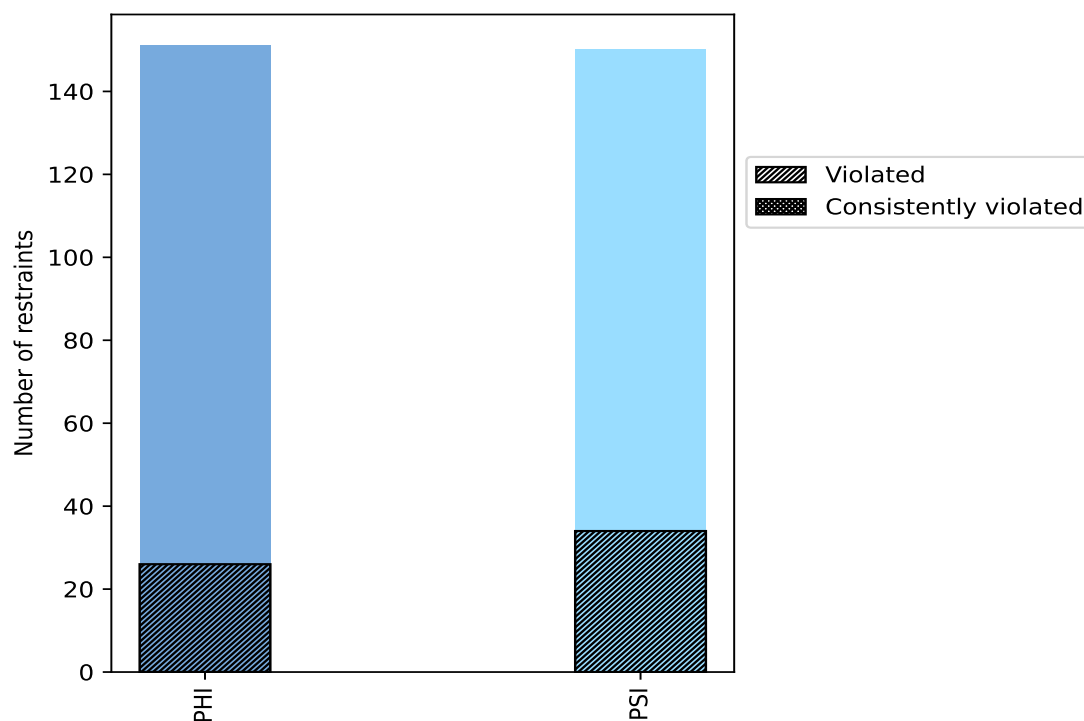
### 10.1 Summary of dihedral-angle violations [i](#)

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

| Angle type | Count | % <sup>1</sup> | Violated <sup>3</sup> |                |                | Consistently Violated <sup>4</sup> |                |                |
|------------|-------|----------------|-----------------------|----------------|----------------|------------------------------------|----------------|----------------|
|            |       |                | Count                 | % <sup>2</sup> | % <sup>1</sup> | Count                              | % <sup>2</sup> | % <sup>1</sup> |
| PHI        | 151   | 50.2           | 26                    | 17.2           | 8.6            | 0                                  | 0.0            | 0.0            |
| PSI        | 150   | 49.8           | 34                    | 22.7           | 11.3           | 0                                  | 0.0            | 0.0            |
| Total      | 301   | 100.0          | 60                    | 19.9           | 19.9           | 0                                  | 0.0            | 0.0            |

<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](#)



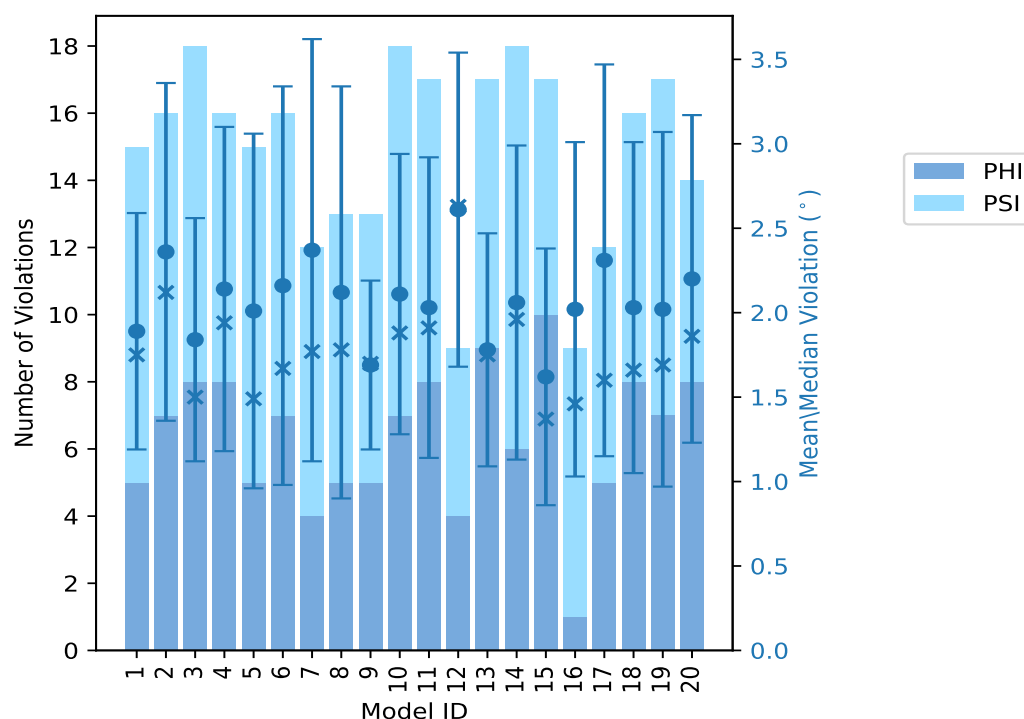
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

## 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        | 5                    | 10  | 15    | 1.89     | 3.61    | 0.7    | 1.75       |
| 2        | 7                    | 9   | 16    | 2.36     | 4.3     | 1.0    | 2.12       |
| 3        | 8                    | 10  | 18    | 1.84     | 3.39    | 0.72   | 1.5        |
| 4        | 8                    | 8   | 16    | 2.14     | 4.68    | 0.96   | 1.94       |
| 5        | 5                    | 10  | 15    | 2.01     | 4.14    | 1.05   | 1.49       |
| 6        | 7                    | 9   | 16    | 2.16     | 4.72    | 1.18   | 1.67       |
| 7        | 4                    | 8   | 12    | 2.37     | 4.74    | 1.25   | 1.77       |
| 8        | 5                    | 8   | 13    | 2.12     | 4.97    | 1.22   | 1.78       |
| 9        | 5                    | 8   | 13    | 1.69     | 2.59    | 0.5    | 1.7        |
| 10       | 7                    | 11  | 18    | 2.11     | 3.87    | 0.83   | 1.88       |
| 11       | 8                    | 9   | 17    | 2.03     | 4.74    | 0.89   | 1.91       |
| 12       | 4                    | 5   | 9     | 2.61     | 4.73    | 0.93   | 2.63       |
| 13       | 9                    | 8   | 17    | 1.78     | 3.56    | 0.69   | 1.75       |
| 14       | 6                    | 12  | 18    | 2.06     | 4.61    | 0.93   | 1.96       |
| 15       | 10                   | 7   | 17    | 1.62     | 4.28    | 0.76   | 1.37       |
| 16       | 1                    | 8   | 9     | 2.02     | 4.15    | 0.99   | 1.46       |
| 17       | 5                    | 7   | 12    | 2.31     | 4.8     | 1.16   | 1.6        |
| 18       | 8                    | 8   | 16    | 2.03     | 4.43    | 0.98   | 1.66       |
| 19       | 7                    | 10  | 17    | 2.02     | 4.86    | 1.05   | 1.69       |
| 20       | 8                    | 6   | 14    | 2.2      | 4.46    | 0.97   | 1.86       |

### 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>       | %    |
| 8                             | 11  | 19    | 1                        | 5.0  |
| 1                             | 3   | 4     | 2                        | 10.0 |
| 4                             | 2   | 6     | 3                        | 15.0 |
| 3                             | 6   | 9     | 4                        | 20.0 |
| 2                             | 1   | 3     | 5                        | 25.0 |
| 1                             | 2   | 3     | 6                        | 30.0 |
| 1                             | 3   | 4     | 7                        | 35.0 |
| 1                             | 1   | 2     | 8                        | 40.0 |
| 1                             | 0   | 1     | 9                        | 45.0 |
| 1                             | 1   | 2     | 10                       | 50.0 |
| 0                             | 0   | 0     | 11                       | 55.0 |

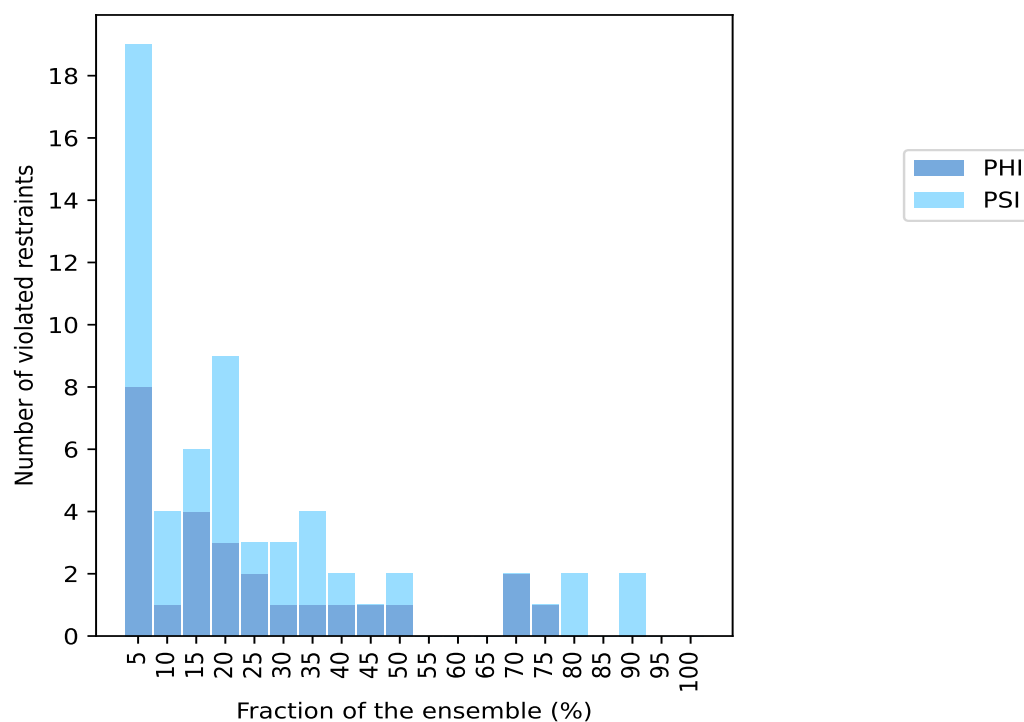
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| Number of violated restraints |     |       | Fraction of the ensemble |       |
|-------------------------------|-----|-------|--------------------------|-------|
| PHI                           | PSI | Total | Count <sup>1</sup>       | %     |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

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

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

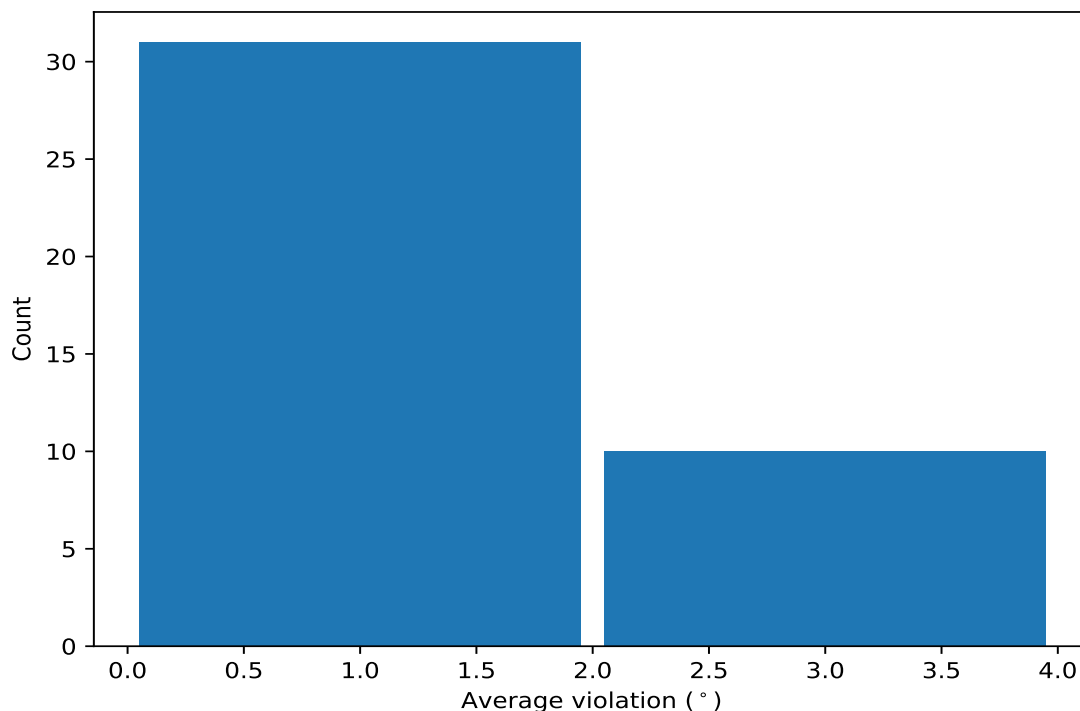


## 10.4 Most violated dihedral-angle restraints in the ensemble [i](#)

### 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 |
|---------|---------------|----------------|----------------|---------------|---------------------|------|-----------------|--------|
| (1,227) | 2:265:B:LYS:N | 2:265:B:LYS:CA | 2:265:B:LYS:C  | 2:266:B:ARG:N | 18                  | 3.76 | 0.99            | 3.98   |
| (1,221) | 2:258:B:LYS:N | 2:258:B:LYS:CA | 2:258:B:LYS:C  | 2:259:B:ASN:N | 18                  | 3.07 | 1.06            | 2.8    |
| (1,194) | 2:225:B:LEU:N | 2:225:B:LEU:CA | 2:225:B:LEU:C  | 2:226:B:LYS:N | 16                  | 2.78 | 0.97            | 2.38   |
| (1,295) | 2:334:B:SER:N | 2:334:B:SER:CA | 2:334:B:SER:C  | 2:335:B:SER:N | 16                  | 2.48 | 0.95            | 2.24   |
| (1,45)  | 2:225:B:LEU:C | 2:226:B:LYS:N  | 2:226:B:LYS:CA | 2:226:B:LYS:C | 15                  | 2.89 | 1.13            | 2.81   |
| (1,40)  | 2:218:B:LEU:C | 2:219:B:GLU:N  | 2:219:B:GLU:CA | 2:219:B:GLU:C | 14                  | 1.93 | 0.55            | 1.8    |
| (1,10)  | 1:187:A:VAL:C | 1:188:A:ASN:N  | 1:188:A:ASN:CA | 1:188:A:ASN:C | 14                  | 1.72 | 0.42            | 1.68   |
| (1,166) | 2:195:B:ILE:N | 2:195:B:ILE:CA | 2:195:B:ILE:C  | 2:196:B:ASN:N | 10                  | 1.69 | 0.22            | 1.75   |
| (1,29)  | 2:207:B:ILE:C | 2:208:B:ASN:N  | 2:208:B:ASN:CA | 2:208:B:ASN:C | 10                  | 1.6  | 0.27            | 1.57   |
| (1,26)  | 2:204:B:THR:C | 2:205:B:SER:N  | 2:205:B:SER:CA | 2:205:B:SER:C | 9                   | 1.39 | 0.23            | 1.41   |
| (1,70)  | 2:256:B:ASN:C | 2:257:B:ASP:N  | 2:257:B:ASP:CA | 2:257:B:ASP:C | 8                   | 1.41 | 0.35            | 1.28   |
| (1,186) | 2:215:B:LEU:N | 2:215:B:LEU:CA | 2:215:B:LEU:C  | 2:216:B:ASP:N | 8                   | 1.36 | 0.33            | 1.23   |
| (1,284) | 2:323:B:LYS:N | 2:323:B:LYS:CA | 2:323:B:LYS:C  | 2:324:B:GLY:N | 7                   | 2.55 | 0.84            | 2.52   |
| (1,19)  | 2:197:B:SER:C | 2:198:B:LYS:N  | 2:198:B:LYS:CA | 2:198:B:LYS:C | 7                   | 2.19 | 0.91            | 1.88   |
| (1,176) | 2:205:B:SER:N | 2:205:B:SER:CA | 2:205:B:SER:C  | 2:206:B:ALA:N | 7                   | 1.82 | 0.37            | 2.0    |
| (1,299) | 2:339:B:ASP:N | 2:339:B:ASP:CA | 2:339:B:ASP:C  | 2:340:B:LEU:N | 7                   | 1.57 | 0.28            | 1.68   |
| (1,193) | 2:224:B:ASP:N | 2:224:B:ASP:CA | 2:224:B:ASP:C  | 2:225:B:LEU:N | 6                   | 1.69 | 0.54            | 1.59   |
| (1,189) | 2:218:B:LEU:N | 2:218:B:LEU:CA | 2:218:B:LEU:C  | 2:219:B:GLU:N | 6                   | 1.67 | 0.42            | 1.8    |
| (1,75)  | 2:261:B:LYS:C | 2:262:B:THR:N  | 2:262:B:THR:CA | 2:262:B:THR:C | 6                   | 1.46 | 0.32            | 1.38   |
| (1,99)  | 2:287:B:ASP:C | 2:288:B:THR:N  | 2:288:B:THR:CA | 2:288:B:THR:C | 5                   | 1.64 | 0.54            | 1.55   |

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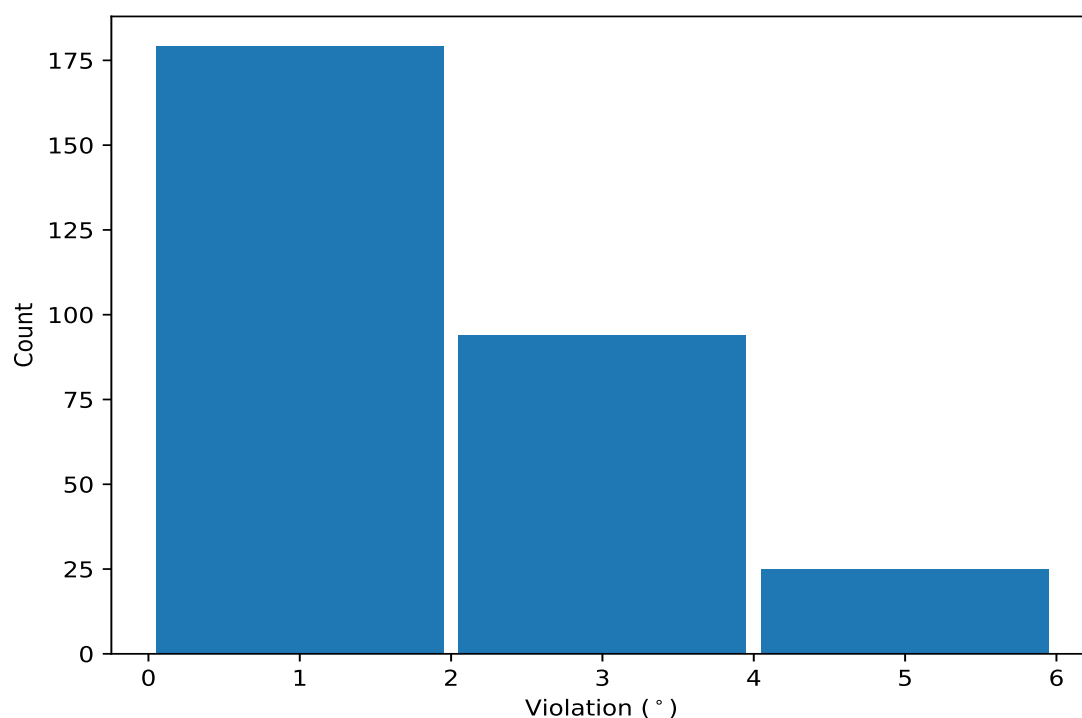
| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Models <sup>1</sup> | Mean | SD <sup>2</sup> | Median |
|---------|---------------|----------------|----------------|---------------|---------------------|------|-----------------|--------|
| (1,36)  | 2:214:B:VAL:C | 2:215:B:LEU:N  | 2:215:B:LEU:CA | 2:215:B:LEU:C | 5                   | 1.47 | 0.32            | 1.43   |
| (1,208) | 2:239:B:LEU:N | 2:239:B:LEU:CA | 2:239:B:LEU:C  | 2:240:B:GLY:N | 5                   | 1.26 | 0.23            | 1.13   |
| (1,190) | 2:219:B:GLU:N | 2:219:B:GLU:CA | 2:219:B:GLU:C  | 2:220:B:LEU:N | 4                   | 2.06 | 0.43            | 2.3    |
| (1,248) | 2:287:B:ASP:N | 2:287:B:ASP:CA | 2:287:B:ASP:C  | 2:288:B:THR:N | 4                   | 1.77 | 0.43            | 1.92   |
| (1,300) | 2:340:B:LEU:N | 2:340:B:LEU:CA | 2:340:B:LEU:C  | 2:341:B:ILE:N | 4                   | 1.74 | 0.45            | 1.83   |
| (1,151) | 2:341:B:ILE:C | 2:342:B:GLU:N  | 2:342:B:GLU:CA | 2:342:B:GLU:C | 4                   | 1.71 | 0.39            | 1.8    |
| (1,61)  | 2:242:B:ILE:C | 2:243:B:SER:N  | 2:243:B:SER:CA | 2:243:B:SER:C | 4                   | 1.71 | 0.57            | 1.61   |
| (1,102) | 2:290:B:VAL:C | 2:291:B:HIS:N  | 2:291:B:HIS:CA | 2:291:B:HIS:C | 4                   | 1.68 | 0.34            | 1.62   |
| (1,187) | 2:216:B:ASP:N | 2:216:B:ASP:CA | 2:216:B:ASP:C  | 2:217:B:GLY:N | 4                   | 1.5  | 0.29            | 1.56   |
| (1,257) | 2:296:B:VAL:N | 2:296:B:VAL:CA | 2:296:B:VAL:C  | 2:297:B:ASP:N | 4                   | 1.34 | 0.32            | 1.23   |
| (1,164) | 2:193:B:PHE:N | 2:193:B:PHE:CA | 2:193:B:PHE:C  | 2:194:B:THR:N | 4                   | 1.18 | 0.12            | 1.15   |
| (1,134) | 2:322:B:GLU:C | 2:323:B:LYS:N  | 2:323:B:LYS:CA | 2:323:B:LYS:C | 3                   | 2.48 | 0.36            | 2.65   |
| (1,2)   | 1:179:A:GLU:C | 1:180:A:TYR:N  | 1:180:A:TYR:CA | 1:180:A:TYR:C | 3                   | 2.09 | 1.09            | 1.54   |
| (1,39)  | 2:217:B:GLY:C | 2:218:B:LEU:N  | 2:218:B:LEU:CA | 2:218:B:LEU:C | 3                   | 1.96 | 0.85            | 1.49   |
| (1,21)  | 2:199:B:HIS:C | 2:200:B:LYS:N  | 2:200:B:LYS:CA | 2:200:B:LYS:C | 3                   | 1.82 | 0.4             | 1.91   |
| (1,159) | 1:186:A:ASP:N | 1:186:A:ASP:CA | 1:186:A:ASP:C  | 1:187:A:VAL:N | 3                   | 1.46 | 0.19            | 1.39   |
| (1,214) | 2:249:B:VAL:N | 2:249:B:VAL:CA | 2:249:B:VAL:C  | 2:250:B:LEU:N | 3                   | 1.3  | 0.15            | 1.31   |
| (1,160) | 1:187:A:VAL:N | 1:187:A:VAL:CA | 1:187:A:VAL:C  | 1:188:A:ASN:N | 2                   | 1.69 | 0.36            | 1.69   |
| (1,11)  | 2:189:B:PRO:C | 2:190:B:SER:N  | 2:190:B:SER:CA | 2:190:B:SER:C | 2                   | 1.29 | 0.06            | 1.29   |
| (1,289) | 2:328:B:THR:N | 2:328:B:THR:CA | 2:328:B:THR:C  | 2:329:B:ILE:N | 2                   | 1.19 | 0.17            | 1.19   |
| (1,218) | 2:253:B:MET:N | 2:253:B:MET:CA | 2:253:B:MET:C  | 2:254:B:ALA:N | 2                   | 1.1  | 0.01            | 1.1    |

<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 (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,227) | 2:265:B:LYS:N | 2:265:B:LYS:CA | 2:265:B:LYS:C  | 2:266:B:ARG:N | 8        | 4.97          |
| (1,221) | 2:258:B:LYS:N | 2:258:B:LYS:CA | 2:258:B:LYS:C  | 2:259:B:ASN:N | 19       | 4.86          |
| (1,221) | 2:258:B:LYS:N | 2:258:B:LYS:CA | 2:258:B:LYS:C  | 2:259:B:ASN:N | 17       | 4.8           |
| (1,227) | 2:265:B:LYS:N | 2:265:B:LYS:CA | 2:265:B:LYS:C  | 2:266:B:ARG:N | 11       | 4.74          |
| (1,45)  | 2:225:B:LEU:C | 2:226:B:LYS:N  | 2:226:B:LYS:CA | 2:226:B:LYS:C | 7        | 4.74          |
| (1,227) | 2:265:B:LYS:N | 2:265:B:LYS:CA | 2:265:B:LYS:C  | 2:266:B:ARG:N | 12       | 4.73          |
| (1,295) | 2:334:B:SER:N | 2:334:B:SER:CA | 2:334:B:SER:C  | 2:335:B:SER:N | 6        | 4.72          |
| (1,45)  | 2:225:B:LEU:C | 2:226:B:LYS:N  | 2:226:B:LYS:CA | 2:226:B:LYS:C | 4        | 4.68          |
| (1,221) | 2:258:B:LYS:N | 2:258:B:LYS:CA | 2:258:B:LYS:C  | 2:259:B:ASN:N | 8        | 4.66          |
| (1,227) | 2:265:B:LYS:N | 2:265:B:LYS:CA | 2:265:B:LYS:C  | 2:266:B:ARG:N | 14       | 4.61          |
| (1,227) | 2:265:B:LYS:N | 2:265:B:LYS:CA | 2:265:B:LYS:C  | 2:266:B:ARG:N | 7        | 4.54          |
| (1,227) | 2:265:B:LYS:N | 2:265:B:LYS:CA | 2:265:B:LYS:C  | 2:266:B:ARG:N | 20       | 4.46          |
| (1,227) | 2:265:B:LYS:N | 2:265:B:LYS:CA | 2:265:B:LYS:C  | 2:266:B:ARG:N | 18       | 4.43          |
| (1,19)  | 2:197:B:SER:C | 2:198:B:LYS:N  | 2:198:B:LYS:CA | 2:198:B:LYS:C | 2        | 4.3           |
| (1,227) | 2:265:B:LYS:N | 2:265:B:LYS:CA | 2:265:B:LYS:C  | 2:266:B:ARG:N | 15       | 4.28          |
| (1,45)  | 2:225:B:LEU:C | 2:226:B:LYS:N  | 2:226:B:LYS:CA | 2:226:B:LYS:C | 18       | 4.26          |
| (1,227) | 2:265:B:LYS:N | 2:265:B:LYS:CA | 2:265:B:LYS:C  | 2:266:B:ARG:N | 19       | 4.21          |
| (1,221) | 2:258:B:LYS:N | 2:258:B:LYS:CA | 2:258:B:LYS:C  | 2:259:B:ASN:N | 16       | 4.15          |
| (1,194) | 2:225:B:LEU:N | 2:225:B:LEU:CA | 2:225:B:LEU:C  | 2:226:B:LYS:N | 5        | 4.14          |
| (1,45)  | 2:225:B:LEU:C | 2:226:B:LYS:N  | 2:226:B:LYS:CA | 2:226:B:LYS:C | 5        | 4.13          |
| (1,194) | 2:225:B:LEU:N | 2:225:B:LEU:CA | 2:225:B:LEU:C  | 2:226:B:LYS:N | 6        | 4.11          |

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| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,194) | 2:225:B:LEU:N | 2:225:B:LEU:CA | 2:225:B:LEU:C  | 2:226:B:LYS:N | 4        | 4.1           |
| (1,194) | 2:225:B:LEU:N | 2:225:B:LEU:CA | 2:225:B:LEU:C  | 2:226:B:LYS:N | 2        | 4.07          |
| (1,221) | 2:258:B:LYS:N | 2:258:B:LYS:CA | 2:258:B:LYS:C  | 2:259:B:ASN:N | 20       | 4.06          |
| (1,251) | 2:290:B:VAL:N | 2:290:B:VAL:CA | 2:290:B:VAL:C  | 2:291:B:HIS:N | 14       | 4.04          |
| (1,284) | 2:323:B:LYS:N | 2:323:B:LYS:CA | 2:323:B:LYS:C  | 2:324:B:GLY:N | 17       | 3.91          |
| (1,295) | 2:334:B:SER:N | 2:334:B:SER:CA | 2:334:B:SER:C  | 2:335:B:SER:N | 10       | 3.87          |
| (1,227) | 2:265:B:LYS:N | 2:265:B:LYS:CA | 2:265:B:LYS:C  | 2:266:B:ARG:N | 10       | 3.76          |
| (1,227) | 2:265:B:LYS:N | 2:265:B:LYS:CA | 2:265:B:LYS:C  | 2:266:B:ARG:N | 6        | 3.66          |
| (1,227) | 2:265:B:LYS:N | 2:265:B:LYS:CA | 2:265:B:LYS:C  | 2:266:B:ARG:N | 2        | 3.64          |
| (1,2)   | 1:179:A:GLU:C | 1:180:A:TYR:N  | 1:180:A:TYR:CA | 1:180:A:TYR:C | 1        | 3.61          |
| (1,45)  | 2:225:B:LEU:C | 2:226:B:LYS:N  | 2:226:B:LYS:CA | 2:226:B:LYS:C | 6        | 3.6           |
| (1,194) | 2:225:B:LEU:N | 2:225:B:LEU:CA | 2:225:B:LEU:C  | 2:226:B:LYS:N | 13       | 3.56          |
| (1,221) | 2:258:B:LYS:N | 2:258:B:LYS:CA | 2:258:B:LYS:C  | 2:259:B:ASN:N | 2        | 3.55          |
| (1,295) | 2:334:B:SER:N | 2:334:B:SER:CA | 2:334:B:SER:C  | 2:335:B:SER:N | 7        | 3.46          |
| (1,194) | 2:225:B:LEU:N | 2:225:B:LEU:CA | 2:225:B:LEU:C  | 2:226:B:LYS:N | 7        | 3.42          |
| (1,227) | 2:265:B:LYS:N | 2:265:B:LYS:CA | 2:265:B:LYS:C  | 2:266:B:ARG:N | 3        | 3.39          |
| (1,227) | 2:265:B:LYS:N | 2:265:B:LYS:CA | 2:265:B:LYS:C  | 2:266:B:ARG:N | 1        | 3.35          |
| (1,221) | 2:258:B:LYS:N | 2:258:B:LYS:CA | 2:258:B:LYS:C  | 2:259:B:ASN:N | 13       | 3.33          |
| (1,284) | 2:323:B:LYS:N | 2:323:B:LYS:CA | 2:323:B:LYS:C  | 2:324:B:GLY:N | 16       | 3.3           |
| (1,227) | 2:265:B:LYS:N | 2:265:B:LYS:CA | 2:265:B:LYS:C  | 2:266:B:ARG:N | 17       | 3.3           |
| (1,221) | 2:258:B:LYS:N | 2:258:B:LYS:CA | 2:258:B:LYS:C  | 2:259:B:ASN:N | 10       | 3.3           |
| (1,295) | 2:334:B:SER:N | 2:334:B:SER:CA | 2:334:B:SER:C  | 2:335:B:SER:N | 5        | 3.25          |
| (1,39)  | 2:217:B:GLY:C | 2:218:B:LEU:N  | 2:218:B:LEU:CA | 2:218:B:LEU:C | 17       | 3.15          |
| (1,194) | 2:225:B:LEU:N | 2:225:B:LEU:CA | 2:225:B:LEU:C  | 2:226:B:LYS:N | 12       | 3.14          |
| (1,295) | 2:334:B:SER:N | 2:334:B:SER:CA | 2:334:B:SER:C  | 2:335:B:SER:N | 3        | 3.13          |
| (1,284) | 2:323:B:LYS:N | 2:323:B:LYS:CA | 2:323:B:LYS:C  | 2:324:B:GLY:N | 11       | 3.02          |
| (1,221) | 2:258:B:LYS:N | 2:258:B:LYS:CA | 2:258:B:LYS:C  | 2:259:B:ASN:N | 5        | 3.0           |
| (1,211) | 2:243:B:SER:N | 2:243:B:SER:CA | 2:243:B:SER:C  | 2:244:B:ASP:N | 4        | 2.98          |
| (1,45)  | 2:225:B:LEU:C | 2:226:B:LYS:N  | 2:226:B:LYS:CA | 2:226:B:LYS:C | 12       | 2.89          |
| (1,40)  | 2:218:B:LEU:C | 2:219:B:GLU:N  | 2:219:B:GLU:CA | 2:219:B:GLU:C | 20       | 2.88          |
| (1,45)  | 2:225:B:LEU:C | 2:226:B:LYS:N  | 2:226:B:LYS:CA | 2:226:B:LYS:C | 3        | 2.85          |
| (1,134) | 2:322:B:GLU:C | 2:323:B:LYS:N  | 2:323:B:LYS:CA | 2:323:B:LYS:C | 18       | 2.82          |
| (1,45)  | 2:225:B:LEU:C | 2:226:B:LYS:N  | 2:226:B:LYS:CA | 2:226:B:LYS:C | 20       | 2.81          |
| (1,45)  | 2:225:B:LEU:C | 2:226:B:LYS:N  | 2:226:B:LYS:CA | 2:226:B:LYS:C | 2        | 2.76          |
| (1,134) | 2:322:B:GLU:C | 2:323:B:LYS:N  | 2:323:B:LYS:CA | 2:323:B:LYS:C | 10       | 2.65          |
| (1,45)  | 2:225:B:LEU:C | 2:226:B:LYS:N  | 2:226:B:LYS:CA | 2:226:B:LYS:C | 19       | 2.64          |
| (1,10)  | 1:187:A:VAL:C | 1:188:A:ASN:N  | 1:188:A:ASN:CA | 1:188:A:ASN:C | 12       | 2.64          |
| (1,295) | 2:334:B:SER:N | 2:334:B:SER:CA | 2:334:B:SER:C  | 2:335:B:SER:N | 2        | 2.63          |
| (1,193) | 2:224:B:ASP:N | 2:224:B:ASP:CA | 2:224:B:ASP:C  | 2:225:B:LEU:N | 12       | 2.63          |
| (1,40)  | 2:218:B:LEU:C | 2:219:B:GLU:N  | 2:219:B:GLU:CA | 2:219:B:GLU:C | 11       | 2.62          |
| (1,221) | 2:258:B:LYS:N | 2:258:B:LYS:CA | 2:258:B:LYS:C  | 2:259:B:ASN:N | 9        | 2.59          |
| (1,99)  | 2:287:B:ASP:C | 2:288:B:THR:N  | 2:288:B:THR:CA | 2:288:B:THR:C | 11       | 2.59          |
| (1,61)  | 2:242:B:ILE:C | 2:243:B:SER:N  | 2:243:B:SER:CA | 2:243:B:SER:C | 17       | 2.59          |
| (1,40)  | 2:218:B:LEU:C | 2:219:B:GLU:N  | 2:219:B:GLU:CA | 2:219:B:GLU:C | 8        | 2.57          |
| (1,221) | 2:258:B:LYS:N | 2:258:B:LYS:CA | 2:258:B:LYS:C  | 2:259:B:ASN:N | 6        | 2.56          |
| (1,221) | 2:258:B:LYS:N | 2:258:B:LYS:CA | 2:258:B:LYS:C  | 2:259:B:ASN:N | 11       | 2.54          |
| (1,284) | 2:323:B:LYS:N | 2:323:B:LYS:CA | 2:323:B:LYS:C  | 2:324:B:GLY:N | 10       | 2.52          |
| (1,40)  | 2:218:B:LEU:C | 2:219:B:GLU:N  | 2:219:B:GLU:CA | 2:219:B:GLU:C | 14       | 2.46          |
| (1,194) | 2:225:B:LEU:N | 2:225:B:LEU:CA | 2:225:B:LEU:C  | 2:226:B:LYS:N | 19       | 2.45          |
| (1,295) | 2:334:B:SER:N | 2:334:B:SER:CA | 2:334:B:SER:C  | 2:335:B:SER:N | 19       | 2.44          |
| (1,40)  | 2:218:B:LEU:C | 2:219:B:GLU:N  | 2:219:B:GLU:CA | 2:219:B:GLU:C | 3        | 2.44          |

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| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,221) | 2:258:B:LYS:N | 2:258:B:LYS:CA | 2:258:B:LYS:C  | 2:259:B:ASN:N | 18       | 2.42          |
| (1,221) | 2:258:B:LYS:N | 2:258:B:LYS:CA | 2:258:B:LYS:C  | 2:259:B:ASN:N | 14       | 2.38          |
| (1,221) | 2:258:B:LYS:N | 2:258:B:LYS:CA | 2:258:B:LYS:C  | 2:259:B:ASN:N | 12       | 2.34          |
| (1,190) | 2:219:B:GLU:N | 2:219:B:GLU:CA | 2:219:B:GLU:C  | 2:220:B:LEU:N | 2        | 2.34          |
| (1,190) | 2:219:B:GLU:N | 2:219:B:GLU:CA | 2:219:B:GLU:C  | 2:220:B:LEU:N | 1        | 2.33          |
| (1,244) | 2:282:B:GLU:N | 2:282:B:GLU:CA | 2:282:B:GLU:C  | 2:283:B:ALA:N | 14       | 2.32          |
| (1,194) | 2:225:B:LEU:N | 2:225:B:LEU:CA | 2:225:B:LEU:C  | 2:226:B:LYS:N | 3        | 2.31          |
| (1,10)  | 1:187:A:VAL:C | 1:188:A:ASN:N  | 1:188:A:ASN:CA | 1:188:A:ASN:C | 6        | 2.31          |
| (1,169) | 2:198:B:LYS:N | 2:198:B:LYS:CA | 2:198:B:LYS:C  | 2:199:B:HIS:N | 10       | 2.3           |
| (1,295) | 2:334:B:SER:N | 2:334:B:SER:CA | 2:334:B:SER:C  | 2:335:B:SER:N | 4        | 2.29          |
| (1,194) | 2:225:B:LEU:N | 2:225:B:LEU:CA | 2:225:B:LEU:C  | 2:226:B:LYS:N | 9        | 2.29          |
| (1,190) | 2:219:B:GLU:N | 2:219:B:GLU:CA | 2:219:B:GLU:C  | 2:220:B:LEU:N | 11       | 2.27          |
| (1,21)  | 2:199:B:HIS:C | 2:200:B:LYS:N  | 2:200:B:LYS:CA | 2:200:B:LYS:C | 14       | 2.27          |
| (1,176) | 2:205:B:SER:N | 2:205:B:SER:CA | 2:205:B:SER:C  | 2:206:B:ALA:N | 16       | 2.25          |
| (1,70)  | 2:256:B:ASN:C | 2:257:B:ASP:N  | 2:257:B:ASP:CA | 2:257:B:ASP:C | 10       | 2.23          |
| (1,300) | 2:340:B:LEU:N | 2:340:B:LEU:CA | 2:340:B:LEU:C  | 2:341:B:ILE:N | 3        | 2.22          |
| (1,295) | 2:334:B:SER:N | 2:334:B:SER:CA | 2:334:B:SER:C  | 2:335:B:SER:N | 14       | 2.2           |
| (1,19)  | 2:197:B:SER:C | 2:198:B:LYS:N  | 2:198:B:LYS:CA | 2:198:B:LYS:C | 15       | 2.2           |
| (1,227) | 2:265:B:LYS:N | 2:265:B:LYS:CA | 2:265:B:LYS:C  | 2:266:B:ARG:N | 5        | 2.19          |
| (1,19)  | 2:197:B:SER:C | 2:198:B:LYS:N  | 2:198:B:LYS:CA | 2:198:B:LYS:C | 19       | 2.18          |
| (1,10)  | 1:187:A:VAL:C | 1:188:A:ASN:N  | 1:188:A:ASN:CA | 1:188:A:ASN:C | 3        | 2.18          |
| (1,248) | 2:287:B:ASP:N | 2:287:B:ASP:CA | 2:287:B:ASP:C  | 2:288:B:THR:N | 18       | 2.15          |
| (1,194) | 2:225:B:LEU:N | 2:225:B:LEU:CA | 2:225:B:LEU:C  | 2:226:B:LYS:N | 10       | 2.15          |
| (1,102) | 2:290:B:VAL:C | 2:291:B:HIS:N  | 2:291:B:HIS:CA | 2:291:B:HIS:C | 12       | 2.15          |
| (1,166) | 2:195:B:ILE:N | 2:195:B:ILE:CA | 2:195:B:ILE:C  | 2:196:B:ASN:N | 6        | 2.14          |
| (1,189) | 2:218:B:LEU:N | 2:218:B:LEU:CA | 2:218:B:LEU:C  | 2:219:B:GLU:N | 14       | 2.12          |
| (1,151) | 2:341:B:ILE:C | 2:342:B:GLU:N  | 2:342:B:GLU:CA | 2:342:B:GLU:C | 2        | 2.12          |
| (1,75)  | 2:261:B:LYS:C | 2:262:B:THR:N  | 2:262:B:THR:CA | 2:262:B:THR:C | 15       | 2.12          |
| (1,176) | 2:205:B:SER:N | 2:205:B:SER:CA | 2:205:B:SER:C  | 2:206:B:ALA:N | 2        | 2.11          |
| (1,40)  | 2:218:B:LEU:C | 2:219:B:GLU:N  | 2:219:B:GLU:CA | 2:219:B:GLU:C | 9        | 2.1           |
| (1,248) | 2:287:B:ASP:N | 2:287:B:ASP:CA | 2:287:B:ASP:C  | 2:288:B:THR:N | 20       | 2.09          |
| (1,189) | 2:218:B:LEU:N | 2:218:B:LEU:CA | 2:218:B:LEU:C  | 2:219:B:GLU:N | 11       | 2.09          |
| (1,300) | 2:340:B:LEU:N | 2:340:B:LEU:CA | 2:340:B:LEU:C  | 2:341:B:ILE:N | 13       | 2.08          |
| (1,295) | 2:334:B:SER:N | 2:334:B:SER:CA | 2:334:B:SER:C  | 2:335:B:SER:N | 9        | 2.07          |
| (1,193) | 2:224:B:ASP:N | 2:224:B:ASP:CA | 2:224:B:ASP:C  | 2:225:B:LEU:N | 4        | 2.07          |
| (1,295) | 2:334:B:SER:N | 2:334:B:SER:CA | 2:334:B:SER:C  | 2:335:B:SER:N | 11       | 2.06          |
| (1,227) | 2:265:B:LYS:N | 2:265:B:LYS:CA | 2:265:B:LYS:C  | 2:266:B:ARG:N | 4        | 2.05          |
| (1,160) | 1:187:A:VAL:N | 1:187:A:VAL:CA | 1:187:A:VAL:C  | 1:188:A:ASN:N | 14       | 2.05          |
| (1,29)  | 2:207:B:ILE:C | 2:208:B:ASN:N  | 2:208:B:ASN:CA | 2:208:B:ASN:C | 13       | 2.05          |
| (1,284) | 2:323:B:LYS:N | 2:323:B:LYS:CA | 2:323:B:LYS:C  | 2:324:B:GLY:N | 9        | 2.03          |
| (1,194) | 2:225:B:LEU:N | 2:225:B:LEU:CA | 2:225:B:LEU:C  | 2:226:B:LYS:N | 8        | 2.03          |
| (1,29)  | 2:207:B:ILE:C | 2:208:B:ASN:N  | 2:208:B:ASN:CA | 2:208:B:ASN:C | 19       | 2.03          |
| (1,221) | 2:258:B:LYS:N | 2:258:B:LYS:CA | 2:258:B:LYS:C  | 2:259:B:ASN:N | 4        | 2.01          |
| (1,176) | 2:205:B:SER:N | 2:205:B:SER:CA | 2:205:B:SER:C  | 2:206:B:ALA:N | 15       | 2.01          |
| (1,151) | 2:341:B:ILE:C | 2:342:B:GLU:N  | 2:342:B:GLU:CA | 2:342:B:GLU:C | 4        | 2.01          |
| (1,295) | 2:334:B:SER:N | 2:334:B:SER:CA | 2:334:B:SER:C  | 2:335:B:SER:N | 1        | 2.0           |
| (1,176) | 2:205:B:SER:N | 2:205:B:SER:CA | 2:205:B:SER:C  | 2:206:B:ALA:N | 8        | 2.0           |
| (1,134) | 2:322:B:GLU:C | 2:323:B:LYS:N  | 2:323:B:LYS:CA | 2:323:B:LYS:C | 20       | 1.98          |
| (1,45)  | 2:225:B:LEU:C | 2:226:B:LYS:N  | 2:226:B:LYS:CA | 2:226:B:LYS:C | 8        | 1.98          |
| (1,299) | 2:339:B:ASP:N | 2:339:B:ASP:CA | 2:339:B:ASP:C  | 2:340:B:LEU:N | 13       | 1.95          |
| (1,189) | 2:218:B:LEU:N | 2:218:B:LEU:CA | 2:218:B:LEU:C  | 2:219:B:GLU:N | 1        | 1.95          |

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| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,194) | 2:225:B:LEU:N | 2:225:B:LEU:CA | 2:225:B:LEU:C  | 2:226:B:LYS:N | 20       | 1.94          |
| (1,21)  | 2:199:B:HIS:C | 2:200:B:LYS:N  | 2:200:B:LYS:CA | 2:200:B:LYS:C | 11       | 1.91          |
| (1,10)  | 1:187:A:VAL:C | 1:188:A:ASN:N  | 1:188:A:ASN:CA | 1:188:A:ASN:C | 9        | 1.91          |
| (1,186) | 2:215:B:LEU:N | 2:215:B:LEU:CA | 2:215:B:LEU:C  | 2:216:B:ASP:N | 16       | 1.9           |
| (1,19)  | 2:197:B:SER:C | 2:198:B:LYS:N  | 2:198:B:LYS:CA | 2:198:B:LYS:C | 4        | 1.88          |
| (1,10)  | 1:187:A:VAL:C | 1:188:A:ASN:N  | 1:188:A:ASN:CA | 1:188:A:ASN:C | 10       | 1.88          |
| (1,166) | 2:195:B:ILE:N | 2:195:B:ILE:CA | 2:195:B:ILE:C  | 2:196:B:ASN:N | 2        | 1.87          |
| (1,102) | 2:290:B:VAL:C | 2:291:B:HIS:N  | 2:291:B:HIS:CA | 2:291:B:HIS:C | 10       | 1.87          |
| (1,36)  | 2:214:B:VAL:C | 2:215:B:LEU:N  | 2:215:B:LEU:CA | 2:215:B:LEU:C | 14       | 1.87          |
| (1,45)  | 2:225:B:LEU:C | 2:226:B:LYS:N  | 2:226:B:LYS:CA | 2:226:B:LYS:C | 10       | 1.86          |
| (1,40)  | 2:218:B:LEU:C | 2:219:B:GLU:N  | 2:219:B:GLU:CA | 2:219:B:GLU:C | 1        | 1.86          |
| (1,257) | 2:296:B:VAL:N | 2:296:B:VAL:CA | 2:296:B:VAL:C  | 2:297:B:ASP:N | 15       | 1.84          |
| (1,186) | 2:215:B:LEU:N | 2:215:B:LEU:CA | 2:215:B:LEU:C  | 2:216:B:ASP:N | 10       | 1.83          |
| (1,62)  | 2:246:B:LYS:C | 2:247:B:ASN:N  | 2:247:B:ASN:CA | 2:247:B:ASN:C | 7        | 1.82          |
| (1,187) | 2:216:B:ASP:N | 2:216:B:ASP:CA | 2:216:B:ASP:C  | 2:217:B:GLY:N | 13       | 1.8           |
| (1,170) | 2:199:B:HIS:N | 2:199:B:HIS:CA | 2:199:B:HIS:C  | 2:200:B:LYS:N | 6        | 1.8           |
| (1,36)  | 2:214:B:VAL:C | 2:215:B:LEU:N  | 2:215:B:LEU:CA | 2:215:B:LEU:C | 3        | 1.8           |
| (1,299) | 2:339:B:ASP:N | 2:339:B:ASP:CA | 2:339:B:ASP:C  | 2:340:B:LEU:N | 1        | 1.79          |
| (1,176) | 2:205:B:SER:N | 2:205:B:SER:CA | 2:205:B:SER:C  | 2:206:B:ALA:N | 7        | 1.79          |
| (1,166) | 2:195:B:ILE:N | 2:195:B:ILE:CA | 2:195:B:ILE:C  | 2:196:B:ASN:N | 5        | 1.78          |
| (1,166) | 2:195:B:ILE:N | 2:195:B:ILE:CA | 2:195:B:ILE:C  | 2:196:B:ASN:N | 13       | 1.78          |
| (1,26)  | 2:204:B:THR:C | 2:205:B:SER:N  | 2:205:B:SER:CA | 2:205:B:SER:C | 8        | 1.78          |
| (1,19)  | 2:197:B:SER:C | 2:198:B:LYS:N  | 2:198:B:LYS:CA | 2:198:B:LYS:C | 20       | 1.78          |
| (1,99)  | 2:287:B:ASP:C | 2:288:B:THR:N  | 2:288:B:THR:CA | 2:288:B:THR:C | 13       | 1.77          |
| (1,248) | 2:287:B:ASP:N | 2:287:B:ASP:CA | 2:287:B:ASP:C  | 2:288:B:THR:N | 7        | 1.75          |
| (1,194) | 2:225:B:LEU:N | 2:225:B:LEU:CA | 2:225:B:LEU:C  | 2:226:B:LYS:N | 1        | 1.75          |
| (1,166) | 2:195:B:ILE:N | 2:195:B:ILE:CA | 2:195:B:ILE:C  | 2:196:B:ASN:N | 18       | 1.75          |
| (1,166) | 2:195:B:ILE:N | 2:195:B:ILE:CA | 2:195:B:ILE:C  | 2:196:B:ASN:N | 19       | 1.75          |
| (1,29)  | 2:207:B:ILE:C | 2:208:B:ASN:N  | 2:208:B:ASN:CA | 2:208:B:ASN:C | 5        | 1.75          |
| (1,10)  | 1:187:A:VAL:C | 1:188:A:ASN:N  | 1:188:A:ASN:CA | 1:188:A:ASN:C | 13       | 1.75          |
| (1,187) | 2:216:B:ASP:N | 2:216:B:ASP:CA | 2:216:B:ASP:C  | 2:217:B:GLY:N | 7        | 1.73          |
| (1,40)  | 2:218:B:LEU:C | 2:219:B:GLU:N  | 2:219:B:GLU:CA | 2:219:B:GLU:C | 10       | 1.73          |
| (1,26)  | 2:204:B:THR:C | 2:205:B:SER:N  | 2:205:B:SER:CA | 2:205:B:SER:C | 20       | 1.73          |
| (1,193) | 2:224:B:ASP:N | 2:224:B:ASP:CA | 2:224:B:ASP:C  | 2:225:B:LEU:N | 14       | 1.72          |
| (1,19)  | 2:197:B:SER:C | 2:198:B:LYS:N  | 2:198:B:LYS:CA | 2:198:B:LYS:C | 18       | 1.72          |
| (1,159) | 1:186:A:ASP:N | 1:186:A:ASP:CA | 1:186:A:ASP:C  | 1:187:A:VAL:N | 1        | 1.71          |
| (1,299) | 2:339:B:ASP:N | 2:339:B:ASP:CA | 2:339:B:ASP:C  | 2:340:B:LEU:N | 9        | 1.7           |
| (1,29)  | 2:207:B:ILE:C | 2:208:B:ASN:N  | 2:208:B:ASN:CA | 2:208:B:ASN:C | 20       | 1.7           |
| (1,61)  | 2:242:B:ILE:C | 2:243:B:SER:N  | 2:243:B:SER:CA | 2:243:B:SER:C | 19       | 1.69          |
| (1,10)  | 1:187:A:VAL:C | 1:188:A:ASN:N  | 1:188:A:ASN:CA | 1:188:A:ASN:C | 18       | 1.69          |
| (1,299) | 2:339:B:ASP:N | 2:339:B:ASP:CA | 2:339:B:ASP:C  | 2:340:B:LEU:N | 12       | 1.68          |
| (1,295) | 2:334:B:SER:N | 2:334:B:SER:CA | 2:334:B:SER:C  | 2:335:B:SER:N | 17       | 1.68          |
| (1,10)  | 1:187:A:VAL:C | 1:188:A:ASN:N  | 1:188:A:ASN:CA | 1:188:A:ASN:C | 20       | 1.68          |
| (1,40)  | 2:218:B:LEU:C | 2:219:B:GLU:N  | 2:219:B:GLU:CA | 2:219:B:GLU:C | 15       | 1.67          |
| (1,194) | 2:225:B:LEU:N | 2:225:B:LEU:CA | 2:225:B:LEU:C  | 2:226:B:LYS:N | 18       | 1.64          |
| (1,189) | 2:218:B:LEU:N | 2:218:B:LEU:CA | 2:218:B:LEU:C  | 2:219:B:GLU:N | 2        | 1.64          |
| (1,208) | 2:239:B:LEU:N | 2:239:B:LEU:CA | 2:239:B:LEU:C  | 2:240:B:GLY:N | 4        | 1.59          |
| (1,70)  | 2:256:B:ASN:C | 2:257:B:ASP:N  | 2:257:B:ASP:CA | 2:257:B:ASP:C | 4        | 1.59          |
| (1,29)  | 2:207:B:ILE:C | 2:208:B:ASN:N  | 2:208:B:ASN:CA | 2:208:B:ASN:C | 11       | 1.59          |
| (1,300) | 2:340:B:LEU:N | 2:340:B:LEU:CA | 2:340:B:LEU:C  | 2:341:B:ILE:N | 1        | 1.58          |
| (1,221) | 2:258:B:LYS:N | 2:258:B:LYS:CA | 2:258:B:LYS:C  | 2:259:B:ASN:N | 3        | 1.58          |

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| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,151) | 2:341:B:ILE:C | 2:342:B:GLU:N  | 2:342:B:GLU:CA | 2:342:B:GLU:C | 8        | 1.58          |
| (1,10)  | 1:187:A:VAL:C | 1:188:A:ASN:N  | 1:188:A:ASN:CA | 1:188:A:ASN:C | 4        | 1.58          |
| (1,99)  | 2:287:B:ASP:C | 2:288:B:THR:N  | 2:288:B:THR:CA | 2:288:B:THR:C | 14       | 1.55          |
| (1,29)  | 2:207:B:ILE:C | 2:208:B:ASN:N  | 2:208:B:ASN:CA | 2:208:B:ASN:C | 9        | 1.55          |
| (1,295) | 2:334:B:SER:N | 2:334:B:SER:CA | 2:334:B:SER:C  | 2:335:B:SER:N | 18       | 1.54          |
| (1,166) | 2:195:B:ILE:N | 2:195:B:ILE:CA | 2:195:B:ILE:C  | 2:196:B:ASN:N | 20       | 1.54          |
| (1,63)  | 2:247:B:ASN:C | 2:248:B:TYR:N  | 2:248:B:TYR:CA | 2:248:B:TYR:C | 13       | 1.54          |
| (1,45)  | 2:225:B:LEU:C | 2:226:B:LYS:N  | 2:226:B:LYS:CA | 2:226:B:LYS:C | 13       | 1.54          |
| (1,2)   | 1:179:A:GLU:C | 1:180:A:TYR:N  | 1:180:A:TYR:CA | 1:180:A:TYR:C | 6        | 1.54          |
| (1,284) | 2:323:B:LYS:N | 2:323:B:LYS:CA | 2:323:B:LYS:C  | 2:324:B:GLY:N | 14       | 1.53          |
| (1,284) | 2:323:B:LYS:N | 2:323:B:LYS:CA | 2:323:B:LYS:C  | 2:324:B:GLY:N | 18       | 1.53          |
| (1,61)  | 2:242:B:ILE:C | 2:243:B:SER:N  | 2:243:B:SER:CA | 2:243:B:SER:C | 11       | 1.53          |
| (1,40)  | 2:218:B:LEU:C | 2:219:B:GLU:N  | 2:219:B:GLU:CA | 2:219:B:GLU:C | 17       | 1.52          |
| (1,186) | 2:215:B:LEU:N | 2:215:B:LEU:CA | 2:215:B:LEU:C  | 2:216:B:ASP:N | 17       | 1.5           |
| (1,166) | 2:195:B:ILE:N | 2:195:B:ILE:CA | 2:195:B:ILE:C  | 2:196:B:ASN:N | 14       | 1.5           |
| (1,10)  | 1:187:A:VAL:C | 1:188:A:ASN:N  | 1:188:A:ASN:CA | 1:188:A:ASN:C | 2        | 1.5           |
| (1,208) | 2:239:B:LEU:N | 2:239:B:LEU:CA | 2:239:B:LEU:C  | 2:240:B:GLY:N | 5        | 1.49          |
| (1,166) | 2:195:B:ILE:N | 2:195:B:ILE:CA | 2:195:B:ILE:C  | 2:196:B:ASN:N | 7        | 1.49          |
| (1,39)  | 2:217:B:GLY:C | 2:218:B:LEU:N  | 2:218:B:LEU:CA | 2:218:B:LEU:C | 15       | 1.49          |
| (1,214) | 2:249:B:VAL:N | 2:249:B:VAL:CA | 2:249:B:VAL:C  | 2:250:B:LEU:N | 8        | 1.47          |
| (1,70)  | 2:256:B:ASN:C | 2:257:B:ASP:N  | 2:257:B:ASP:CA | 2:257:B:ASP:C | 2        | 1.47          |
| (1,299) | 2:339:B:ASP:N | 2:339:B:ASP:CA | 2:339:B:ASP:C  | 2:340:B:LEU:N | 16       | 1.46          |
| (1,193) | 2:224:B:ASP:N | 2:224:B:ASP:CA | 2:224:B:ASP:C  | 2:225:B:LEU:N | 19       | 1.46          |
| (1,75)  | 2:261:B:LYS:C | 2:262:B:THR:N  | 2:262:B:THR:CA | 2:262:B:THR:C | 18       | 1.46          |
| (1,29)  | 2:207:B:ILE:C | 2:208:B:ASN:N  | 2:208:B:ASN:CA | 2:208:B:ASN:C | 17       | 1.46          |
| (1,176) | 2:205:B:SER:N | 2:205:B:SER:CA | 2:205:B:SER:C  | 2:206:B:ALA:N | 3        | 1.43          |
| (1,40)  | 2:218:B:LEU:C | 2:219:B:GLU:N  | 2:219:B:GLU:CA | 2:219:B:GLU:C | 2        | 1.43          |
| (1,36)  | 2:214:B:VAL:C | 2:215:B:LEU:N  | 2:215:B:LEU:CA | 2:215:B:LEU:C | 4        | 1.43          |
| (1,75)  | 2:261:B:LYS:C | 2:262:B:THR:N  | 2:262:B:THR:CA | 2:262:B:THR:C | 13       | 1.42          |
| (1,26)  | 2:204:B:THR:C | 2:205:B:SER:N  | 2:205:B:SER:CA | 2:205:B:SER:C | 9        | 1.42          |
| (1,40)  | 2:218:B:LEU:C | 2:219:B:GLU:N  | 2:219:B:GLU:CA | 2:219:B:GLU:C | 19       | 1.41          |
| (1,26)  | 2:204:B:THR:C | 2:205:B:SER:N  | 2:205:B:SER:CA | 2:205:B:SER:C | 13       | 1.41          |
| (1,26)  | 2:204:B:THR:C | 2:205:B:SER:N  | 2:205:B:SER:CA | 2:205:B:SER:C | 16       | 1.41          |
| (1,10)  | 1:187:A:VAL:C | 1:188:A:ASN:N  | 1:188:A:ASN:CA | 1:188:A:ASN:C | 11       | 1.4           |
| (1,257) | 2:296:B:VAL:N | 2:296:B:VAL:CA | 2:296:B:VAL:C  | 2:297:B:ASP:N | 1        | 1.39          |
| (1,159) | 1:186:A:ASP:N | 1:186:A:ASP:CA | 1:186:A:ASP:C  | 1:187:A:VAL:N | 15       | 1.39          |
| (1,29)  | 2:207:B:ILE:C | 2:208:B:ASN:N  | 2:208:B:ASN:CA | 2:208:B:ASN:C | 18       | 1.39          |
| (1,187) | 2:216:B:ASP:N | 2:216:B:ASP:CA | 2:216:B:ASP:C  | 2:217:B:GLY:N | 4        | 1.38          |
| (1,102) | 2:290:B:VAL:C | 2:291:B:HIS:N  | 2:291:B:HIS:CA | 2:291:B:HIS:C | 11       | 1.38          |
| (1,288) | 2:327:B:ILE:N | 2:327:B:ILE:CA | 2:327:B:ILE:C  | 2:328:B:THR:N | 6        | 1.37          |
| (1,45)  | 2:225:B:LEU:C | 2:226:B:LYS:N  | 2:226:B:LYS:CA | 2:226:B:LYS:C | 15       | 1.37          |
| (1,40)  | 2:218:B:LEU:C | 2:219:B:GLU:N  | 2:219:B:GLU:CA | 2:219:B:GLU:C | 7        | 1.37          |
| (1,289) | 2:328:B:THR:N | 2:328:B:THR:CA | 2:328:B:THR:C  | 2:329:B:ILE:N | 3        | 1.36          |
| (1,227) | 2:265:B:LYS:N | 2:265:B:LYS:CA | 2:265:B:LYS:C  | 2:266:B:ARG:N | 16       | 1.36          |
| (1,164) | 2:193:B:PHE:N | 2:193:B:PHE:CA | 2:193:B:PHE:C  | 2:194:B:THR:N | 17       | 1.36          |
| (1,22)  | 2:200:B:LYS:C | 2:201:B:VAL:N  | 2:201:B:VAL:CA | 2:201:B:VAL:C | 11       | 1.36          |
| (1,10)  | 1:187:A:VAL:C | 1:188:A:ASN:N  | 1:188:A:ASN:CA | 1:188:A:ASN:C | 17       | 1.36          |
| (1,75)  | 2:261:B:LYS:C | 2:262:B:THR:N  | 2:262:B:THR:CA | 2:262:B:THR:C | 1        | 1.35          |
| (1,11)  | 2:189:B:PRO:C | 2:190:B:SER:N  | 2:190:B:SER:CA | 2:190:B:SER:C | 6        | 1.35          |
| (1,166) | 2:195:B:ILE:N | 2:195:B:ILE:CA | 2:195:B:ILE:C  | 2:196:B:ASN:N | 16       | 1.34          |
| (1,29)  | 2:207:B:ILE:C | 2:208:B:ASN:N  | 2:208:B:ASN:CA | 2:208:B:ASN:C | 4        | 1.34          |

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| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,160) | 1:187:A:VAL:N | 1:187:A:VAL:CA | 1:187:A:VAL:C  | 1:188:A:ASN:N | 2        | 1.33          |
| (1,102) | 2:290:B:VAL:C | 2:291:B:HIS:N  | 2:291:B:HIS:CA | 2:291:B:HIS:C | 1        | 1.33          |
| (1,190) | 2:219:B:GLU:N | 2:219:B:GLU:CA | 2:219:B:GLU:C  | 2:220:B:LEU:N | 5        | 1.32          |
| (1,26)  | 2:204:B:THR:C | 2:205:B:SER:N  | 2:205:B:SER:CA | 2:205:B:SER:C | 18       | 1.32          |
| (1,214) | 2:249:B:VAL:N | 2:249:B:VAL:CA | 2:249:B:VAL:C  | 2:250:B:LEU:N | 19       | 1.31          |
| (1,70)  | 2:256:B:ASN:C | 2:257:B:ASP:N  | 2:257:B:ASP:CA | 2:257:B:ASP:C | 3        | 1.31          |
| (1,45)  | 2:225:B:LEU:C | 2:226:B:LYS:N  | 2:226:B:LYS:CA | 2:226:B:LYS:C | 1        | 1.31          |
| (1,194) | 2:225:B:LEU:N | 2:225:B:LEU:CA | 2:225:B:LEU:C  | 2:226:B:LYS:N | 11       | 1.3           |
| (1,175) | 2:204:B:THR:N | 2:204:B:THR:CA | 2:204:B:THR:C  | 2:205:B:SER:N | 3        | 1.29          |
| (1,21)  | 2:199:B:HIS:C | 2:200:B:LYS:N  | 2:200:B:LYS:CA | 2:200:B:LYS:C | 3        | 1.29          |
| (1,19)  | 2:197:B:SER:C | 2:198:B:LYS:N  | 2:198:B:LYS:CA | 2:198:B:LYS:C | 12       | 1.29          |
| (1,299) | 2:339:B:ASP:N | 2:339:B:ASP:CA | 2:339:B:ASP:C  | 2:340:B:LEU:N | 10       | 1.28          |
| (1,159) | 1:186:A:ASP:N | 1:186:A:ASP:CA | 1:186:A:ASP:C  | 1:187:A:VAL:N | 10       | 1.27          |
| (1,26)  | 2:204:B:THR:C | 2:205:B:SER:N  | 2:205:B:SER:CA | 2:205:B:SER:C | 7        | 1.27          |
| (1,295) | 2:334:B:SER:N | 2:334:B:SER:CA | 2:334:B:SER:C  | 2:335:B:SER:N | 15       | 1.25          |
| (1,75)  | 2:261:B:LYS:C | 2:262:B:THR:N  | 2:262:B:THR:CA | 2:262:B:THR:C | 5        | 1.25          |
| (1,70)  | 2:256:B:ASN:C | 2:257:B:ASP:N  | 2:257:B:ASP:CA | 2:257:B:ASP:C | 18       | 1.25          |
| (1,186) | 2:215:B:LEU:N | 2:215:B:LEU:CA | 2:215:B:LEU:C  | 2:216:B:ASP:N | 15       | 1.24          |
| (1,99)  | 2:287:B:ASP:C | 2:288:B:THR:N  | 2:288:B:THR:CA | 2:288:B:THR:C | 19       | 1.24          |
| (1,39)  | 2:217:B:GLY:C | 2:218:B:LEU:N  | 2:218:B:LEU:CA | 2:218:B:LEU:C | 4        | 1.23          |
| (1,23)  | 2:201:B:VAL:C | 2:202:B:ILE:N  | 2:202:B:ILE:CA | 2:202:B:ILE:C | 19       | 1.23          |
| (1,11)  | 2:189:B:PRO:C | 2:190:B:SER:N  | 2:190:B:SER:CA | 2:190:B:SER:C | 8        | 1.23          |
| (1,193) | 2:224:B:ASP:N | 2:224:B:ASP:CA | 2:224:B:ASP:C  | 2:225:B:LEU:N | 5        | 1.22          |
| (1,186) | 2:215:B:LEU:N | 2:215:B:LEU:CA | 2:215:B:LEU:C  | 2:216:B:ASP:N | 5        | 1.22          |
| (1,219) | 2:254:B:ALA:N | 2:254:B:ALA:CA | 2:254:B:ALA:C  | 2:255:B:LEU:N | 19       | 1.21          |
| (1,100) | 2:288:B:THR:C | 2:289:B:ILE:N  | 2:289:B:ILE:CA | 2:289:B:ILE:C | 10       | 1.21          |
| (1,221) | 2:258:B:LYS:N | 2:258:B:LYS:CA | 2:258:B:LYS:C  | 2:259:B:ASN:N | 15       | 1.2           |
| (1,70)  | 2:256:B:ASN:C | 2:257:B:ASP:N  | 2:257:B:ASP:CA | 2:257:B:ASP:C | 14       | 1.2           |
| (1,164) | 2:193:B:PHE:N | 2:193:B:PHE:CA | 2:193:B:PHE:C  | 2:194:B:THR:N | 9        | 1.18          |
| (1,36)  | 2:214:B:VAL:C | 2:215:B:LEU:N  | 2:215:B:LEU:CA | 2:215:B:LEU:C | 20       | 1.17          |
| (1,146) | 2:334:B:SER:C | 2:335:B:SER:N  | 2:335:B:SER:CA | 2:335:B:SER:C | 3        | 1.16          |
| (1,29)  | 2:207:B:ILE:C | 2:208:B:ASN:N  | 2:208:B:ASN:CA | 2:208:B:ASN:C | 6        | 1.16          |
| (1,10)  | 1:187:A:VAL:C | 1:188:A:ASN:N  | 1:188:A:ASN:CA | 1:188:A:ASN:C | 15       | 1.16          |
| (1,189) | 2:218:B:LEU:N | 2:218:B:LEU:CA | 2:218:B:LEU:C  | 2:219:B:GLU:N | 10       | 1.15          |
| (1,26)  | 2:204:B:THR:C | 2:205:B:SER:N  | 2:205:B:SER:CA | 2:205:B:SER:C | 15       | 1.15          |
| (1,151) | 2:341:B:ILE:C | 2:342:B:GLU:N  | 2:342:B:GLU:CA | 2:342:B:GLU:C | 15       | 1.14          |
| (1,145) | 2:333:B:LYS:C | 2:334:B:SER:N  | 2:334:B:SER:CA | 2:334:B:SER:C | 13       | 1.14          |
| (1,75)  | 2:261:B:LYS:C | 2:262:B:THR:N  | 2:262:B:THR:CA | 2:262:B:THR:C | 3        | 1.14          |
| (1,208) | 2:239:B:LEU:N | 2:239:B:LEU:CA | 2:239:B:LEU:C  | 2:240:B:GLY:N | 6        | 1.13          |
| (1,164) | 2:193:B:PHE:N | 2:193:B:PHE:CA | 2:193:B:PHE:C  | 2:194:B:THR:N | 8        | 1.13          |
| (1,70)  | 2:256:B:ASN:C | 2:257:B:ASP:N  | 2:257:B:ASP:CA | 2:257:B:ASP:C | 5        | 1.13          |
| (1,2)   | 1:179:A:GLU:C | 1:180:A:TYR:N  | 1:180:A:TYR:CA | 1:180:A:TYR:C | 5        | 1.13          |
| (1,295) | 2:334:B:SER:N | 2:334:B:SER:CA | 2:334:B:SER:C  | 2:335:B:SER:N | 8        | 1.12          |
| (1,176) | 2:205:B:SER:N | 2:205:B:SER:CA | 2:205:B:SER:C  | 2:206:B:ALA:N | 14       | 1.12          |
| (1,299) | 2:339:B:ASP:N | 2:339:B:ASP:CA | 2:339:B:ASP:C  | 2:340:B:LEU:N | 5        | 1.11          |
| (1,214) | 2:249:B:VAL:N | 2:249:B:VAL:CA | 2:249:B:VAL:C  | 2:250:B:LEU:N | 13       | 1.11          |
| (1,10)  | 1:187:A:VAL:C | 1:188:A:ASN:N  | 1:188:A:ASN:CA | 1:188:A:ASN:C | 14       | 1.11          |
| (1,218) | 2:253:B:MET:N | 2:253:B:MET:CA | 2:253:B:MET:C  | 2:254:B:ALA:N | 19       | 1.1           |
| (1,208) | 2:239:B:LEU:N | 2:239:B:LEU:CA | 2:239:B:LEU:C  | 2:240:B:GLY:N | 11       | 1.1           |
| (1,70)  | 2:256:B:ASN:C | 2:257:B:ASP:N  | 2:257:B:ASP:CA | 2:257:B:ASP:C | 6        | 1.1           |
| (1,300) | 2:340:B:LEU:N | 2:340:B:LEU:CA | 2:340:B:LEU:C  | 2:341:B:ILE:N | 10       | 1.09          |

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| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,218) | 2:253:B:MET:N | 2:253:B:MET:CA | 2:253:B:MET:C  | 2:254:B:ALA:N | 8        | 1.09          |
| (1,189) | 2:218:B:LEU:N | 2:218:B:LEU:CA | 2:218:B:LEU:C  | 2:219:B:GLU:N | 9        | 1.09          |
| (1,187) | 2:216:B:ASP:N | 2:216:B:ASP:CA | 2:216:B:ASP:C  | 2:217:B:GLY:N | 17       | 1.09          |
| (1,248) | 2:287:B:ASP:N | 2:287:B:ASP:CA | 2:287:B:ASP:C  | 2:288:B:THR:N | 1        | 1.08          |
| (1,186) | 2:215:B:LEU:N | 2:215:B:LEU:CA | 2:215:B:LEU:C  | 2:216:B:ASP:N | 3        | 1.08          |
| (1,152) | 1:179:A:GLU:N | 1:179:A:GLU:CA | 1:179:A:GLU:C  | 1:180:A:TYR:N | 3        | 1.08          |
| (1,65)  | 2:249:B:VAL:C | 2:250:B:LEU:N  | 2:250:B:LEU:CA | 2:250:B:LEU:C | 15       | 1.08          |
| (1,257) | 2:296:B:VAL:N | 2:296:B:VAL:CA | 2:296:B:VAL:C  | 2:297:B:ASP:N | 7        | 1.07          |
| (1,216) | 2:251:B:VAL:N | 2:251:B:VAL:CA | 2:251:B:VAL:C  | 2:252:B:SER:N | 19       | 1.07          |
| (1,36)  | 2:214:B:VAL:C | 2:215:B:LEU:N  | 2:215:B:LEU:CA | 2:215:B:LEU:C | 9        | 1.07          |
| (1,186) | 2:215:B:LEU:N | 2:215:B:LEU:CA | 2:215:B:LEU:C  | 2:216:B:ASP:N | 13       | 1.06          |
| (1,99)  | 2:287:B:ASP:C | 2:288:B:THR:N  | 2:288:B:THR:CA | 2:288:B:THR:C | 6        | 1.05          |
| (1,257) | 2:296:B:VAL:N | 2:296:B:VAL:CA | 2:296:B:VAL:C  | 2:297:B:ASP:N | 20       | 1.04          |
| (1,193) | 2:224:B:ASP:N | 2:224:B:ASP:CA | 2:224:B:ASP:C  | 2:225:B:LEU:N | 18       | 1.04          |
| (1,164) | 2:193:B:PHE:N | 2:193:B:PHE:CA | 2:193:B:PHE:C  | 2:194:B:THR:N | 6        | 1.04          |
| (1,285) | 2:324:B:GLY:N | 2:324:B:GLY:CA | 2:324:B:GLY:C  | 2:325:B:MET:N | 16       | 1.03          |
| (1,26)  | 2:204:B:THR:C | 2:205:B:SER:N  | 2:205:B:SER:CA | 2:205:B:SER:C | 2        | 1.03          |
| (1,289) | 2:328:B:THR:N | 2:328:B:THR:CA | 2:328:B:THR:C  | 2:329:B:ILE:N | 14       | 1.02          |
| (1,186) | 2:215:B:LEU:N | 2:215:B:LEU:CA | 2:215:B:LEU:C  | 2:216:B:ASP:N | 11       | 1.02          |
| (1,61)  | 2:242:B:ILE:C | 2:243:B:SER:N  | 2:243:B:SER:CA | 2:243:B:SER:C | 15       | 1.02          |
| (1,40)  | 2:218:B:LEU:C | 2:219:B:GLU:N  | 2:219:B:GLU:CA | 2:219:B:GLU:C | 13       | 1.02          |
| (1,208) | 2:239:B:LEU:N | 2:239:B:LEU:CA | 2:239:B:LEU:C  | 2:240:B:GLY:N | 9        | 1.01          |