



# Full wwPDB NMR Structure Validation Report ⓘ

Mar 1, 2026 – 11:05 AM UTC

PDB ID : 2N5X / pdb\_00002n5x  
BMRB ID : 25740  
Title : C-terminal domain of Cdc37 cochaperone  
Authors : Keramisanou, D.; Dudhat, A.; Pare, M.  
Deposited on : 2015-08-02

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

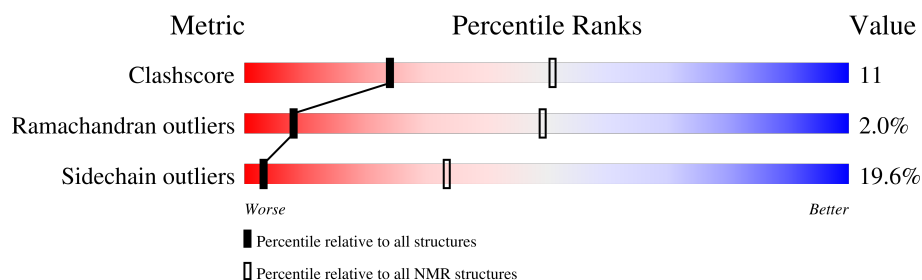
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 90%.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



| Metric                | Whole archive<br>(#Entries) | NMR archive<br>(#Entries) |
|-----------------------|-----------------------------|---------------------------|
| Clashscore            | 229148                      | 14424                     |
| Ramachandran outliers | 224038                      | 12848                     |
| Sidechain outliers    | 223484                      | 12823                     |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$

| Mol | Chain | Length | Quality of chain                                                       |
|-----|-------|--------|------------------------------------------------------------------------|
| 1   | A     | 94     | <div> <div>35%</div> <div>16%</div> <div>.</div> <div>48%</div> </div> |

## 2 Ensemble composition and analysis

This entry contains 10 models. Model 10 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:292-A:340 (49)      | 0.21              | 10           |

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 2 clusters. No single-model clusters were found.

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

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1390 atoms, of which 680 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Hsp90 co-chaperone Cdc37.

| Mol | Chain | Residues | Atoms |     |     |     |     |   | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|-------|
| 1   | A     | 94       | Total | C   | H   | N   | O   | S | 0     |
|     |       |          | 1390  | 440 | 680 | 115 | 149 | 6 |       |

There are 3 discrepancies between the modelled and reference sequences:

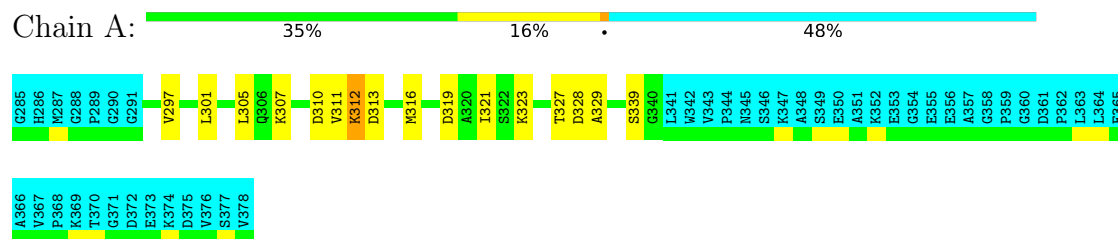
| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | 285     | GLY      | -      | expression tag | UNP Q16543 |
| A     | 286     | HIS      | -      | expression tag | UNP Q16543 |
| A     | 287     | MET      | -      | expression tag | UNP Q16543 |

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

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

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

- Molecule 1: Hsp90 co-chaperone Cdc37

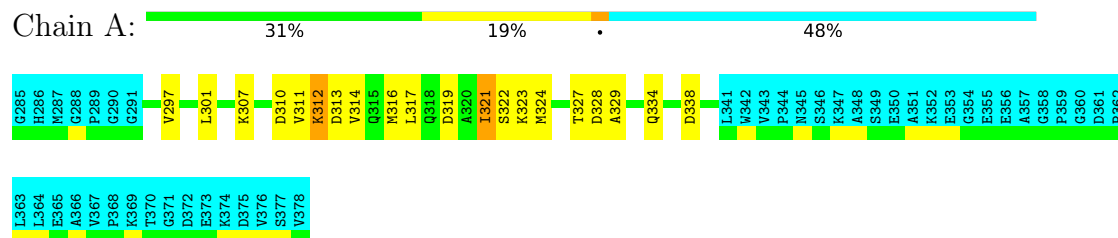


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

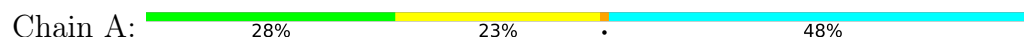
#### 4.2.1 Score per residue for model 1

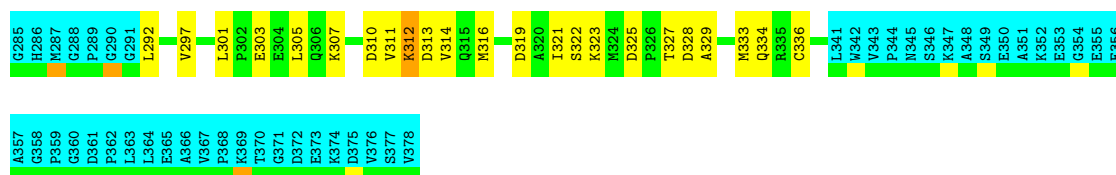
- Molecule 1: Hsp90 co-chaperone Cdc37



#### 4.2.2 Score per residue for model 2

- Molecule 1: Hsp90 co-chaperone Cdc37





#### 4.2.3 Score per residue for model 3

- Molecule 1: Hsp90 co-chaperone Cdc37

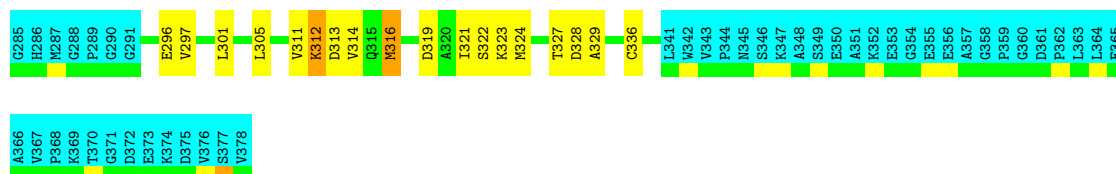
Chain A: 31% 20% 48%



#### 4.2.4 Score per residue for model 4

- Molecule 1: Hsp90 co-chaperone Cdc37

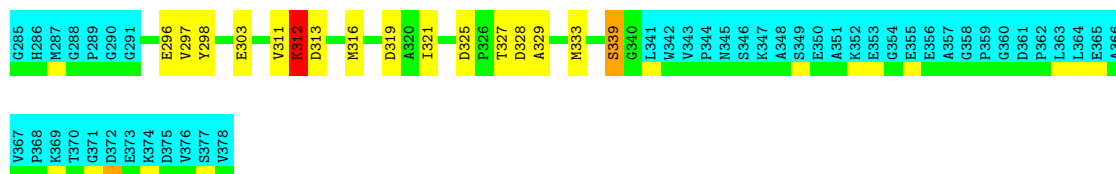
Chain A: 33% 17% 48%



#### 4.2.5 Score per residue for model 5

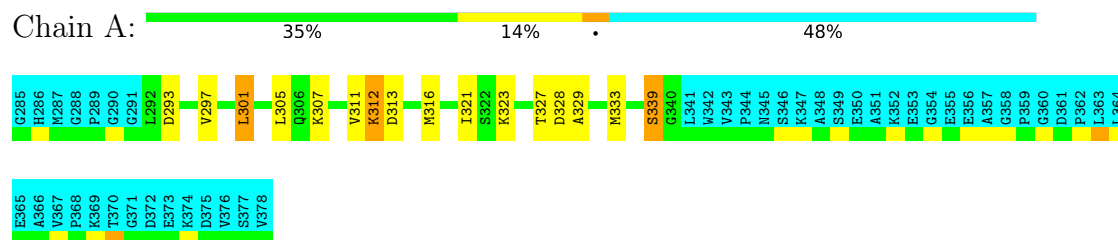
- Molecule 1: Hsp90 co-chaperone Cdc37

Chain A: 35% 15% 48%



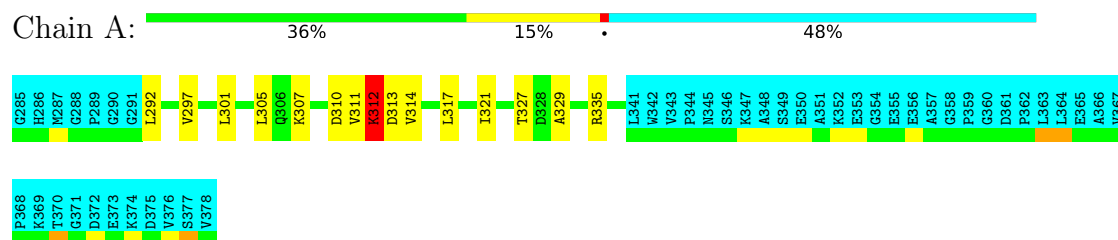
#### 4.2.6 Score per residue for model 6

- Molecule 1: Hsp90 co-chaperone Cdc37



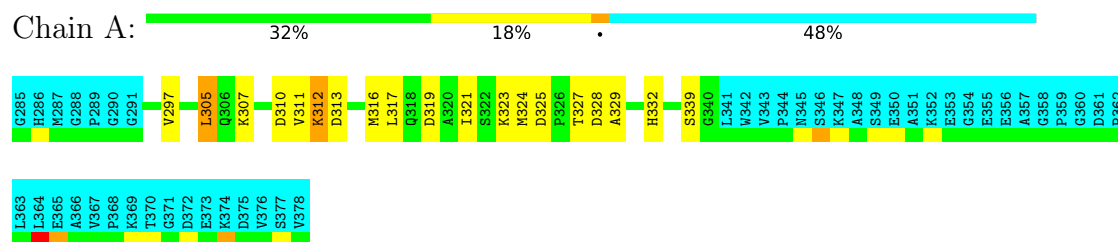
#### 4.2.7 Score per residue for model 7

- Molecule 1: Hsp90 co-chaperone Cdc37



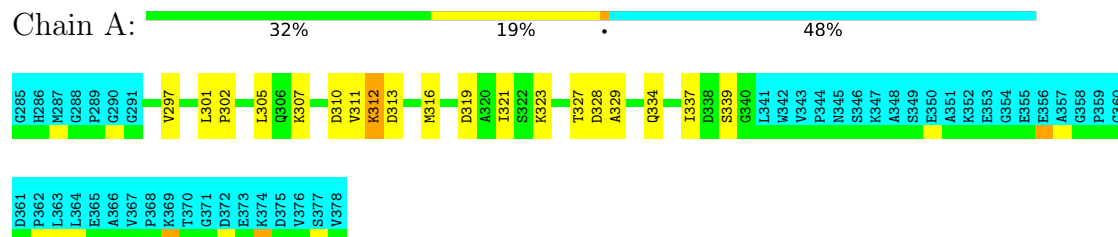
#### 4.2.8 Score per residue for model 8

- Molecule 1: Hsp90 co-chaperone Cdc37



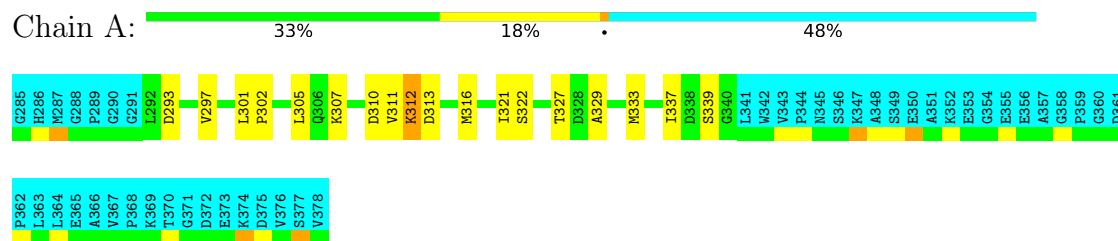
#### 4.2.9 Score per residue for model 9

- Molecule 1: Hsp90 co-chaperone Cdc37



#### 4.2.10 Score per residue for model 10 (medoid)

- Molecule 1: Hsp90 co-chaperone Cdc37



## 5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 10 were deposited, based on the following criterion: *structures with the lowest energy*.

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

| Software name | Classification     | Version |
|---------------|--------------------|---------|
| CYANA         | structure solution | 3.97    |
| CYANA         | 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                       | 1020           |
| Number of shifts mapped to atoms             | 1020           |
| Number of unparsed shifts                    | 0              |
| Number of shifts with mapping errors         | 0              |
| Number of shifts with mapping warnings       | 0              |
| Assignment completeness (well-defined parts) | 90%            |

## 6 Model quality [i](#)

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

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes |
|-----|-------|-------|----------|----------|---------|
| 1   | A     | 392   | 378      | 378      | 8±2     |
| All | All   | 3920  | 3780     | 3780     | 83      |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

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

| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:321:ILE:HG21 | 1:A:333:MET:HE3  | 0.70     | 1.63        | 10     | 3     |
| 1:A:317:LEU:O    | 1:A:321:ILE:HD12 | 0.63     | 1.93        | 1      | 4     |
| 1:A:321:ILE:HG23 | 1:A:329:ALA:HB1  | 0.61     | 1.71        | 3      | 6     |
| 1:A:321:ILE:HG21 | 1:A:333:MET:CE   | 0.60     | 2.24        | 10     | 3     |
| 1:A:292:LEU:HD13 | 1:A:338:ASP:HB3  | 0.60     | 1.72        | 3      | 1     |
| 1:A:321:ILE:HG23 | 1:A:329:ALA:CB   | 0.60     | 2.27        | 7      | 10    |
| 1:A:311:VAL:O    | 1:A:313:ASP:N    | 0.59     | 2.36        | 7      | 10    |
| 1:A:297:VAL:O    | 1:A:301:LEU:HD13 | 0.56     | 2.00        | 10     | 8     |
| 1:A:297:VAL:HG21 | 1:A:339:SER:HB3  | 0.54     | 1.79        | 5      | 5     |
| 1:A:301:LEU:HD23 | 1:A:305:LEU:HB3  | 0.53     | 1.79        | 3      | 4     |
| 1:A:311:VAL:O    | 1:A:312:LYS:C    | 0.52     | 2.51        | 7      | 10    |
| 1:A:316:MET:O    | 1:A:316:MET:HE2  | 0.52     | 2.04        | 4      | 1     |
| 1:A:305:LEU:HD11 | 1:A:332:HIS:CE1  | 0.49     | 2.42        | 8      | 1     |
| 1:A:311:VAL:C    | 1:A:313:ASP:N    | 0.49     | 2.70        | 7      | 10    |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:292:LEU:HD21 | 1:A:335:ARG:NH1  | 0.48     | 2.23        | 7      | 1     |
| 1:A:302:PRO:HG2  | 1:A:305:LEU:HD23 | 0.47     | 1.87        | 9      | 2     |
| 1:A:301:LEU:HD23 | 1:A:305:LEU:HD12 | 0.45     | 1.87        | 2      | 1     |
| 1:A:334:GLN:HA   | 1:A:337:ILE:HD12 | 0.42     | 1.91        | 9      | 1     |
| 1:A:292:LEU:HD13 | 1:A:338:ASP:CB   | 0.42     | 2.43        | 3      | 1     |
| 1:A:297:VAL:HG21 | 1:A:339:SER:CB   | 0.42     | 2.44        | 9      | 1     |

## 6.3 Torsion angles [i](#)

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

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

| Mol | Chain | Analysed      | Favoured     | Allowed    | Outliers   | Percentiles |    |
|-----|-------|---------------|--------------|------------|------------|-------------|----|
| 1   | A     | 49/94 (52%)   | 47±0 (95±1%) | 1±0 (3±1%) | 1±0 (2±0%) | 8           | 49 |
| All | All   | 490/940 (52%) | 466 (95%)    | 14 (3%)    | 10 (2%)    | 8           | 49 |

All 1 unique Ramachandran outliers are listed below.

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 312 | LYS  | 10             |

### 6.3.2 Protein sidechains [i](#)

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     | 46/79 (58%)   | 37±2 (80±5%) | 9±2 (20±5%) | 3           | 33 |
| All | All   | 460/790 (58%) | 370 (80%)    | 90 (20%)    | 3           | 33 |

All 23 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 327 | THR  | 10             |
| 1   | A     | 316 | MET  | 9              |
| 1   | A     | 307 | LYS  | 8              |
| 1   | A     | 328 | ASP  | 8              |
| 1   | A     | 310 | ASP  | 7              |
| 1   | A     | 323 | LYS  | 7              |
| 1   | A     | 319 | ASP  | 6              |
| 1   | A     | 322 | SER  | 4              |
| 1   | A     | 324 | MET  | 4              |
| 1   | A     | 325 | ASP  | 4              |
| 1   | A     | 312 | LYS  | 3              |
| 1   | A     | 305 | LEU  | 3              |
| 1   | A     | 334 | GLN  | 2              |
| 1   | A     | 303 | GLU  | 2              |
| 1   | A     | 336 | CYS  | 2              |
| 1   | A     | 296 | GLU  | 2              |
| 1   | A     | 339 | SER  | 2              |
| 1   | A     | 293 | ASP  | 2              |
| 1   | A     | 321 | ILE  | 1              |
| 1   | A     | 333 | MET  | 1              |
| 1   | A     | 315 | GLN  | 1              |
| 1   | A     | 301 | LEU  | 1              |
| 1   | A     | 314 | VAL  | 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 90% for the well-defined parts and 86% for the entire structure.

### 7.1 Chemical shift list 1

File name: working\_cs.cif

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

#### 7.1.1 Bookkeeping

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

|                                         |      |
|-----------------------------------------|------|
| Total number of shifts                  | 1020 |
| Number of shifts mapped to atoms        | 1020 |
| Number of unparsed shifts               | 0    |
| Number of shifts with mapping errors    | 0    |
| Number of shifts with mapping warnings  | 0    |
| Number of shift outliers (ShiftChecker) | 0    |

#### 7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

| Nucleus                | # values | Correction $\pm$ precision, ppm | Suggested action           |
|------------------------|----------|---------------------------------|----------------------------|
| $^{13}\text{C}_\alpha$ | 84       | $-0.22 \pm 0.10$                | None needed ( $< 0.5$ ppm) |
| $^{13}\text{C}_\beta$  | 77       | $0.01 \pm 0.09$                 | None needed ( $< 0.5$ ppm) |
| $^{13}\text{C}'$       | 79       | $-0.34 \pm 0.11$                | None needed ( $< 0.5$ ppm) |
| $^{15}\text{N}$        | 80       | $-0.39 \pm 0.45$                | None needed ( $< 0.5$ ppm) |

#### 7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 90%, i.e. 590 atoms were assigned a chemical shift out of a possible 657. 0 out of 8 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total         | $^1\text{H}$  | $^{13}\text{C}$ | $^{15}\text{N}$ |
|-----------|---------------|---------------|-----------------|-----------------|
| Backbone  | 235/240 (98%) | 95/96 (99%)   | 94/98 (96%)     | 46/46 (100%)    |
| Sidechain | 338/382 (88%) | 231/246 (94%) | 103/125 (82%)   | 4/11 (36%)      |

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|          | Total         | <sup>1</sup> H | <sup>13</sup> C | <sup>15</sup> N |
|----------|---------------|----------------|-----------------|-----------------|
| Aromatic | 17/35 (49%)   | 9/17 (53%)     | 8/17 (47%)      | 0/1 (0%)        |
| Overall  | 590/657 (90%) | 335/359 (93%)  | 205/240 (85%)   | 50/58 (86%)     |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 86%, i.e. 1020 atoms were assigned a chemical shift out of a possible 1183. 0 out of 15 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total           | <sup>1</sup> H | <sup>13</sup> C | <sup>15</sup> N |
|-----------|-----------------|----------------|-----------------|-----------------|
| Backbone  | 417/463 (90%)   | 174/189 (92%)  | 163/188 (87%)   | 80/86 (93%)     |
| Sidechain | 574/666 (86%)   | 394/430 (92%)  | 175/220 (80%)   | 5/16 (31%)      |
| Aromatic  | 29/54 (54%)     | 15/27 (56%)    | 13/24 (54%)     | 1/3 (33%)       |
| Overall   | 1020/1183 (86%) | 583/646 (90%)  | 351/432 (81%)   | 86/105 (82%)    |

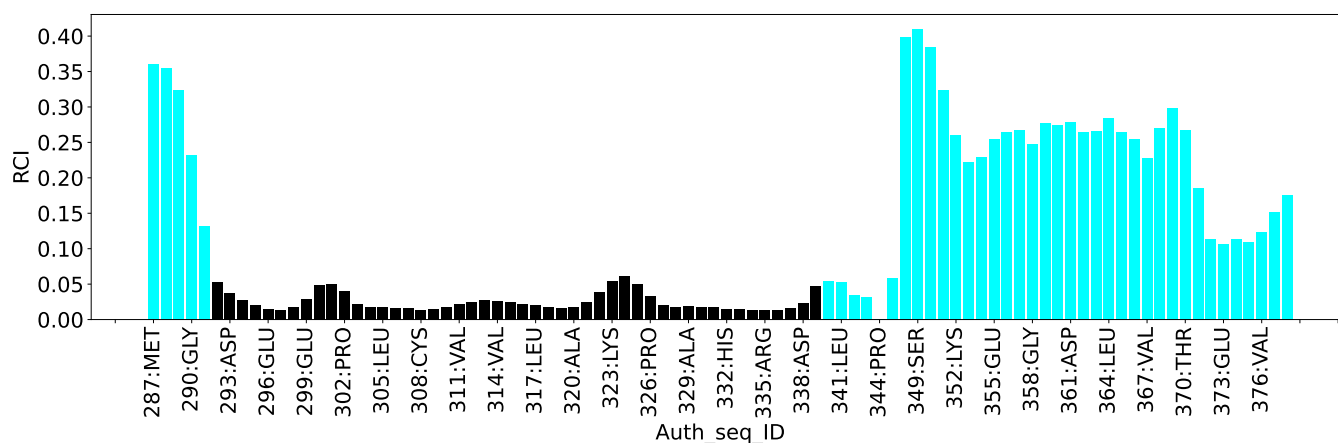
#### 7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

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

Random coil index (RCI) for chain A:



## 8 NMR restraints analysis

### 8.1 Conformationally restricting restraints

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

| Description                                              | Value |
|----------------------------------------------------------|-------|
| Total distance restraints                                | 934   |
| Intra-residue ( $ i-j =0$ )                              | 204   |
| Sequential ( $ i-j =1$ )                                 | 249   |
| Medium range ( $ i-j >1$ and $ i-j <5$ )                 | 249   |
| Long range ( $ i-j \geq 5$ )                             | 166   |
| Inter-chain                                              | 0     |
| Hydrogen bond restraints                                 | 66    |
| Disulfide bond restraints                                | 0     |
| Total dihedral-angle restraints                          | 90    |
| Number of unmapped restraints                            | 0     |
| Number of restraints per residue                         | 10.9  |
| Number of long range restraints per residue <sup>1</sup> | 1.8   |

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

### 8.2 Residual restraint violations

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

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

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

| Bins (Å)         | Average number of violations per model | Max (Å) |
|------------------|----------------------------------------|---------|
| 0.1-0.2 (Small)  | 15.0                                   | 0.2     |
| 0.2-0.5 (Medium) | 29.9                                   | 0.5     |
| >0.5 (Large)     | 19.3                                   | 3.91    |

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

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

| Bins (°)           | Average number of violations per model | Max (°) |
|--------------------|----------------------------------------|---------|
| 1.0-10.0 (Small)   | 45.3                                   | 6.78    |
| 10.0-20.0 (Medium) | 1.0                                    | 19.61   |
| >20.0 (Large)      | 1.0                                    | 24.21   |

## 9 Distance violation analysis ⓘ

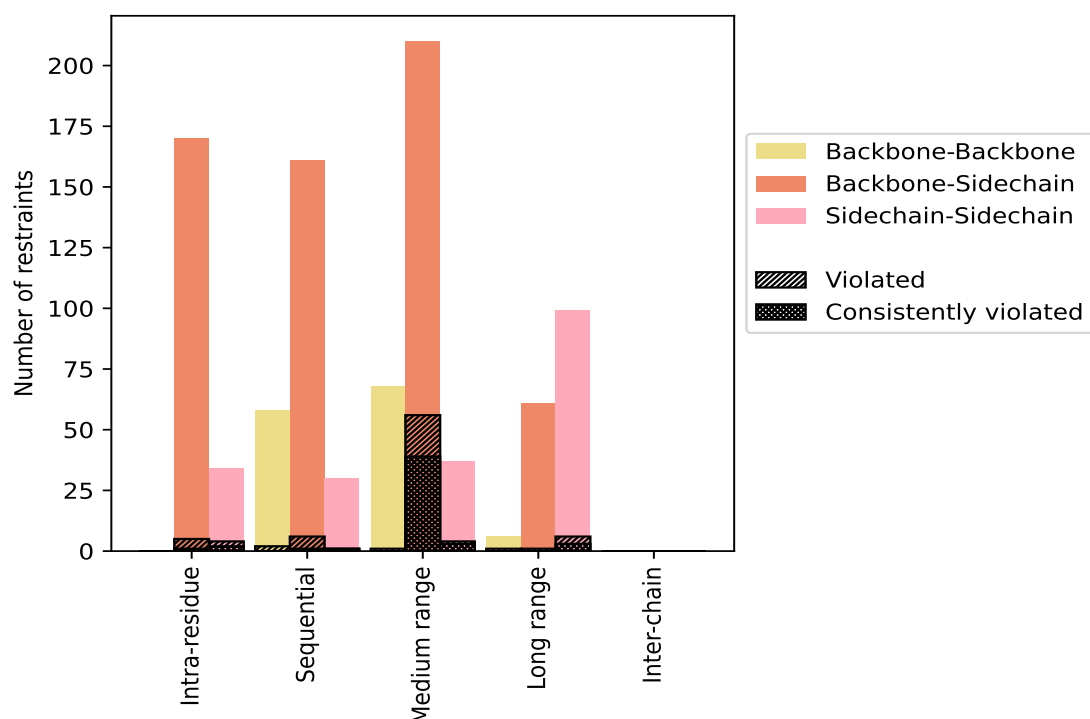
### 9.1 Summary of distance violations ⓘ

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.

| Restraints type                                            | Count               | % <sup>1</sup>        | Violated <sup>3</sup> |                      |                     | Consistently Violated <sup>4</sup> |                      |                     |
|------------------------------------------------------------|---------------------|-----------------------|-----------------------|----------------------|---------------------|------------------------------------|----------------------|---------------------|
|                                                            |                     |                       | Count                 | % <sup>2</sup>       | % <sup>1</sup>      | Count                              | % <sup>2</sup>       | % <sup>1</sup>      |
| <a href="#">Intra-residue ( i-j =0)</a>                    | <a href="#">204</a> | <a href="#">21.8</a>  | <a href="#">9</a>     | <a href="#">4.4</a>  | <a href="#">1.0</a> | <a href="#">3</a>                  | <a href="#">1.5</a>  | <a href="#">0.3</a> |
| Backbone-Backbone                                          | 0                   | 0.0                   | 0                     | 0.0                  | 0.0                 | 0                                  | 0.0                  | 0.0                 |
| Backbone-Sidechain                                         | 170                 | 18.2                  | 5                     | 2.9                  | 0.5                 | 1                                  | 0.6                  | 0.1                 |
| Sidechain-Sidechain                                        | 34                  | 3.6                   | 4                     | 11.8                 | 0.4                 | 2                                  | 5.9                  | 0.2                 |
| <a href="#">Sequential ( i-j =1)</a>                       | <a href="#">249</a> | <a href="#">26.7</a>  | <a href="#">9</a>     | <a href="#">3.6</a>  | <a href="#">1.0</a> | <a href="#">2</a>                  | <a href="#">0.8</a>  | <a href="#">0.2</a> |
| Backbone-Backbone                                          | 58                  | 6.2                   | 2                     | 3.4                  | 0.2                 | 0                                  | 0.0                  | 0.0                 |
| Backbone-Sidechain                                         | 161                 | 17.2                  | 6                     | 3.7                  | 0.6                 | 1                                  | 0.6                  | 0.1                 |
| Sidechain-Sidechain                                        | 30                  | 3.2                   | 1                     | 3.3                  | 0.1                 | 1                                  | 3.3                  | 0.1                 |
| <a href="#">Medium range ( i-j &gt;1 &amp;  i-j &lt;5)</a> | <a href="#">249</a> | <a href="#">26.7</a>  | <a href="#">9</a>     | <a href="#">3.6</a>  | <a href="#">1.0</a> | <a href="#">4</a>                  | <a href="#">1.6</a>  | <a href="#">0.4</a> |
| Backbone-Backbone                                          | 68                  | 7.3                   | 1                     | 1.5                  | 0.1                 | 0                                  | 0.0                  | 0.0                 |
| Backbone-Sidechain                                         | 144                 | 15.4                  | 4                     | 2.8                  | 0.4                 | 1                                  | 0.7                  | 0.1                 |
| Sidechain-Sidechain                                        | 37                  | 4.0                   | 4                     | 10.8                 | 0.4                 | 3                                  | 8.1                  | 0.3                 |
| <a href="#">Long range ( i-j ≥5)</a>                       | <a href="#">166</a> | <a href="#">17.8</a>  | <a href="#">8</a>     | <a href="#">4.8</a>  | <a href="#">0.9</a> | <a href="#">3</a>                  | <a href="#">1.8</a>  | <a href="#">0.3</a> |
| Backbone-Backbone                                          | 6                   | 0.6                   | 1                     | 16.7                 | 0.1                 | 0                                  | 0.0                  | 0.0                 |
| Backbone-Sidechain                                         | 61                  | 6.5                   | 1                     | 1.6                  | 0.1                 | 0                                  | 0.0                  | 0.0                 |
| Sidechain-Sidechain                                        | 99                  | 10.6                  | 6                     | 6.1                  | 0.6                 | 3                                  | 3.0                  | 0.3                 |
| <a href="#">Inter-chain</a>                                | <a href="#">0</a>   | <a href="#">0.0</a>   | <a href="#">0</a>     | <a href="#">0.0</a>  | <a href="#">0.0</a> | <a href="#">0</a>                  | <a href="#">0.0</a>  | <a href="#">0.0</a> |
| Backbone-Backbone                                          | 0                   | 0.0                   | 0                     | 0.0                  | 0.0                 | 0                                  | 0.0                  | 0.0                 |
| Backbone-Sidechain                                         | 0                   | 0.0                   | 0                     | 0.0                  | 0.0                 | 0                                  | 0.0                  | 0.0                 |
| Sidechain-Sidechain                                        | 0                   | 0.0                   | 0                     | 0.0                  | 0.0                 | 0                                  | 0.0                  | 0.0                 |
| <a href="#">Hydrogen bond</a>                              | <a href="#">66</a>  | <a href="#">7.1</a>   | <a href="#">52</a>    | <a href="#">78.8</a> | <a href="#">5.6</a> | <a href="#">38</a>                 | <a href="#">57.6</a> | <a href="#">4.1</a> |
| <a href="#">Disulfide bond</a>                             | <a href="#">0</a>   | <a href="#">0.0</a>   | <a href="#">0</a>     | <a href="#">0.0</a>  | <a href="#">0.0</a> | <a href="#">0</a>                  | <a href="#">0.0</a>  | <a href="#">0.0</a> |
| <a href="#">Total</a>                                      | <a href="#">934</a> | <a href="#">100.0</a> | <a href="#">87</a>    | <a href="#">9.3</a>  | <a href="#">9.3</a> | <a href="#">50</a>                 | <a href="#">5.4</a>  | <a href="#">5.4</a> |
| Backbone-Backbone                                          | 132                 | 14.1                  | 4                     | 3.0                  | 0.4                 | 0                                  | 0.0                  | 0.0                 |
| Backbone-Sidechain                                         | 602                 | 64.5                  | 68                    | 11.3                 | 7.3                 | 41                                 | 6.8                  | 4.4                 |
| Sidechain-Sidechain                                        | 200                 | 21.4                  | 15                    | 7.5                  | 1.6                 | 9                                  | 4.5                  | 1.0                 |

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

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



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

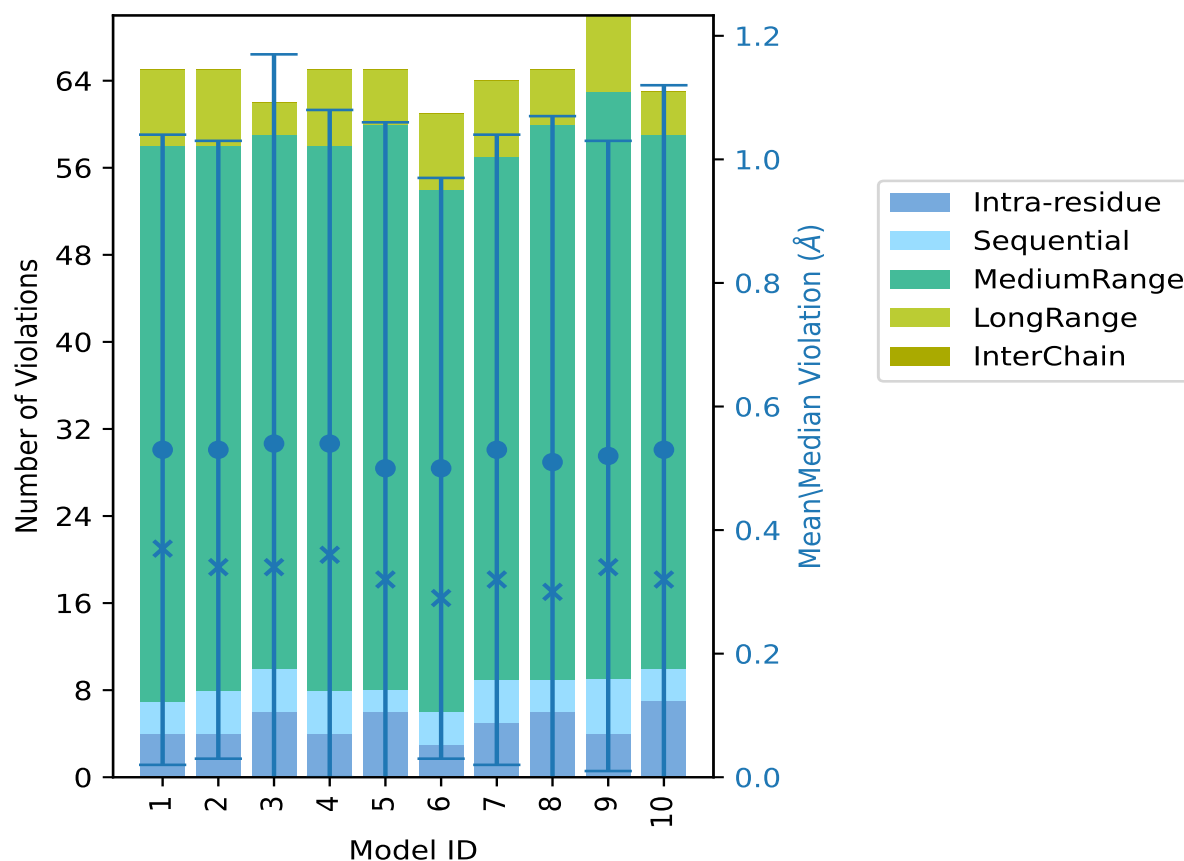
## 9.2 Distance violation statistics for each model [i](#)

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

| Model ID | Number of violations |                 |                 |                 |                 |       | Mean (Å) | Max (Å) | SD <sup>6</sup> (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
|          | IR <sup>1</sup>      | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total |          |         |                     |            |
| 1        | 4                    | 3               | 51              | 7               | 0               | 65    | 0.53     | 2.63    | 0.51                | 0.37       |
| 2        | 4                    | 4               | 50              | 7               | 0               | 65    | 0.53     | 2.78    | 0.5                 | 0.34       |
| 3        | 6                    | 4               | 49              | 3               | 0               | 62    | 0.54     | 3.91    | 0.63                | 0.34       |
| 4        | 4                    | 4               | 50              | 7               | 0               | 65    | 0.54     | 2.83    | 0.54                | 0.36       |
| 5        | 6                    | 2               | 52              | 5               | 0               | 65    | 0.5      | 3.42    | 0.56                | 0.32       |
| 6        | 3                    | 3               | 48              | 7               | 0               | 61    | 0.5      | 2.46    | 0.47                | 0.29       |
| 7        | 5                    | 4               | 48              | 7               | 0               | 64    | 0.53     | 2.19    | 0.51                | 0.32       |
| 8        | 6                    | 3               | 51              | 5               | 0               | 65    | 0.51     | 3.33    | 0.56                | 0.3        |
| 9        | 4                    | 5               | 54              | 7               | 0               | 70    | 0.52     | 2.78    | 0.51                | 0.34       |
| 10       | 7                    | 3               | 49              | 4               | 0               | 63    | 0.53     | 3.65    | 0.59                | 0.32       |

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

### 9.2.1 Bar graph : Distance Violation statistics for each model [i](#)



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

### 9.3 Distance violation statistics for the ensemble [i](#)

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 833(IR:195, SQ:240, MR:240, LR:158, IC:0) restraints are not violated in the ensemble.

| Number of violated restraints |                 |                 |                 |                 |       | Fraction of the ensemble |      |
|-------------------------------|-----------------|-----------------|-----------------|-----------------|-------|--------------------------|------|
| IR <sup>1</sup>               | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total | Count <sup>6</sup>       | %    |
| 3                             | 4               | 3               | 1               | 0               | 11    | 1                        | 10.0 |
| 0                             | 1               | 0               | 0               | 0               | 1     | 2                        | 20.0 |
| 0                             | 0               | 0               | 0               | 0               | 0     | 3                        | 30.0 |

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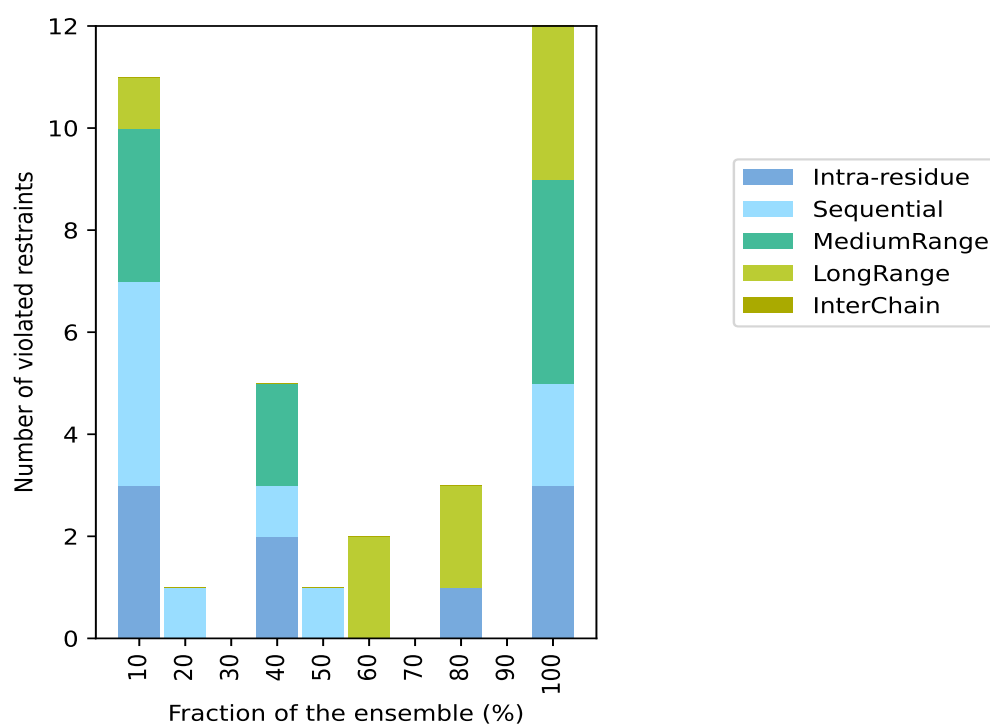
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| Number of violated restraints |                 |                 |                 |                 |       | Fraction of the ensemble |       |
|-------------------------------|-----------------|-----------------|-----------------|-----------------|-------|--------------------------|-------|
| IR <sup>1</sup>               | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total | Count <sup>6</sup>       | %     |
| 2                             | 1               | 2               | 0               | 0               | 5     | 4                        | 40.0  |
| 0                             | 1               | 0               | 0               | 0               | 1     | 5                        | 50.0  |
| 0                             | 0               | 0               | 2               | 0               | 2     | 6                        | 60.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 7                        | 70.0  |
| 1                             | 0               | 0               | 2               | 0               | 3     | 8                        | 80.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 9                        | 90.0  |
| 3                             | 2               | 4               | 3               | 0               | 12    | 10                       | 100.0 |

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

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

### 9.3.1 Bar graph : Distance violation statistics for the ensemble ⓘ

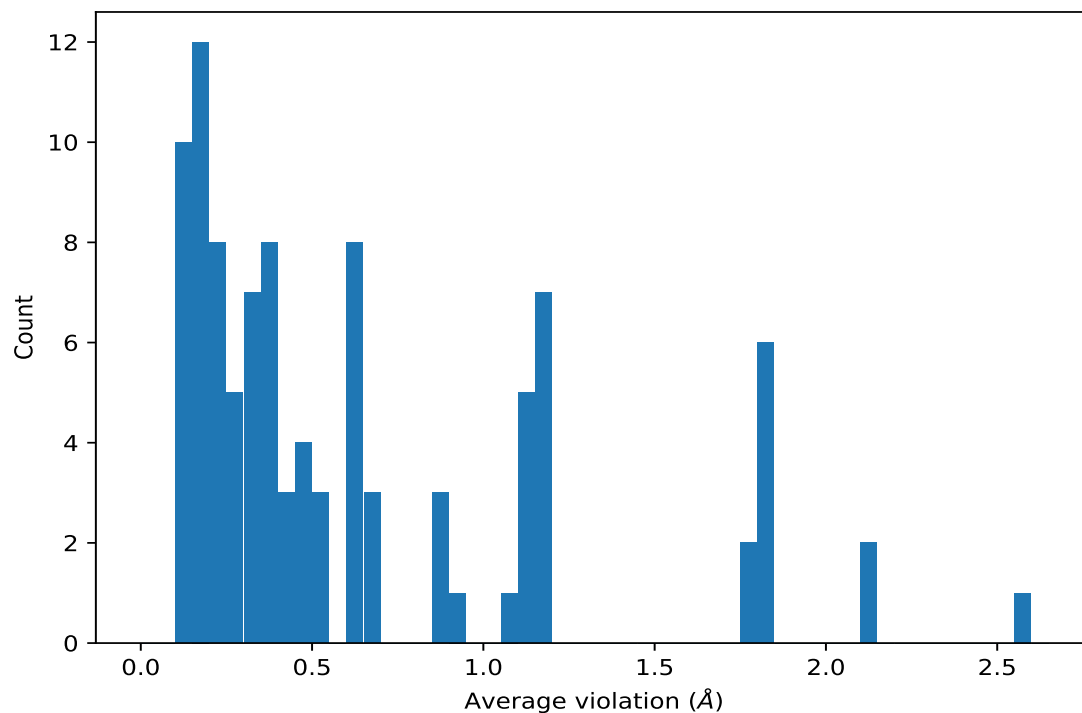


## 9.4 Most violated distance restraints in the ensemble ⓘ

### 9.4.1 Histogram : Distribution of mean distance violations ⓘ

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

in the ensemble



#### 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) |
|---------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (3,204) | 1:305:A:LEU:HG   | 1:309:A:PHE:HE1 | 10                  | 2.57     | 1.26                | 2.8        |
| (3,649) | 1:331:A:TYR:HE2  | 1:335:A:ARG:HD2 | 10                  | 2.14     | 0.25                | 2.18       |
| (3,649) | 1:331:A:TYR:HE2  | 1:335:A:ARG:HD3 | 10                  | 2.14     | 0.25                | 2.18       |
| (3,730) | 1:301:A:LEU:HD11 | 1:309:A:PHE:HD1 | 10                  | 1.81     | 0.32                | 1.9        |
| (3,730) | 1:301:A:LEU:HD12 | 1:309:A:PHE:HD1 | 10                  | 1.81     | 0.32                | 1.9        |
| (3,730) | 1:301:A:LEU:HD13 | 1:309:A:PHE:HD1 | 10                  | 1.81     | 0.32                | 1.9        |
| (3,730) | 1:301:A:LEU:HD21 | 1:309:A:PHE:HD1 | 10                  | 1.81     | 0.32                | 1.9        |
| (3,730) | 1:301:A:LEU:HD22 | 1:309:A:PHE:HD1 | 10                  | 1.81     | 0.32                | 1.9        |
| (3,730) | 1:301:A:LEU:HD23 | 1:309:A:PHE:HD1 | 10                  | 1.81     | 0.32                | 1.9        |
| (3,206) | 1:331:A:TYR:HE1  | 1:332:A:HIS:HB2 | 10                  | 1.79     | 0.25                | 1.88       |
| (3,206) | 1:331:A:TYR:HE1  | 1:332:A:HIS:HB3 | 10                  | 1.79     | 0.25                | 1.88       |
| (3,656) | 1:306:A:GLN:HA   | 1:309:A:PHE:HD1 | 10                  | 1.18     | 0.39                | 1.29       |
| (3,731) | 1:301:A:LEU:HD11 | 1:309:A:PHE:HE1 | 10                  | 1.16     | 0.39                | 1.24       |
| (3,731) | 1:301:A:LEU:HD12 | 1:309:A:PHE:HE1 | 10                  | 1.16     | 0.39                | 1.24       |
| (3,731) | 1:301:A:LEU:HD13 | 1:309:A:PHE:HE1 | 10                  | 1.16     | 0.39                | 1.24       |

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| Key     | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|------------------|------------------|---------------------|----------|---------------------|------------|
| (3,731) | 1:301:A:LEU:HD21 | 1:309:A:PHE:HE1  | 10                  | 1.16     | 0.39                | 1.24       |
| (3,731) | 1:301:A:LEU:HD22 | 1:309:A:PHE:HE1  | 10                  | 1.16     | 0.39                | 1.24       |
| (3,731) | 1:301:A:LEU:HD23 | 1:309:A:PHE:HE1  | 10                  | 1.16     | 0.39                | 1.24       |
| (3,640) | 1:331:A:TYR:HA   | 1:331:A:TYR:HD2  | 10                  | 1.12     | 0.02                | 1.11       |
| (3,660) | 1:309:A:PHE:HD1  | 1:341:A:LEU:HD21 | 10                  | 1.12     | 0.41                | 1.14       |
| (3,660) | 1:309:A:PHE:HD1  | 1:341:A:LEU:HD22 | 10                  | 1.12     | 0.41                | 1.14       |
| (3,660) | 1:309:A:PHE:HD1  | 1:341:A:LEU:HD23 | 10                  | 1.12     | 0.41                | 1.14       |
| (3,572) | 1:331:A:TYR:HE1  | 1:332:A:HIS:H    | 10                  | 1.06     | 0.05                | 1.06       |
| (2,9)   | 1:315:A:GLN:O    | 1:319:A:ASP:N    | 10                  | 0.68     | 0.12                | 0.66       |
| (2,10)  | 1:316:A:MET:O    | 1:320:A:ALA:N    | 10                  | 0.66     | 0.13                | 0.68       |
| (2,7)   | 1:307:A:LYS:O    | 1:311:A:VAL:N    | 10                  | 0.66     | 0.02                | 0.65       |
| (2,13)  | 1:319:A:ASP:O    | 1:323:A:LYS:N    | 10                  | 0.61     | 0.24                | 0.52       |
| (2,11)  | 1:317:A:LEU:O    | 1:321:A:ILE:N    | 10                  | 0.61     | 0.06                | 0.61       |
| (2,39)  | 1:315:A:GLN:O    | 1:319:A:ASP:H    | 10                  | 0.54     | 0.13                | 0.52       |
| (2,6)   | 1:306:A:GLN:O    | 1:310:A:ASP:N    | 10                  | 0.53     | 0.05                | 0.54       |
| (2,14)  | 1:327:A:THR:O    | 1:331:A:TYR:N    | 10                  | 0.51     | 0.04                | 0.52       |
| (2,47)  | 1:319:A:ASP:O    | 1:323:A:LYS:H    | 10                  | 0.49     | 0.28                | 0.38       |
| (2,35)  | 1:307:A:LYS:O    | 1:311:A:VAL:H    | 10                  | 0.48     | 0.02                | 0.48       |
| (2,41)  | 1:316:A:MET:O    | 1:320:A:ALA:H    | 10                  | 0.48     | 0.13                | 0.5        |
| (3,672) | 1:331:A:TYR:HE2  | 1:335:A:ARG:HG2  | 10                  | 0.48     | 0.12                | 0.43       |
| (2,43)  | 1:317:A:LEU:O    | 1:321:A:ILE:H    | 10                  | 0.43     | 0.07                | 0.44       |
| (2,15)  | 1:328:A:ASP:O    | 1:332:A:HIS:N    | 10                  | 0.42     | 0.02                | 0.42       |
| (2,12)  | 1:318:A:GLN:O    | 1:322:A:SER:N    | 10                  | 0.4      | 0.16                | 0.36       |
| (2,40)  | 1:315:A:GLN:O    | 1:319:A:ASP:N    | 10                  | 0.38     | 0.12                | 0.36       |
| (2,21)  | 1:334:A:GLN:O    | 1:338:A:ASP:N    | 10                  | 0.38     | 0.12                | 0.4        |
| (2,42)  | 1:316:A:MET:O    | 1:320:A:ALA:N    | 10                  | 0.36     | 0.13                | 0.38       |
| (2,19)  | 1:332:A:HIS:O    | 1:336:A:CYS:N    | 10                  | 0.36     | 0.11                | 0.4        |
| (2,36)  | 1:307:A:LYS:O    | 1:311:A:VAL:N    | 10                  | 0.36     | 0.02                | 0.35       |
| (2,18)  | 1:331:A:TYR:O    | 1:335:A:ARG:N    | 10                  | 0.36     | 0.04                | 0.36       |
| (2,33)  | 1:306:A:GLN:O    | 1:310:A:ASP:H    | 10                  | 0.35     | 0.04                | 0.36       |
| (2,49)  | 1:327:A:THR:O    | 1:331:A:TYR:H    | 10                  | 0.34     | 0.04                | 0.34       |
| (2,5)   | 1:305:A:LEU:O    | 1:309:A:PHE:N    | 10                  | 0.33     | 0.06                | 0.36       |
| (2,20)  | 1:333:A:MET:O    | 1:337:A:ILE:N    | 10                  | 0.31     | 0.03                | 0.3        |
| (2,44)  | 1:317:A:LEU:O    | 1:321:A:ILE:N    | 10                  | 0.31     | 0.06                | 0.31       |
| (3,671) | 1:331:A:TYR:HB2  | 1:331:A:TYR:HE2  | 10                  | 0.3      | 0.02                | 0.3        |
| (2,8)   | 1:314:A:VAL:O    | 1:318:A:GLN:N    | 10                  | 0.26     | 0.01                | 0.27       |
| (3,641) | 1:331:A:TYR:HB2  | 1:331:A:TYR:HD2  | 10                  | 0.26     | 0.03                | 0.27       |
| (2,25)  | 1:296:A:GLU:O    | 1:300:A:SER:H    | 10                  | 0.25     | 0.03                | 0.26       |
| (2,16)  | 1:329:A:ALA:O    | 1:333:A:MET:N    | 10                  | 0.23     | 0.04                | 0.22       |
| (2,34)  | 1:306:A:GLN:O    | 1:310:A:ASP:N    | 10                  | 0.23     | 0.05                | 0.24       |
| (2,4)   | 1:304:A:GLU:O    | 1:308:A:CYS:N    | 10                  | 0.23     | 0.03                | 0.23       |
| (2,17)  | 1:330:A:LYS:O    | 1:334:A:GLN:N    | 10                  | 0.23     | 0.04                | 0.22       |

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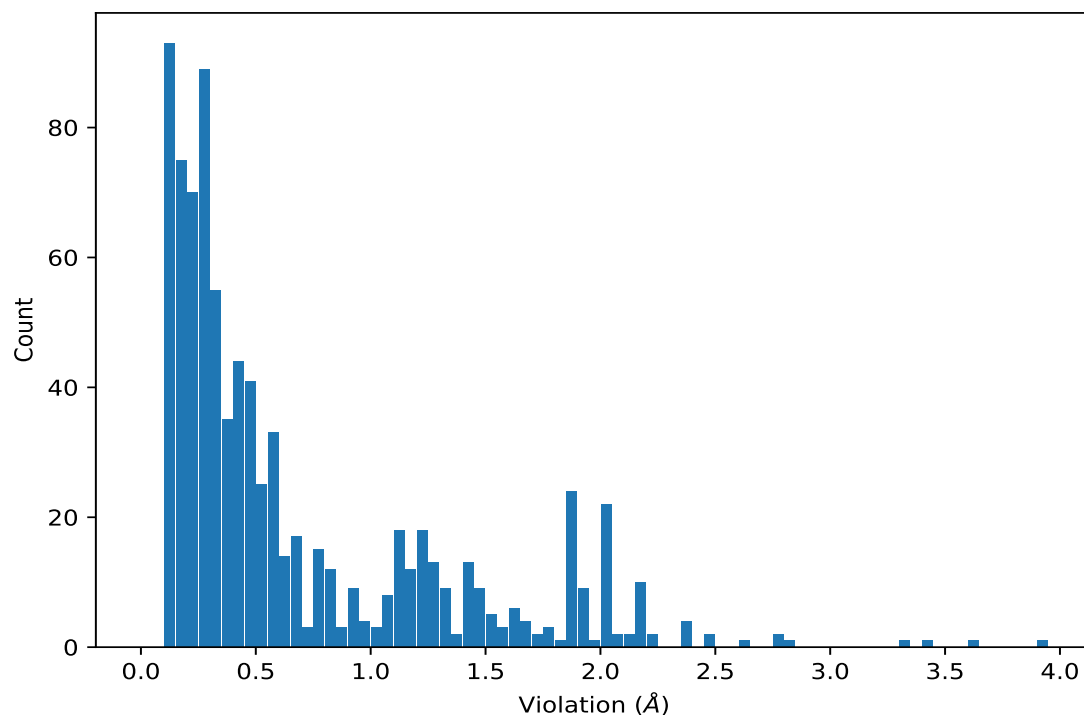
| Key     | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|------------------|------------------|---------------------|----------|---------------------|------------|
| (2,50)  | 1:327:A:THR:O    | 1:331:A:TYR:N    | 10                  | 0.21     | 0.04                | 0.22       |
| (2,2)   | 1:296:A:GLU:O    | 1:300:A:SER:N    | 10                  | 0.2      | 0.03                | 0.2        |
| (2,57)  | 1:331:A:TYR:O    | 1:335:A:ARG:H    | 10                  | 0.19     | 0.05                | 0.2        |
| (2,1)   | 1:295:A:VAL:O    | 1:299:A:GLU:N    | 10                  | 0.19     | 0.02                | 0.18       |
| (2,3)   | 1:303:A:GLU:O    | 1:307:A:LYS:N    | 10                  | 0.18     | 0.03                | 0.18       |
| (2,51)  | 1:328:A:ASP:O    | 1:332:A:HIS:H    | 10                  | 0.18     | 0.02                | 0.18       |
| (2,22)  | 1:335:A:ARG:O    | 1:339:A:SER:N    | 10                  | 0.17     | 0.06                | 0.16       |
| (3,662) | 1:309:A:PHE:HE1  | 1:341:A:LEU:HD21 | 8                   | 0.89     | 0.42                | 0.89       |
| (3,662) | 1:309:A:PHE:HE1  | 1:341:A:LEU:HD22 | 8                   | 0.89     | 0.42                | 0.89       |
| (3,662) | 1:309:A:PHE:HE1  | 1:341:A:LEU:HD23 | 8                   | 0.89     | 0.42                | 0.89       |
| (2,48)  | 1:319:A:ASP:O    | 1:323:A:LYS:N    | 8                   | 0.38     | 0.21                | 0.38       |
| (3,657) | 1:309:A:PHE:HB2  | 1:309:A:PHE:HD1  | 8                   | 0.16     | 0.01                | 0.16       |
| (3,609) | 1:308:A:CYS:HA   | 1:313:A:ASP:H    | 8                   | 0.13     | 0.02                | 0.13       |
| (2,52)  | 1:328:A:ASP:O    | 1:332:A:HIS:N    | 8                   | 0.12     | 0.01                | 0.12       |
| (2,31)  | 1:305:A:LEU:O    | 1:309:A:PHE:H    | 7                   | 0.14     | 0.01                | 0.14       |
| (2,61)  | 1:333:A:MET:O    | 1:337:A:ILE:H    | 7                   | 0.13     | 0.02                | 0.11       |
| (3,661) | 1:309:A:PHE:HE1  | 1:341:A:LEU:HG   | 6                   | 1.12     | 0.55                | 0.86       |
| (3,659) | 1:309:A:PHE:HD1  | 1:341:A:LEU:HG   | 6                   | 0.92     | 0.54                | 0.59       |
| (2,45)  | 1:318:A:GLN:O    | 1:322:A:SER:H    | 6                   | 0.32     | 0.12                | 0.36       |
| (2,63)  | 1:334:A:GLN:O    | 1:338:A:ASP:H    | 6                   | 0.23     | 0.06                | 0.22       |
| (2,59)  | 1:332:A:HIS:O    | 1:336:A:CYS:H    | 6                   | 0.21     | 0.05                | 0.22       |
| (3,442) | 1:363:A:LEU:HA   | 1:364:A:LEU:H    | 5                   | 0.31     | 0.02                | 0.32       |
| (2,64)  | 1:334:A:GLN:O    | 1:338:A:ASP:N    | 5                   | 0.19     | 0.03                | 0.17       |
| (2,60)  | 1:332:A:HIS:O    | 1:336:A:CYS:N    | 5                   | 0.16     | 0.02                | 0.16       |
| (3,745) | 1:305:A:LEU:HD11 | 1:309:A:PHE:HE1  | 4                   | 0.62     | 0.25                | 0.62       |
| (3,745) | 1:305:A:LEU:HD12 | 1:309:A:PHE:HE1  | 4                   | 0.62     | 0.25                | 0.62       |
| (3,745) | 1:305:A:LEU:HD13 | 1:309:A:PHE:HE1  | 4                   | 0.62     | 0.25                | 0.62       |
| (3,745) | 1:305:A:LEU:HD21 | 1:309:A:PHE:HE1  | 4                   | 0.62     | 0.25                | 0.62       |
| (3,745) | 1:305:A:LEU:HD22 | 1:309:A:PHE:HE1  | 4                   | 0.62     | 0.25                | 0.62       |
| (3,745) | 1:305:A:LEU:HD23 | 1:309:A:PHE:HE1  | 4                   | 0.62     | 0.25                | 0.62       |
| (2,46)  | 1:318:A:GLN:O    | 1:322:A:SER:N    | 4                   | 0.29     | 0.04                | 0.3        |
| (3,29)  | 1:342:A:TRP:HA   | 1:342:A:TRP:HE3  | 4                   | 0.26     | 0.07                | 0.24       |
| (3,420) | 1:342:A:TRP:HB3  | 1:342:A:TRP:HE1  | 4                   | 0.19     | 0.0                 | 0.19       |
| (3,791) | 1:323:A:LYS:HD2  | 1:324:A:MET:H    | 4                   | 0.19     | 0.0                 | 0.19       |
| (3,791) | 1:323:A:LYS:HD3  | 1:324:A:MET:H    | 4                   | 0.19     | 0.0                 | 0.19       |
| (3,547) | 1:321:A:ILE:H    | 1:323:A:LYS:HG2  | 4                   | 0.14     | 0.0                 | 0.14       |
| (3,547) | 1:321:A:ILE:H    | 1:323:A:LYS:HG3  | 4                   | 0.14     | 0.0                 | 0.14       |
| (2,29)  | 1:304:A:GLU:O    | 1:308:A:CYS:H    | 3                   | 0.16     | 0.03                | 0.18       |
| (2,65)  | 1:335:A:ARG:O    | 1:339:A:SER:H    | 3                   | 0.14     | 0.02                | 0.14       |
| (3,347) | 1:324:A:MET:HG3  | 1:325:A:ASP:H    | 2                   | 0.11     | 0.0                 | 0.11       |
| (3,347) | 1:324:A:MET:HG2  | 1:325:A:ASP:H    | 2                   | 0.11     | 0.0                 | 0.11       |
| (2,58)  | 1:331:A:TYR:O    | 1:335:A:ARG:N    | 2                   | 0.11     | 0.0                 | 0.11       |

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

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

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

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



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

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

| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (3,204) | 1:305:A:LEU:HG | 1:309:A:PHE:HE1 | 3        | 3.91          |
| (3,204) | 1:305:A:LEU:HG | 1:309:A:PHE:HE1 | 10       | 3.65          |
| (3,204) | 1:305:A:LEU:HG | 1:309:A:PHE:HE1 | 5        | 3.42          |
| (3,204) | 1:305:A:LEU:HG | 1:309:A:PHE:HE1 | 8        | 3.33          |
| (3,204) | 1:305:A:LEU:HG | 1:309:A:PHE:HE1 | 4        | 2.83          |
| (3,204) | 1:305:A:LEU:HG | 1:309:A:PHE:HE1 | 2        | 2.78          |
| (3,204) | 1:305:A:LEU:HG | 1:309:A:PHE:HE1 | 9        | 2.78          |

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| Key     | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|---------|------------------|-----------------|----------|---------------|
| (3,204) | 1:305:A:LEU:HG   | 1:309:A:PHE:HE1 | 1        | 2.63          |
| (3,649) | 1:331:A:TYR:HE2  | 1:335:A:ARG:HD2 | 6        | 2.46          |
| (3,649) | 1:331:A:TYR:HE2  | 1:335:A:ARG:HD3 | 6        | 2.46          |
| (3,649) | 1:331:A:TYR:HE2  | 1:335:A:ARG:HD2 | 5        | 2.39          |
| (3,649) | 1:331:A:TYR:HE2  | 1:335:A:ARG:HD3 | 5        | 2.39          |
| (3,649) | 1:331:A:TYR:HE2  | 1:335:A:ARG:HD2 | 8        | 2.38          |
| (3,649) | 1:331:A:TYR:HE2  | 1:335:A:ARG:HD3 | 8        | 2.38          |
| (3,649) | 1:331:A:TYR:HE2  | 1:335:A:ARG:HD2 | 4        | 2.23          |
| (3,649) | 1:331:A:TYR:HE2  | 1:335:A:ARG:HD3 | 4        | 2.23          |
| (3,649) | 1:331:A:TYR:HE2  | 1:335:A:ARG:HD2 | 7        | 2.19          |
| (3,649) | 1:331:A:TYR:HE2  | 1:335:A:ARG:HD3 | 7        | 2.19          |
| (3,730) | 1:301:A:LEU:HD11 | 1:309:A:PHE:HD1 | 3        | 2.18          |
| (3,730) | 1:301:A:LEU:HD12 | 1:309:A:PHE:HD1 | 3        | 2.18          |
| (3,730) | 1:301:A:LEU:HD13 | 1:309:A:PHE:HD1 | 3        | 2.18          |
| (3,730) | 1:301:A:LEU:HD21 | 1:309:A:PHE:HD1 | 3        | 2.18          |
| (3,730) | 1:301:A:LEU:HD22 | 1:309:A:PHE:HD1 | 3        | 2.18          |
| (3,730) | 1:301:A:LEU:HD23 | 1:309:A:PHE:HD1 | 3        | 2.18          |
| (3,649) | 1:331:A:TYR:HE2  | 1:335:A:ARG:HD2 | 1        | 2.18          |
| (3,649) | 1:331:A:TYR:HE2  | 1:335:A:ARG:HD3 | 1        | 2.18          |
| (3,649) | 1:331:A:TYR:HE2  | 1:335:A:ARG:HD2 | 10       | 2.13          |
| (3,649) | 1:331:A:TYR:HE2  | 1:335:A:ARG:HD3 | 10       | 2.13          |
| (3,649) | 1:331:A:TYR:HE2  | 1:335:A:ARG:HD2 | 9        | 2.08          |
| (3,649) | 1:331:A:TYR:HE2  | 1:335:A:ARG:HD3 | 9        | 2.08          |
| (3,730) | 1:301:A:LEU:HD11 | 1:309:A:PHE:HD1 | 8        | 2.02          |
| (3,730) | 1:301:A:LEU:HD12 | 1:309:A:PHE:HD1 | 8        | 2.02          |
| (3,730) | 1:301:A:LEU:HD13 | 1:309:A:PHE:HD1 | 8        | 2.02          |
| (3,730) | 1:301:A:LEU:HD21 | 1:309:A:PHE:HD1 | 8        | 2.02          |
| (3,730) | 1:301:A:LEU:HD22 | 1:309:A:PHE:HD1 | 8        | 2.02          |
| (3,730) | 1:301:A:LEU:HD23 | 1:309:A:PHE:HD1 | 8        | 2.02          |
| (3,730) | 1:301:A:LEU:HD11 | 1:309:A:PHE:HD1 | 10       | 2.02          |
| (3,730) | 1:301:A:LEU:HD12 | 1:309:A:PHE:HD1 | 10       | 2.02          |
| (3,730) | 1:301:A:LEU:HD13 | 1:309:A:PHE:HD1 | 10       | 2.02          |
| (3,730) | 1:301:A:LEU:HD21 | 1:309:A:PHE:HD1 | 10       | 2.02          |
| (3,730) | 1:301:A:LEU:HD22 | 1:309:A:PHE:HD1 | 10       | 2.02          |
| (3,730) | 1:301:A:LEU:HD23 | 1:309:A:PHE:HD1 | 10       | 2.02          |
| (3,206) | 1:331:A:TYR:HE1  | 1:332:A:HIS:HB2 | 3        | 2.02          |
| (3,206) | 1:331:A:TYR:HE1  | 1:332:A:HIS:HB3 | 3        | 2.02          |
| (3,206) | 1:331:A:TYR:HE1  | 1:332:A:HIS:HB2 | 4        | 2.02          |
| (3,206) | 1:331:A:TYR:HE1  | 1:332:A:HIS:HB3 | 4        | 2.02          |
| (3,206) | 1:331:A:TYR:HE1  | 1:332:A:HIS:HB2 | 7        | 2.02          |
| (3,206) | 1:331:A:TYR:HE1  | 1:332:A:HIS:HB3 | 7        | 2.02          |
| (3,206) | 1:331:A:TYR:HE1  | 1:332:A:HIS:HB2 | 1        | 2.01          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,206) | 1:331:A:TYR:HE1  | 1:332:A:HIS:HB3  | 1        | 2.01          |
| (3,206) | 1:331:A:TYR:HE1  | 1:332:A:HIS:HB2  | 2        | 2.01          |
| (3,206) | 1:331:A:TYR:HE1  | 1:332:A:HIS:HB3  | 2        | 2.01          |
| (3,661) | 1:309:A:PHE:HE1  | 1:341:A:LEU:HG   | 7        | 1.96          |
| (3,730) | 1:301:A:LEU:HD11 | 1:309:A:PHE:HD1  | 9        | 1.92          |
| (3,730) | 1:301:A:LEU:HD12 | 1:309:A:PHE:HD1  | 9        | 1.92          |
| (3,730) | 1:301:A:LEU:HD13 | 1:309:A:PHE:HD1  | 9        | 1.92          |
| (3,730) | 1:301:A:LEU:HD21 | 1:309:A:PHE:HD1  | 9        | 1.92          |
| (3,730) | 1:301:A:LEU:HD22 | 1:309:A:PHE:HD1  | 9        | 1.92          |
| (3,730) | 1:301:A:LEU:HD23 | 1:309:A:PHE:HD1  | 9        | 1.92          |
| (3,660) | 1:309:A:PHE:HD1  | 1:341:A:LEU:HD21 | 7        | 1.91          |
| (3,660) | 1:309:A:PHE:HD1  | 1:341:A:LEU:HD22 | 7        | 1.91          |
| (3,660) | 1:309:A:PHE:HD1  | 1:341:A:LEU:HD23 | 7        | 1.91          |
| (3,730) | 1:301:A:LEU:HD11 | 1:309:A:PHE:HD1  | 2        | 1.9           |
| (3,730) | 1:301:A:LEU:HD12 | 1:309:A:PHE:HD1  | 2        | 1.9           |
| (3,730) | 1:301:A:LEU:HD13 | 1:309:A:PHE:HD1  | 2        | 1.9           |
| (3,730) | 1:301:A:LEU:HD21 | 1:309:A:PHE:HD1  | 2        | 1.9           |
| (3,730) | 1:301:A:LEU:HD22 | 1:309:A:PHE:HD1  | 2        | 1.9           |
| (3,730) | 1:301:A:LEU:HD23 | 1:309:A:PHE:HD1  | 2        | 1.9           |
| (3,730) | 1:301:A:LEU:HD11 | 1:309:A:PHE:HD1  | 4        | 1.9           |
| (3,730) | 1:301:A:LEU:HD12 | 1:309:A:PHE:HD1  | 4        | 1.9           |
| (3,730) | 1:301:A:LEU:HD13 | 1:309:A:PHE:HD1  | 4        | 1.9           |
| (3,730) | 1:301:A:LEU:HD21 | 1:309:A:PHE:HD1  | 4        | 1.9           |
| (3,730) | 1:301:A:LEU:HD22 | 1:309:A:PHE:HD1  | 4        | 1.9           |
| (3,730) | 1:301:A:LEU:HD23 | 1:309:A:PHE:HD1  | 4        | 1.9           |
| (3,730) | 1:301:A:LEU:HD11 | 1:309:A:PHE:HD1  | 1        | 1.89          |
| (3,730) | 1:301:A:LEU:HD12 | 1:309:A:PHE:HD1  | 1        | 1.89          |
| (3,730) | 1:301:A:LEU:HD13 | 1:309:A:PHE:HD1  | 1        | 1.89          |
| (3,730) | 1:301:A:LEU:HD21 | 1:309:A:PHE:HD1  | 1        | 1.89          |
| (3,730) | 1:301:A:LEU:HD22 | 1:309:A:PHE:HD1  | 1        | 1.89          |
| (3,730) | 1:301:A:LEU:HD23 | 1:309:A:PHE:HD1  | 1        | 1.89          |
| (3,730) | 1:301:A:LEU:HD11 | 1:309:A:PHE:HD1  | 5        | 1.89          |
| (3,730) | 1:301:A:LEU:HD12 | 1:309:A:PHE:HD1  | 5        | 1.89          |
| (3,730) | 1:301:A:LEU:HD13 | 1:309:A:PHE:HD1  | 5        | 1.89          |
| (3,730) | 1:301:A:LEU:HD21 | 1:309:A:PHE:HD1  | 5        | 1.89          |
| (3,730) | 1:301:A:LEU:HD22 | 1:309:A:PHE:HD1  | 5        | 1.89          |
| (3,730) | 1:301:A:LEU:HD23 | 1:309:A:PHE:HD1  | 5        | 1.89          |
| (3,659) | 1:309:A:PHE:HD1  | 1:341:A:LEU:HG   | 7        | 1.83          |
| (3,661) | 1:309:A:PHE:HE1  | 1:341:A:LEU:HG   | 6        | 1.79          |
| (3,206) | 1:331:A:TYR:HE1  | 1:332:A:HIS:HB2  | 9        | 1.75          |
| (3,206) | 1:331:A:TYR:HE1  | 1:332:A:HIS:HB3  | 9        | 1.75          |
| (3,206) | 1:331:A:TYR:HE1  | 1:332:A:HIS:HB2  | 10       | 1.72          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,206) | 1:331:A:TYR:HE1  | 1:332:A:HIS:HB3  | 10       | 1.72          |
| (3,649) | 1:331:A:TYR:HE2  | 1:335:A:ARG:HD2  | 2        | 1.69          |
| (3,649) | 1:331:A:TYR:HE2  | 1:335:A:ARG:HD3  | 2        | 1.69          |
| (3,649) | 1:331:A:TYR:HE2  | 1:335:A:ARG:HD2  | 3        | 1.69          |
| (3,649) | 1:331:A:TYR:HE2  | 1:335:A:ARG:HD3  | 3        | 1.69          |
| (3,731) | 1:301:A:LEU:HD11 | 1:309:A:PHE:HE1  | 3        | 1.62          |
| (3,731) | 1:301:A:LEU:HD12 | 1:309:A:PHE:HE1  | 3        | 1.62          |
| (3,731) | 1:301:A:LEU:HD13 | 1:309:A:PHE:HE1  | 3        | 1.62          |
| (3,731) | 1:301:A:LEU:HD21 | 1:309:A:PHE:HE1  | 3        | 1.62          |
| (3,731) | 1:301:A:LEU:HD22 | 1:309:A:PHE:HE1  | 3        | 1.62          |
| (3,731) | 1:301:A:LEU:HD23 | 1:309:A:PHE:HE1  | 3        | 1.62          |
| (3,662) | 1:309:A:PHE:HE1  | 1:341:A:LEU:HD21 | 7        | 1.58          |
| (3,662) | 1:309:A:PHE:HE1  | 1:341:A:LEU:HD22 | 7        | 1.58          |
| (3,662) | 1:309:A:PHE:HE1  | 1:341:A:LEU:HD23 | 7        | 1.58          |
| (3,656) | 1:306:A:GLN:HA   | 1:309:A:PHE:HD1  | 3        | 1.53          |
| (3,660) | 1:309:A:PHE:HD1  | 1:341:A:LEU:HD21 | 6        | 1.51          |
| (3,660) | 1:309:A:PHE:HD1  | 1:341:A:LEU:HD22 | 6        | 1.51          |
| (3,660) | 1:309:A:PHE:HD1  | 1:341:A:LEU:HD23 | 6        | 1.51          |
| (3,656) | 1:306:A:GLN:HA   | 1:309:A:PHE:HD1  | 8        | 1.51          |
| (3,659) | 1:309:A:PHE:HD1  | 1:341:A:LEU:HG   | 6        | 1.49          |
| (3,731) | 1:301:A:LEU:HD11 | 1:309:A:PHE:HE1  | 10       | 1.46          |
| (3,731) | 1:301:A:LEU:HD12 | 1:309:A:PHE:HE1  | 10       | 1.46          |
| (3,731) | 1:301:A:LEU:HD13 | 1:309:A:PHE:HE1  | 10       | 1.46          |
| (3,731) | 1:301:A:LEU:HD21 | 1:309:A:PHE:HE1  | 10       | 1.46          |
| (3,731) | 1:301:A:LEU:HD22 | 1:309:A:PHE:HE1  | 10       | 1.46          |
| (3,731) | 1:301:A:LEU:HD23 | 1:309:A:PHE:HE1  | 10       | 1.46          |
| (3,206) | 1:331:A:TYR:HE1  | 1:332:A:HIS:HB2  | 5        | 1.46          |
| (3,206) | 1:331:A:TYR:HE1  | 1:332:A:HIS:HB3  | 5        | 1.46          |
| (3,731) | 1:301:A:LEU:HD11 | 1:309:A:PHE:HE1  | 8        | 1.45          |
| (3,731) | 1:301:A:LEU:HD12 | 1:309:A:PHE:HE1  | 8        | 1.45          |
| (3,731) | 1:301:A:LEU:HD13 | 1:309:A:PHE:HE1  | 8        | 1.45          |
| (3,731) | 1:301:A:LEU:HD21 | 1:309:A:PHE:HE1  | 8        | 1.45          |
| (3,731) | 1:301:A:LEU:HD22 | 1:309:A:PHE:HE1  | 8        | 1.45          |
| (3,731) | 1:301:A:LEU:HD23 | 1:309:A:PHE:HE1  | 8        | 1.45          |
| (3,206) | 1:331:A:TYR:HE1  | 1:332:A:HIS:HB2  | 8        | 1.45          |
| (3,206) | 1:331:A:TYR:HE1  | 1:332:A:HIS:HB3  | 8        | 1.45          |
| (3,660) | 1:309:A:PHE:HD1  | 1:341:A:LEU:HD21 | 4        | 1.42          |
| (3,660) | 1:309:A:PHE:HD1  | 1:341:A:LEU:HD22 | 4        | 1.42          |
| (3,660) | 1:309:A:PHE:HD1  | 1:341:A:LEU:HD23 | 4        | 1.42          |
| (3,656) | 1:306:A:GLN:HA   | 1:309:A:PHE:HD1  | 5        | 1.42          |
| (3,656) | 1:306:A:GLN:HA   | 1:309:A:PHE:HD1  | 10       | 1.41          |
| (3,206) | 1:331:A:TYR:HE1  | 1:332:A:HIS:HB2  | 6        | 1.4           |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,206) | 1:331:A:TYR:HE1  | 1:332:A:HIS:HB3  | 6        | 1.4           |
| (3,731) | 1:301:A:LEU:HD11 | 1:309:A:PHE:HE1  | 5        | 1.34          |
| (3,731) | 1:301:A:LEU:HD12 | 1:309:A:PHE:HE1  | 5        | 1.34          |
| (3,731) | 1:301:A:LEU:HD13 | 1:309:A:PHE:HE1  | 5        | 1.34          |
| (3,731) | 1:301:A:LEU:HD21 | 1:309:A:PHE:HE1  | 5        | 1.34          |
| (3,731) | 1:301:A:LEU:HD22 | 1:309:A:PHE:HE1  | 5        | 1.34          |
| (3,731) | 1:301:A:LEU:HD23 | 1:309:A:PHE:HE1  | 5        | 1.34          |
| (3,660) | 1:309:A:PHE:HD1  | 1:341:A:LEU:HD21 | 9        | 1.34          |
| (3,660) | 1:309:A:PHE:HD1  | 1:341:A:LEU:HD22 | 9        | 1.34          |
| (3,660) | 1:309:A:PHE:HD1  | 1:341:A:LEU:HD23 | 9        | 1.34          |
| (3,656) | 1:306:A:GLN:HA   | 1:309:A:PHE:HD1  | 1        | 1.29          |
| (3,656) | 1:306:A:GLN:HA   | 1:309:A:PHE:HD1  | 2        | 1.29          |
| (3,662) | 1:309:A:PHE:HE1  | 1:341:A:LEU:HD21 | 6        | 1.28          |
| (3,662) | 1:309:A:PHE:HE1  | 1:341:A:LEU:HD22 | 6        | 1.28          |
| (3,662) | 1:309:A:PHE:HE1  | 1:341:A:LEU:HD23 | 6        | 1.28          |
| (3,656) | 1:306:A:GLN:HA   | 1:309:A:PHE:HD1  | 4        | 1.28          |
| (3,656) | 1:306:A:GLN:HA   | 1:309:A:PHE:HD1  | 9        | 1.28          |
| (3,731) | 1:301:A:LEU:HD11 | 1:309:A:PHE:HE1  | 9        | 1.25          |
| (3,731) | 1:301:A:LEU:HD12 | 1:309:A:PHE:HE1  | 9        | 1.25          |
| (3,731) | 1:301:A:LEU:HD13 | 1:309:A:PHE:HE1  | 9        | 1.25          |
| (3,731) | 1:301:A:LEU:HD21 | 1:309:A:PHE:HE1  | 9        | 1.25          |
| (3,731) | 1:301:A:LEU:HD22 | 1:309:A:PHE:HE1  | 9        | 1.25          |
| (3,731) | 1:301:A:LEU:HD23 | 1:309:A:PHE:HE1  | 9        | 1.25          |
| (3,731) | 1:301:A:LEU:HD11 | 1:309:A:PHE:HE1  | 2        | 1.23          |
| (3,731) | 1:301:A:LEU:HD12 | 1:309:A:PHE:HE1  | 2        | 1.23          |
| (3,731) | 1:301:A:LEU:HD13 | 1:309:A:PHE:HE1  | 2        | 1.23          |
| (3,731) | 1:301:A:LEU:HD21 | 1:309:A:PHE:HE1  | 2        | 1.23          |
| (3,731) | 1:301:A:LEU:HD22 | 1:309:A:PHE:HE1  | 2        | 1.23          |
| (3,731) | 1:301:A:LEU:HD23 | 1:309:A:PHE:HE1  | 2        | 1.23          |
| (3,731) | 1:301:A:LEU:HD11 | 1:309:A:PHE:HE1  | 4        | 1.21          |
| (3,731) | 1:301:A:LEU:HD12 | 1:309:A:PHE:HE1  | 4        | 1.21          |
| (3,731) | 1:301:A:LEU:HD13 | 1:309:A:PHE:HE1  | 4        | 1.21          |
| (3,731) | 1:301:A:LEU:HD21 | 1:309:A:PHE:HE1  | 4        | 1.21          |
| (3,731) | 1:301:A:LEU:HD22 | 1:309:A:PHE:HE1  | 4        | 1.21          |
| (3,731) | 1:301:A:LEU:HD23 | 1:309:A:PHE:HE1  | 4        | 1.21          |
| (3,730) | 1:301:A:LEU:HD11 | 1:309:A:PHE:HD1  | 6        | 1.21          |
| (3,730) | 1:301:A:LEU:HD12 | 1:309:A:PHE:HD1  | 6        | 1.21          |
| (3,730) | 1:301:A:LEU:HD13 | 1:309:A:PHE:HD1  | 6        | 1.21          |
| (3,730) | 1:301:A:LEU:HD21 | 1:309:A:PHE:HD1  | 6        | 1.21          |
| (3,730) | 1:301:A:LEU:HD22 | 1:309:A:PHE:HD1  | 6        | 1.21          |
| (3,730) | 1:301:A:LEU:HD23 | 1:309:A:PHE:HD1  | 6        | 1.21          |
| (3,731) | 1:301:A:LEU:HD11 | 1:309:A:PHE:HE1  | 1        | 1.2           |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,731) | 1:301:A:LEU:HD12 | 1:309:A:PHE:HE1  | 1        | 1.2           |
| (3,731) | 1:301:A:LEU:HD13 | 1:309:A:PHE:HE1  | 1        | 1.2           |
| (3,731) | 1:301:A:LEU:HD21 | 1:309:A:PHE:HE1  | 1        | 1.2           |
| (3,731) | 1:301:A:LEU:HD22 | 1:309:A:PHE:HE1  | 1        | 1.2           |
| (3,731) | 1:301:A:LEU:HD23 | 1:309:A:PHE:HE1  | 1        | 1.2           |
| (3,730) | 1:301:A:LEU:HD11 | 1:309:A:PHE:HD1  | 7        | 1.2           |
| (3,730) | 1:301:A:LEU:HD12 | 1:309:A:PHE:HD1  | 7        | 1.2           |
| (3,730) | 1:301:A:LEU:HD13 | 1:309:A:PHE:HD1  | 7        | 1.2           |
| (3,730) | 1:301:A:LEU:HD21 | 1:309:A:PHE:HD1  | 7        | 1.2           |
| (3,730) | 1:301:A:LEU:HD22 | 1:309:A:PHE:HD1  | 7        | 1.2           |
| (3,730) | 1:301:A:LEU:HD23 | 1:309:A:PHE:HD1  | 7        | 1.2           |
| (3,660) | 1:309:A:PHE:HD1  | 1:341:A:LEU:HD21 | 2        | 1.15          |
| (3,660) | 1:309:A:PHE:HD1  | 1:341:A:LEU:HD22 | 2        | 1.15          |
| (3,660) | 1:309:A:PHE:HD1  | 1:341:A:LEU:HD23 | 2        | 1.15          |
| (3,640) | 1:331:A:TYR:HA   | 1:331:A:TYR:HD2  | 9        | 1.15          |
| (3,640) | 1:331:A:TYR:HA   | 1:331:A:TYR:HD2  | 10       | 1.15          |
| (3,572) | 1:331:A:TYR:HE1  | 1:332:A:HIS:H    | 9        | 1.15          |
| (3,572) | 1:331:A:TYR:HE1  | 1:332:A:HIS:H    | 10       | 1.15          |
| (3,660) | 1:309:A:PHE:HD1  | 1:341:A:LEU:HD21 | 1        | 1.13          |
| (3,660) | 1:309:A:PHE:HD1  | 1:341:A:LEU:HD22 | 1        | 1.13          |
| (3,660) | 1:309:A:PHE:HD1  | 1:341:A:LEU:HD23 | 1        | 1.13          |
| (3,640) | 1:331:A:TYR:HA   | 1:331:A:TYR:HD2  | 1        | 1.12          |
| (3,640) | 1:331:A:TYR:HA   | 1:331:A:TYR:HD2  | 4        | 1.12          |
| (3,640) | 1:331:A:TYR:HA   | 1:331:A:TYR:HD2  | 2        | 1.11          |
| (3,640) | 1:331:A:TYR:HA   | 1:331:A:TYR:HD2  | 3        | 1.11          |
| (3,640) | 1:331:A:TYR:HA   | 1:331:A:TYR:HD2  | 5        | 1.11          |
| (3,640) | 1:331:A:TYR:HA   | 1:331:A:TYR:HD2  | 7        | 1.11          |
| (3,640) | 1:331:A:TYR:HA   | 1:331:A:TYR:HD2  | 8        | 1.11          |
| (3,640) | 1:331:A:TYR:HA   | 1:331:A:TYR:HD2  | 6        | 1.1           |
| (3,572) | 1:331:A:TYR:HE1  | 1:332:A:HIS:H    | 3        | 1.07          |
| (3,572) | 1:331:A:TYR:HE1  | 1:332:A:HIS:H    | 4        | 1.07          |
| (3,662) | 1:309:A:PHE:HE1  | 1:341:A:LEU:HD21 | 4        | 1.06          |
| (3,662) | 1:309:A:PHE:HE1  | 1:341:A:LEU:HD22 | 4        | 1.06          |
| (3,662) | 1:309:A:PHE:HE1  | 1:341:A:LEU:HD23 | 4        | 1.06          |
| (3,572) | 1:331:A:TYR:HE1  | 1:332:A:HIS:H    | 1        | 1.06          |
| (3,572) | 1:331:A:TYR:HE1  | 1:332:A:HIS:H    | 7        | 1.06          |
| (3,572) | 1:331:A:TYR:HE1  | 1:332:A:HIS:H    | 2        | 1.05          |
| (3,572) | 1:331:A:TYR:HE1  | 1:332:A:HIS:H    | 5        | 1.02          |
| (3,572) | 1:331:A:TYR:HE1  | 1:332:A:HIS:H    | 8        | 1.02          |
| (3,572) | 1:331:A:TYR:HE1  | 1:332:A:HIS:H    | 6        | 1.0           |
| (3,662) | 1:309:A:PHE:HE1  | 1:341:A:LEU:HD21 | 9        | 0.97          |
| (3,662) | 1:309:A:PHE:HE1  | 1:341:A:LEU:HD22 | 9        | 0.97          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,662) | 1:309:A:PHE:HE1  | 1:341:A:LEU:HD23 | 9        | 0.97          |
| (2,13)  | 1:319:A:ASP:O    | 1:323:A:LYS:N    | 9        | 0.97          |
| (3,745) | 1:305:A:LEU:HD11 | 1:309:A:PHE:HE1  | 3        | 0.93          |
| (3,745) | 1:305:A:LEU:HD12 | 1:309:A:PHE:HE1  | 3        | 0.93          |
| (3,745) | 1:305:A:LEU:HD13 | 1:309:A:PHE:HE1  | 3        | 0.93          |
| (3,745) | 1:305:A:LEU:HD21 | 1:309:A:PHE:HE1  | 3        | 0.93          |
| (3,745) | 1:305:A:LEU:HD22 | 1:309:A:PHE:HE1  | 3        | 0.93          |
| (3,745) | 1:305:A:LEU:HD23 | 1:309:A:PHE:HE1  | 3        | 0.93          |
| (2,9)   | 1:315:A:GLN:O    | 1:319:A:ASP:N    | 7        | 0.91          |
| (3,661) | 1:309:A:PHE:HE1  | 1:341:A:LEU:HG   | 4        | 0.9           |
| (2,47)  | 1:319:A:ASP:O    | 1:323:A:LYS:H    | 9        | 0.9           |
| (2,13)  | 1:319:A:ASP:O    | 1:323:A:LYS:N    | 2        | 0.89          |
| (2,9)   | 1:315:A:GLN:O    | 1:319:A:ASP:N    | 6        | 0.87          |
| (2,13)  | 1:319:A:ASP:O    | 1:323:A:LYS:N    | 4        | 0.86          |
| (2,10)  | 1:316:A:MET:O    | 1:320:A:ALA:N    | 6        | 0.85          |
| (2,10)  | 1:316:A:MET:O    | 1:320:A:ALA:N    | 7        | 0.85          |
| (2,47)  | 1:319:A:ASP:O    | 1:323:A:LYS:H    | 2        | 0.83          |
| (3,661) | 1:309:A:PHE:HE1  | 1:341:A:LEU:HG   | 9        | 0.82          |
| (2,13)  | 1:319:A:ASP:O    | 1:323:A:LYS:N    | 1        | 0.82          |
| (3,662) | 1:309:A:PHE:HE1  | 1:341:A:LEU:HD21 | 2        | 0.81          |
| (3,662) | 1:309:A:PHE:HE1  | 1:341:A:LEU:HD22 | 2        | 0.81          |
| (3,662) | 1:309:A:PHE:HE1  | 1:341:A:LEU:HD23 | 2        | 0.81          |
| (3,662) | 1:309:A:PHE:HE1  | 1:341:A:LEU:HD21 | 1        | 0.8           |
| (3,662) | 1:309:A:PHE:HE1  | 1:341:A:LEU:HD22 | 1        | 0.8           |
| (3,662) | 1:309:A:PHE:HE1  | 1:341:A:LEU:HD23 | 1        | 0.8           |
| (2,47)  | 1:319:A:ASP:O    | 1:323:A:LYS:H    | 4        | 0.8           |
| (3,745) | 1:305:A:LEU:HD11 | 1:309:A:PHE:HE1  | 10       | 0.78          |
| (3,745) | 1:305:A:LEU:HD12 | 1:309:A:PHE:HE1  | 10       | 0.78          |
| (3,745) | 1:305:A:LEU:HD13 | 1:309:A:PHE:HE1  | 10       | 0.78          |
| (3,745) | 1:305:A:LEU:HD21 | 1:309:A:PHE:HE1  | 10       | 0.78          |
| (3,745) | 1:305:A:LEU:HD22 | 1:309:A:PHE:HE1  | 10       | 0.78          |
| (3,745) | 1:305:A:LEU:HD23 | 1:309:A:PHE:HE1  | 10       | 0.78          |
| (3,660) | 1:309:A:PHE:HD1  | 1:341:A:LEU:HD21 | 8        | 0.78          |
| (3,660) | 1:309:A:PHE:HD1  | 1:341:A:LEU:HD22 | 8        | 0.78          |
| (3,660) | 1:309:A:PHE:HD1  | 1:341:A:LEU:HD23 | 8        | 0.78          |
| (2,39)  | 1:315:A:GLN:O    | 1:319:A:ASP:H    | 7        | 0.78          |
| (3,660) | 1:309:A:PHE:HD1  | 1:341:A:LEU:HD21 | 3        | 0.77          |
| (3,660) | 1:309:A:PHE:HD1  | 1:341:A:LEU:HD22 | 3        | 0.77          |
| (3,660) | 1:309:A:PHE:HD1  | 1:341:A:LEU:HD23 | 3        | 0.77          |
| (2,47)  | 1:319:A:ASP:O    | 1:323:A:LYS:H    | 1        | 0.76          |
| (2,39)  | 1:315:A:GLN:O    | 1:319:A:ASP:H    | 6        | 0.75          |
| (2,10)  | 1:316:A:MET:O    | 1:320:A:ALA:N    | 3        | 0.74          |

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| Key     | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (2,9)   | 1:315:A:GLN:O   | 1:319:A:ASP:N    | 3        | 0.73          |
| (2,10)  | 1:316:A:MET:O   | 1:320:A:ALA:N    | 10       | 0.71          |
| (2,10)  | 1:316:A:MET:O   | 1:320:A:ALA:N    | 8        | 0.7           |
| (2,9)   | 1:315:A:GLN:O   | 1:319:A:ASP:N    | 8        | 0.7           |
| (2,9)   | 1:315:A:GLN:O   | 1:319:A:ASP:N    | 10       | 0.7           |
| (2,41)  | 1:316:A:MET:O   | 1:320:A:ALA:H    | 6        | 0.68          |
| (2,11)  | 1:317:A:LEU:O   | 1:321:A:ILE:N    | 1        | 0.68          |
| (2,7)   | 1:307:A:LYS:O   | 1:311:A:VAL:N    | 6        | 0.68          |
| (2,7)   | 1:307:A:LYS:O   | 1:311:A:VAL:N    | 7        | 0.68          |
| (2,48)  | 1:319:A:ASP:O   | 1:323:A:LYS:N    | 9        | 0.67          |
| (2,41)  | 1:316:A:MET:O   | 1:320:A:ALA:H    | 7        | 0.67          |
| (2,7)   | 1:307:A:LYS:O   | 1:311:A:VAL:N    | 9        | 0.67          |
| (3,672) | 1:331:A:TYR:HE2 | 1:335:A:ARG:HG2  | 6        | 0.66          |
| (2,11)  | 1:317:A:LEU:O   | 1:321:A:ILE:N    | 4        | 0.66          |
| (2,7)   | 1:307:A:LYS:O   | 1:311:A:VAL:N    | 10       | 0.66          |
| (2,11)  | 1:317:A:LEU:O   | 1:321:A:ILE:N    | 3        | 0.65          |
| (2,10)  | 1:316:A:MET:O   | 1:320:A:ALA:N    | 5        | 0.65          |
| (2,7)   | 1:307:A:LYS:O   | 1:311:A:VAL:N    | 1        | 0.65          |
| (2,7)   | 1:307:A:LYS:O   | 1:311:A:VAL:N    | 5        | 0.65          |
| (3,672) | 1:331:A:TYR:HE2 | 1:335:A:ARG:HG2  | 5        | 0.64          |
| (2,12)  | 1:318:A:GLN:O   | 1:322:A:SER:N    | 4        | 0.64          |
| (2,11)  | 1:317:A:LEU:O   | 1:321:A:ILE:N    | 2        | 0.64          |
| (2,7)   | 1:307:A:LYS:O   | 1:311:A:VAL:N    | 2        | 0.64          |
| (2,7)   | 1:307:A:LYS:O   | 1:311:A:VAL:N    | 3        | 0.64          |
| (2,7)   | 1:307:A:LYS:O   | 1:311:A:VAL:N    | 4        | 0.64          |
| (2,7)   | 1:307:A:LYS:O   | 1:311:A:VAL:N    | 8        | 0.64          |
| (3,672) | 1:331:A:TYR:HE2 | 1:335:A:ARG:HG2  | 8        | 0.63          |
| (3,661) | 1:309:A:PHE:HE1 | 1:341:A:LEU:HG   | 2        | 0.62          |
| (2,12)  | 1:318:A:GLN:O   | 1:322:A:SER:N    | 2        | 0.62          |
| (2,11)  | 1:317:A:LEU:O   | 1:321:A:ILE:N    | 8        | 0.62          |
| (2,9)   | 1:315:A:GLN:O   | 1:319:A:ASP:N    | 5        | 0.62          |
| (2,40)  | 1:315:A:GLN:O   | 1:319:A:ASP:N    | 7        | 0.61          |
| (2,6)   | 1:306:A:GLN:O   | 1:310:A:ASP:N    | 3        | 0.61          |
| (3,661) | 1:309:A:PHE:HE1 | 1:341:A:LEU:HG   | 1        | 0.6           |
| (3,660) | 1:309:A:PHE:HD1 | 1:341:A:LEU:HD21 | 5        | 0.6           |
| (3,660) | 1:309:A:PHE:HD1 | 1:341:A:LEU:HD22 | 5        | 0.6           |
| (3,660) | 1:309:A:PHE:HD1 | 1:341:A:LEU:HD23 | 5        | 0.6           |
| (3,659) | 1:309:A:PHE:HD1 | 1:341:A:LEU:HG   | 4        | 0.6           |
| (2,39)  | 1:315:A:GLN:O   | 1:319:A:ASP:H    | 3        | 0.6           |
| (2,11)  | 1:317:A:LEU:O   | 1:321:A:ILE:N    | 5        | 0.6           |
| (2,11)  | 1:317:A:LEU:O   | 1:321:A:ILE:N    | 9        | 0.6           |
| (2,6)   | 1:306:A:GLN:O   | 1:310:A:ASP:N    | 8        | 0.6           |

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| Key     | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (2,48)  | 1:319:A:ASP:O   | 1:323:A:LYS:N    | 2        | 0.59          |
| (3,660) | 1:309:A:PHE:HD1 | 1:341:A:LEU:HD21 | 10       | 0.58          |
| (3,660) | 1:309:A:PHE:HD1 | 1:341:A:LEU:HD22 | 10       | 0.58          |
| (3,660) | 1:309:A:PHE:HD1 | 1:341:A:LEU:HD23 | 10       | 0.58          |
| (3,659) | 1:309:A:PHE:HD1 | 1:341:A:LEU:HG   | 9        | 0.58          |
| (2,12)  | 1:318:A:GLN:O   | 1:322:A:SER:N    | 1        | 0.58          |
| (2,11)  | 1:317:A:LEU:O   | 1:321:A:ILE:N    | 10       | 0.58          |
| (2,10)  | 1:316:A:MET:O   | 1:320:A:ALA:N    | 9        | 0.58          |
| (2,41)  | 1:316:A:MET:O   | 1:320:A:ALA:H    | 3        | 0.57          |
| (2,40)  | 1:315:A:GLN:O   | 1:319:A:ASP:N    | 6        | 0.57          |
| (2,39)  | 1:315:A:GLN:O   | 1:319:A:ASP:H    | 8        | 0.57          |
| (2,39)  | 1:315:A:GLN:O   | 1:319:A:ASP:H    | 10       | 0.57          |
| (2,14)  | 1:327:A:THR:O   | 1:331:A:TYR:N    | 4        | 0.57          |
| (2,11)  | 1:317:A:LEU:O   | 1:321:A:ILE:N    | 7        | 0.57          |
| (2,9)   | 1:315:A:GLN:O   | 1:319:A:ASP:N    | 9        | 0.57          |
| (2,48)  | 1:319:A:ASP:O   | 1:323:A:LYS:N    | 4        | 0.56          |
| (2,9)   | 1:315:A:GLN:O   | 1:319:A:ASP:N    | 2        | 0.56          |
| (2,9)   | 1:315:A:GLN:O   | 1:319:A:ASP:N    | 4        | 0.56          |
| (2,42)  | 1:316:A:MET:O   | 1:320:A:ALA:N    | 6        | 0.55          |
| (2,42)  | 1:316:A:MET:O   | 1:320:A:ALA:N    | 7        | 0.55          |
| (2,14)  | 1:327:A:THR:O   | 1:331:A:TYR:N    | 1        | 0.55          |
| (2,14)  | 1:327:A:THR:O   | 1:331:A:TYR:N    | 2        | 0.55          |
| (2,6)   | 1:306:A:GLN:O   | 1:310:A:ASP:N    | 5        | 0.55          |
| (2,6)   | 1:306:A:GLN:O   | 1:310:A:ASP:N    | 10       | 0.55          |
| (2,21)  | 1:334:A:GLN:O   | 1:338:A:ASP:N    | 8        | 0.54          |
| (2,13)  | 1:319:A:ASP:O   | 1:323:A:LYS:N    | 5        | 0.54          |
| (2,9)   | 1:315:A:GLN:O   | 1:319:A:ASP:N    | 1        | 0.54          |
| (2,6)   | 1:306:A:GLN:O   | 1:310:A:ASP:N    | 1        | 0.54          |
| (2,41)  | 1:316:A:MET:O   | 1:320:A:ALA:H    | 10       | 0.53          |
| (2,14)  | 1:327:A:THR:O   | 1:331:A:TYR:N    | 9        | 0.53          |
| (2,14)  | 1:327:A:THR:O   | 1:331:A:TYR:N    | 10       | 0.53          |
| (2,12)  | 1:318:A:GLN:O   | 1:322:A:SER:N    | 9        | 0.53          |
| (2,10)  | 1:316:A:MET:O   | 1:320:A:ALA:N    | 2        | 0.53          |
| (2,6)   | 1:306:A:GLN:O   | 1:310:A:ASP:N    | 9        | 0.53          |
| (3,672) | 1:331:A:TYR:HE2 | 1:335:A:ARG:HG2  | 3        | 0.52          |
| (2,48)  | 1:319:A:ASP:O   | 1:323:A:LYS:N    | 1        | 0.52          |
| (2,41)  | 1:316:A:MET:O   | 1:320:A:ALA:H    | 8        | 0.52          |
| (2,21)  | 1:334:A:GLN:O   | 1:338:A:ASP:N    | 5        | 0.52          |
| (2,14)  | 1:327:A:THR:O   | 1:331:A:TYR:N    | 3        | 0.52          |
| (2,43)  | 1:317:A:LEU:O   | 1:321:A:ILE:H    | 1        | 0.51          |
| (2,43)  | 1:317:A:LEU:O   | 1:321:A:ILE:H    | 4        | 0.51          |
| (2,35)  | 1:307:A:LYS:O   | 1:311:A:VAL:H    | 6        | 0.51          |

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| Key     | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|---------|------------------|-----------------|----------|---------------|
| (2,35)  | 1:307:A:LYS:O    | 1:311:A:VAL:H   | 7        | 0.51          |
| (2,10)  | 1:316:A:MET:O    | 1:320:A:ALA:N   | 4        | 0.51          |
| (3,659) | 1:309:A:PHE:HD1  | 1:341:A:LEU:HG  | 2        | 0.5           |
| (2,35)  | 1:307:A:LYS:O    | 1:311:A:VAL:H   | 9        | 0.5           |
| (2,19)  | 1:332:A:HIS:O    | 1:336:A:CYS:N   | 1        | 0.5           |
| (2,14)  | 1:327:A:THR:O    | 1:331:A:TYR:N   | 5        | 0.5           |
| (2,13)  | 1:319:A:ASP:O    | 1:323:A:LYS:N   | 10       | 0.5           |
| (3,659) | 1:309:A:PHE:HD1  | 1:341:A:LEU:HG  | 1        | 0.49          |
| (2,43)  | 1:317:A:LEU:O    | 1:321:A:ILE:H   | 2        | 0.49          |
| (2,41)  | 1:316:A:MET:O    | 1:320:A:ALA:H   | 5        | 0.49          |
| (2,35)  | 1:307:A:LYS:O    | 1:311:A:VAL:H   | 10       | 0.49          |
| (2,10)  | 1:316:A:MET:O    | 1:320:A:ALA:N   | 1        | 0.49          |
| (2,6)   | 1:306:A:GLN:O    | 1:310:A:ASP:N   | 4        | 0.49          |
| (2,39)  | 1:315:A:GLN:O    | 1:319:A:ASP:H   | 5        | 0.48          |
| (2,35)  | 1:307:A:LYS:O    | 1:311:A:VAL:H   | 1        | 0.48          |
| (2,35)  | 1:307:A:LYS:O    | 1:311:A:VAL:H   | 2        | 0.48          |
| (2,14)  | 1:327:A:THR:O    | 1:331:A:TYR:N   | 8        | 0.48          |
| (2,6)   | 1:306:A:GLN:O    | 1:310:A:ASP:N   | 2        | 0.48          |
| (2,35)  | 1:307:A:LYS:O    | 1:311:A:VAL:H   | 3        | 0.47          |
| (2,35)  | 1:307:A:LYS:O    | 1:311:A:VAL:H   | 4        | 0.47          |
| (2,35)  | 1:307:A:LYS:O    | 1:311:A:VAL:H   | 5        | 0.47          |
| (2,21)  | 1:334:A:GLN:O    | 1:338:A:ASP:N   | 9        | 0.47          |
| (2,21)  | 1:334:A:GLN:O    | 1:338:A:ASP:N   | 10       | 0.47          |
| (2,19)  | 1:332:A:HIS:O    | 1:336:A:CYS:N   | 9        | 0.47          |
| (2,13)  | 1:319:A:ASP:O    | 1:323:A:LYS:N   | 7        | 0.47          |
| (2,11)  | 1:317:A:LEU:O    | 1:321:A:ILE:N   | 6        | 0.47          |
| (2,6)   | 1:306:A:GLN:O    | 1:310:A:ASP:N   | 7        | 0.47          |
| (2,43)  | 1:317:A:LEU:O    | 1:321:A:ILE:H   | 3        | 0.46          |
| (2,35)  | 1:307:A:LYS:O    | 1:311:A:VAL:H   | 8        | 0.46          |
| (2,19)  | 1:332:A:HIS:O    | 1:336:A:CYS:N   | 7        | 0.46          |
| (2,14)  | 1:327:A:THR:O    | 1:331:A:TYR:N   | 6        | 0.46          |
| (2,6)   | 1:306:A:GLN:O    | 1:310:A:ASP:N   | 6        | 0.46          |
| (3,745) | 1:305:A:LEU:HD11 | 1:309:A:PHE:HE1 | 5        | 0.45          |
| (3,745) | 1:305:A:LEU:HD12 | 1:309:A:PHE:HE1 | 5        | 0.45          |
| (3,745) | 1:305:A:LEU:HD13 | 1:309:A:PHE:HE1 | 5        | 0.45          |
| (3,745) | 1:305:A:LEU:HD21 | 1:309:A:PHE:HE1 | 5        | 0.45          |
| (3,745) | 1:305:A:LEU:HD22 | 1:309:A:PHE:HE1 | 5        | 0.45          |
| (3,745) | 1:305:A:LEU:HD23 | 1:309:A:PHE:HE1 | 5        | 0.45          |
| (3,731) | 1:301:A:LEU:HD11 | 1:309:A:PHE:HE1 | 6        | 0.45          |
| (3,731) | 1:301:A:LEU:HD12 | 1:309:A:PHE:HE1 | 6        | 0.45          |
| (3,731) | 1:301:A:LEU:HD13 | 1:309:A:PHE:HE1 | 6        | 0.45          |
| (3,731) | 1:301:A:LEU:HD21 | 1:309:A:PHE:HE1 | 6        | 0.45          |

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| Key     | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|---------|------------------|-----------------|----------|---------------|
| (3,731) | 1:301:A:LEU:HD22 | 1:309:A:PHE:HE1 | 6        | 0.45          |
| (3,731) | 1:301:A:LEU:HD23 | 1:309:A:PHE:HE1 | 6        | 0.45          |
| (2,45)  | 1:318:A:GLN:O    | 1:322:A:SER:H   | 4        | 0.45          |
| (2,43)  | 1:317:A:LEU:O    | 1:321:A:ILE:H   | 9        | 0.45          |
| (2,21)  | 1:334:A:GLN:O    | 1:338:A:ASP:N   | 6        | 0.45          |
| (2,19)  | 1:332:A:HIS:O    | 1:336:A:CYS:N   | 2        | 0.45          |
| (2,45)  | 1:318:A:GLN:O    | 1:322:A:SER:H   | 2        | 0.44          |
| (2,42)  | 1:316:A:MET:O    | 1:320:A:ALA:N   | 3        | 0.44          |
| (2,19)  | 1:332:A:HIS:O    | 1:336:A:CYS:N   | 4        | 0.44          |
| (2,15)  | 1:328:A:ASP:O    | 1:332:A:HIS:N   | 5        | 0.44          |
| (2,15)  | 1:328:A:ASP:O    | 1:332:A:HIS:N   | 8        | 0.44          |
| (2,14)  | 1:327:A:THR:O    | 1:331:A:TYR:N   | 7        | 0.44          |
| (3,672) | 1:331:A:TYR:HE2  | 1:335:A:ARG:HG2 | 2        | 0.43          |
| (3,672) | 1:331:A:TYR:HE2  | 1:335:A:ARG:HG2 | 10       | 0.43          |
| (2,43)  | 1:317:A:LEU:O    | 1:321:A:ILE:H   | 5        | 0.43          |
| (2,43)  | 1:317:A:LEU:O    | 1:321:A:ILE:H   | 8        | 0.43          |
| (2,40)  | 1:315:A:GLN:O    | 1:319:A:ASP:N   | 3        | 0.43          |
| (2,39)  | 1:315:A:GLN:O    | 1:319:A:ASP:H   | 9        | 0.43          |
| (2,15)  | 1:328:A:ASP:O    | 1:332:A:HIS:N   | 7        | 0.43          |
| (3,672) | 1:331:A:TYR:HE2  | 1:335:A:ARG:HG2 | 4        | 0.42          |
| (3,656) | 1:306:A:GLN:HA   | 1:309:A:PHE:HD1 | 6        | 0.42          |
| (3,656) | 1:306:A:GLN:HA   | 1:309:A:PHE:HD1 | 7        | 0.42          |
| (2,39)  | 1:315:A:GLN:O    | 1:319:A:ASP:H   | 2        | 0.42          |
| (2,33)  | 1:306:A:GLN:O    | 1:310:A:ASP:H   | 3        | 0.42          |
| (2,15)  | 1:328:A:ASP:O    | 1:332:A:HIS:N   | 6        | 0.42          |
| (2,15)  | 1:328:A:ASP:O    | 1:332:A:HIS:N   | 9        | 0.42          |
| (2,13)  | 1:319:A:ASP:O    | 1:323:A:LYS:N   | 6        | 0.42          |
| (3,731) | 1:301:A:LEU:HD11 | 1:309:A:PHE:HE1 | 7        | 0.41          |
| (3,731) | 1:301:A:LEU:HD12 | 1:309:A:PHE:HE1 | 7        | 0.41          |
| (3,731) | 1:301:A:LEU:HD13 | 1:309:A:PHE:HE1 | 7        | 0.41          |
| (3,731) | 1:301:A:LEU:HD21 | 1:309:A:PHE:HE1 | 7        | 0.41          |
| (3,731) | 1:301:A:LEU:HD22 | 1:309:A:PHE:HE1 | 7        | 0.41          |
| (3,731) | 1:301:A:LEU:HD23 | 1:309:A:PHE:HE1 | 7        | 0.41          |
| (2,42)  | 1:316:A:MET:O    | 1:320:A:ALA:N   | 10       | 0.41          |
| (2,39)  | 1:315:A:GLN:O    | 1:319:A:ASP:H   | 4        | 0.41          |
| (2,33)  | 1:306:A:GLN:O    | 1:310:A:ASP:H   | 8        | 0.41          |
| (2,18)  | 1:331:A:TYR:O    | 1:335:A:ARG:N   | 3        | 0.41          |
| (2,15)  | 1:328:A:ASP:O    | 1:332:A:HIS:N   | 1        | 0.41          |
| (2,15)  | 1:328:A:ASP:O    | 1:332:A:HIS:N   | 2        | 0.41          |
| (3,443) | 1:364:A:LEU:H    | 1:364:A:LEU:HG  | 7        | 0.4           |
| (2,47)  | 1:319:A:ASP:O    | 1:323:A:LYS:H   | 5        | 0.4           |
| (2,43)  | 1:317:A:LEU:O    | 1:321:A:ILE:H   | 10       | 0.4           |

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| Key     | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (2,42)  | 1:316:A:MET:O   | 1:320:A:ALA:N    | 8        | 0.4           |
| (2,41)  | 1:316:A:MET:O   | 1:320:A:ALA:H    | 9        | 0.4           |
| (2,40)  | 1:315:A:GLN:O   | 1:319:A:ASP:N    | 8        | 0.4           |
| (2,40)  | 1:315:A:GLN:O   | 1:319:A:ASP:N    | 10       | 0.4           |
| (2,18)  | 1:331:A:TYR:O   | 1:335:A:ARG:N    | 2        | 0.4           |
| (2,18)  | 1:331:A:TYR:O   | 1:335:A:ARG:N    | 4        | 0.4           |
| (2,15)  | 1:328:A:ASP:O   | 1:332:A:HIS:N    | 4        | 0.4           |
| (2,15)  | 1:328:A:ASP:O   | 1:332:A:HIS:N    | 10       | 0.4           |
| (2,49)  | 1:327:A:THR:O   | 1:331:A:TYR:H    | 4        | 0.39          |
| (2,45)  | 1:318:A:GLN:O   | 1:322:A:SER:H    | 1        | 0.39          |
| (2,39)  | 1:315:A:GLN:O   | 1:319:A:ASP:H    | 1        | 0.39          |
| (2,15)  | 1:328:A:ASP:O   | 1:332:A:HIS:N    | 3        | 0.39          |
| (2,49)  | 1:327:A:THR:O   | 1:331:A:TYR:H    | 1        | 0.38          |
| (2,44)  | 1:317:A:LEU:O   | 1:321:A:ILE:N    | 1        | 0.38          |
| (2,36)  | 1:307:A:LYS:O   | 1:311:A:VAL:N    | 6        | 0.38          |
| (2,36)  | 1:307:A:LYS:O   | 1:311:A:VAL:N    | 7        | 0.38          |
| (2,33)  | 1:306:A:GLN:O   | 1:310:A:ASP:H    | 5        | 0.38          |
| (2,33)  | 1:306:A:GLN:O   | 1:310:A:ASP:H    | 10       | 0.38          |
| (2,18)  | 1:331:A:TYR:O   | 1:335:A:ARG:N    | 1        | 0.38          |
| (3,672) | 1:331:A:TYR:HE2 | 1:335:A:ARG:HG2  | 7        | 0.37          |
| (3,29)  | 1:342:A:TRP:HA  | 1:342:A:TRP:HE3  | 5        | 0.37          |
| (2,49)  | 1:327:A:THR:O   | 1:331:A:TYR:H    | 2        | 0.37          |
| (2,49)  | 1:327:A:THR:O   | 1:331:A:TYR:H    | 9        | 0.37          |
| (2,43)  | 1:317:A:LEU:O   | 1:321:A:ILE:H    | 7        | 0.37          |
| (2,36)  | 1:307:A:LYS:O   | 1:311:A:VAL:N    | 9        | 0.37          |
| (2,33)  | 1:306:A:GLN:O   | 1:310:A:ASP:H    | 1        | 0.37          |
| (2,18)  | 1:331:A:TYR:O   | 1:335:A:ARG:N    | 7        | 0.37          |
| (2,5)   | 1:305:A:LEU:O   | 1:309:A:PHE:N    | 1        | 0.37          |
| (2,5)   | 1:305:A:LEU:O   | 1:309:A:PHE:N    | 2        | 0.37          |
| (2,5)   | 1:305:A:LEU:O   | 1:309:A:PHE:N    | 3        | 0.37          |
| (2,5)   | 1:305:A:LEU:O   | 1:309:A:PHE:N    | 8        | 0.37          |
| (3,672) | 1:331:A:TYR:HE2 | 1:335:A:ARG:HG2  | 1        | 0.36          |
| (3,662) | 1:309:A:PHE:HE1 | 1:341:A:LEU:HD21 | 8        | 0.36          |
| (3,662) | 1:309:A:PHE:HE1 | 1:341:A:LEU:HD22 | 8        | 0.36          |
| (3,662) | 1:309:A:PHE:HE1 | 1:341:A:LEU:HD23 | 8        | 0.36          |
| (2,47)  | 1:319:A:ASP:O   | 1:323:A:LYS:H    | 10       | 0.36          |
| (2,44)  | 1:317:A:LEU:O   | 1:321:A:ILE:N    | 4        | 0.36          |
| (2,36)  | 1:307:A:LYS:O   | 1:311:A:VAL:N    | 10       | 0.36          |
| (2,33)  | 1:306:A:GLN:O   | 1:310:A:ASP:H    | 9        | 0.36          |
| (2,20)  | 1:333:A:MET:O   | 1:337:A:ILE:N    | 1        | 0.36          |
| (2,12)  | 1:318:A:GLN:O   | 1:322:A:SER:N    | 10       | 0.36          |
| (2,5)   | 1:305:A:LEU:O   | 1:309:A:PHE:N    | 4        | 0.36          |

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| Key     | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|---------|------------------|-----------------|----------|---------------|
| (2,5)   | 1:305:A:LEU:O    | 1:309:A:PHE:N   | 5        | 0.36          |
| (3,672) | 1:331:A:TYR:HE2  | 1:335:A:ARG:HG2 | 9        | 0.35          |
| (2,49)  | 1:327:A:THR:O    | 1:331:A:TYR:H   | 10       | 0.35          |
| (2,44)  | 1:317:A:LEU:O    | 1:321:A:ILE:N   | 3        | 0.35          |
| (2,42)  | 1:316:A:MET:O    | 1:320:A:ALA:N   | 5        | 0.35          |
| (2,36)  | 1:307:A:LYS:O    | 1:311:A:VAL:N   | 1        | 0.35          |
| (2,36)  | 1:307:A:LYS:O    | 1:311:A:VAL:N   | 5        | 0.35          |
| (2,20)  | 1:333:A:MET:O    | 1:337:A:ILE:N   | 7        | 0.35          |
| (2,19)  | 1:332:A:HIS:O    | 1:336:A:CYS:N   | 3        | 0.35          |
| (2,18)  | 1:331:A:TYR:O    | 1:335:A:ARG:N   | 9        | 0.35          |
| (2,12)  | 1:318:A:GLN:O    | 1:322:A:SER:N   | 5        | 0.35          |
| (2,5)   | 1:305:A:LEU:O    | 1:309:A:PHE:N   | 9        | 0.35          |
| (2,49)  | 1:327:A:THR:O    | 1:331:A:TYR:H   | 3        | 0.34          |
| (2,46)  | 1:318:A:GLN:O    | 1:322:A:SER:N   | 4        | 0.34          |
| (2,45)  | 1:318:A:GLN:O    | 1:322:A:SER:H   | 9        | 0.34          |
| (2,44)  | 1:317:A:LEU:O    | 1:321:A:ILE:N   | 2        | 0.34          |
| (2,41)  | 1:316:A:MET:O    | 1:320:A:ALA:H   | 2        | 0.34          |
| (2,36)  | 1:307:A:LYS:O    | 1:311:A:VAL:N   | 2        | 0.34          |
| (2,36)  | 1:307:A:LYS:O    | 1:311:A:VAL:N   | 3        | 0.34          |
| (2,36)  | 1:307:A:LYS:O    | 1:311:A:VAL:N   | 4        | 0.34          |
| (2,36)  | 1:307:A:LYS:O    | 1:311:A:VAL:N   | 8        | 0.34          |
| (2,21)  | 1:334:A:GLN:O    | 1:338:A:ASP:N   | 3        | 0.34          |
| (2,47)  | 1:319:A:ASP:O    | 1:323:A:LYS:H   | 7        | 0.33          |
| (2,20)  | 1:333:A:MET:O    | 1:337:A:ILE:N   | 2        | 0.33          |
| (2,20)  | 1:333:A:MET:O    | 1:337:A:ILE:N   | 4        | 0.33          |
| (2,13)  | 1:319:A:ASP:O    | 1:323:A:LYS:N   | 8        | 0.33          |
| (3,745) | 1:305:A:LEU:HD11 | 1:309:A:PHE:HE1 | 8        | 0.32          |
| (3,745) | 1:305:A:LEU:HD12 | 1:309:A:PHE:HE1 | 8        | 0.32          |
| (3,745) | 1:305:A:LEU:HD13 | 1:309:A:PHE:HE1 | 8        | 0.32          |
| (3,745) | 1:305:A:LEU:HD21 | 1:309:A:PHE:HE1 | 8        | 0.32          |
| (3,745) | 1:305:A:LEU:HD22 | 1:309:A:PHE:HE1 | 8        | 0.32          |
| (3,745) | 1:305:A:LEU:HD23 | 1:309:A:PHE:HE1 | 8        | 0.32          |
| (3,671) | 1:331:A:TYR:HB2  | 1:331:A:TYR:HE2 | 6        | 0.32          |
| (3,671) | 1:331:A:TYR:HB2  | 1:331:A:TYR:HE2 | 8        | 0.32          |
| (3,442) | 1:363:A:LEU:HA   | 1:364:A:LEU:H   | 3        | 0.32          |
| (3,442) | 1:363:A:LEU:HA   | 1:364:A:LEU:H   | 7        | 0.32          |
| (3,442) | 1:363:A:LEU:HA   | 1:364:A:LEU:H   | 9        | 0.32          |
| (3,442) | 1:363:A:LEU:HA   | 1:364:A:LEU:H   | 10       | 0.32          |
| (3,380) | 1:314:A:VAL:HB   | 1:315:A:GLN:H   | 7        | 0.32          |
| (2,49)  | 1:327:A:THR:O    | 1:331:A:TYR:H   | 5        | 0.32          |
| (2,46)  | 1:318:A:GLN:O    | 1:322:A:SER:N   | 2        | 0.32          |
| (2,44)  | 1:317:A:LEU:O    | 1:321:A:ILE:N   | 8        | 0.32          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (2,41)  | 1:316:A:MET:O   | 1:320:A:ALA:H   | 4        | 0.32          |
| (2,40)  | 1:315:A:GLN:O   | 1:319:A:ASP:N   | 5        | 0.32          |
| (2,33)  | 1:306:A:GLN:O   | 1:310:A:ASP:H   | 4        | 0.32          |
| (2,20)  | 1:333:A:MET:O   | 1:337:A:ILE:N   | 10       | 0.32          |
| (2,18)  | 1:331:A:TYR:O   | 1:335:A:ARG:N   | 6        | 0.32          |
| (2,5)   | 1:305:A:LEU:O   | 1:309:A:PHE:N   | 10       | 0.32          |
| (3,671) | 1:331:A:TYR:HB2 | 1:331:A:TYR:HE2 | 2        | 0.31          |
| (3,671) | 1:331:A:TYR:HB2 | 1:331:A:TYR:HE2 | 5        | 0.31          |
| (3,671) | 1:331:A:TYR:HB2 | 1:331:A:TYR:HE2 | 7        | 0.31          |
| (2,34)  | 1:306:A:GLN:O   | 1:310:A:ASP:N   | 3        | 0.31          |
| (2,33)  | 1:306:A:GLN:O   | 1:310:A:ASP:H   | 2        | 0.31          |
| (2,18)  | 1:331:A:TYR:O   | 1:335:A:ARG:N   | 5        | 0.31          |
| (2,18)  | 1:331:A:TYR:O   | 1:335:A:ARG:N   | 10       | 0.31          |
| (2,16)  | 1:329:A:ALA:O   | 1:333:A:MET:N   | 9        | 0.31          |
| (3,799) | 1:334:A:GLN:H   | 1:334:A:GLN:HG2 | 10       | 0.3           |
| (3,799) | 1:334:A:GLN:H   | 1:334:A:GLN:HG3 | 10       | 0.3           |
| (3,671) | 1:331:A:TYR:HB2 | 1:331:A:TYR:HE2 | 1        | 0.3           |
| (3,671) | 1:331:A:TYR:HB2 | 1:331:A:TYR:HE2 | 3        | 0.3           |
| (3,671) | 1:331:A:TYR:HB2 | 1:331:A:TYR:HE2 | 4        | 0.3           |
| (2,63)  | 1:334:A:GLN:O   | 1:338:A:ASP:H   | 8        | 0.3           |
| (2,49)  | 1:327:A:THR:O   | 1:331:A:TYR:H   | 8        | 0.3           |
| (2,44)  | 1:317:A:LEU:O   | 1:321:A:ILE:N   | 5        | 0.3           |
| (2,44)  | 1:317:A:LEU:O   | 1:321:A:ILE:N   | 9        | 0.3           |
| (2,34)  | 1:306:A:GLN:O   | 1:310:A:ASP:N   | 8        | 0.3           |
| (2,33)  | 1:306:A:GLN:O   | 1:310:A:ASP:H   | 6        | 0.3           |
| (2,33)  | 1:306:A:GLN:O   | 1:310:A:ASP:H   | 7        | 0.3           |
| (2,18)  | 1:331:A:TYR:O   | 1:335:A:ARG:N   | 8        | 0.3           |
| (3,641) | 1:331:A:TYR:HB2 | 1:331:A:TYR:HD2 | 6        | 0.29          |
| (3,641) | 1:331:A:TYR:HB2 | 1:331:A:TYR:HD2 | 8        | 0.29          |
| (2,63)  | 1:334:A:GLN:O   | 1:338:A:ASP:H   | 5        | 0.29          |
| (2,49)  | 1:327:A:THR:O   | 1:331:A:TYR:H   | 6        | 0.29          |
| (2,41)  | 1:316:A:MET:O   | 1:320:A:ALA:H   | 1        | 0.29          |
| (2,25)  | 1:296:A:GLU:O   | 1:300:A:SER:H   | 5        | 0.29          |
| (2,20)  | 1:333:A:MET:O   | 1:337:A:ILE:N   | 6        | 0.29          |
| (2,20)  | 1:333:A:MET:O   | 1:337:A:ILE:N   | 8        | 0.29          |
| (2,17)  | 1:330:A:LYS:O   | 1:334:A:GLN:N   | 3        | 0.29          |
| (2,16)  | 1:329:A:ALA:O   | 1:333:A:MET:N   | 7        | 0.29          |
| (2,13)  | 1:319:A:ASP:O   | 1:323:A:LYS:N   | 3        | 0.29          |
| (2,12)  | 1:318:A:GLN:O   | 1:322:A:SER:N   | 7        | 0.29          |
| (3,641) | 1:331:A:TYR:HB2 | 1:331:A:TYR:HD2 | 2        | 0.28          |
| (3,641) | 1:331:A:TYR:HB2 | 1:331:A:TYR:HD2 | 5        | 0.28          |
| (3,442) | 1:363:A:LEU:HA  | 1:364:A:LEU:H   | 6        | 0.28          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (2,46)  | 1:318:A:GLN:O   | 1:322:A:SER:N   | 1        | 0.28          |
| (2,44)  | 1:317:A:LEU:O   | 1:321:A:ILE:N   | 10       | 0.28          |
| (2,42)  | 1:316:A:MET:O   | 1:320:A:ALA:N   | 9        | 0.28          |
| (2,25)  | 1:296:A:GLU:O   | 1:300:A:SER:H   | 6        | 0.28          |
| (2,25)  | 1:296:A:GLU:O   | 1:300:A:SER:H   | 8        | 0.28          |
| (2,20)  | 1:333:A:MET:O   | 1:337:A:ILE:N   | 5        | 0.28          |
| (2,20)  | 1:333:A:MET:O   | 1:337:A:ILE:N   | 9        | 0.28          |
| (2,8)   | 1:314:A:VAL:O   | 1:318:A:GLN:N   | 1        | 0.28          |
| (3,641) | 1:331:A:TYR:HB2 | 1:331:A:TYR:HD2 | 1        | 0.27          |
| (3,641) | 1:331:A:TYR:HB2 | 1:331:A:TYR:HD2 | 3        | 0.27          |
| (3,641) | 1:331:A:TYR:HB2 | 1:331:A:TYR:HD2 | 4        | 0.27          |
| (3,641) | 1:331:A:TYR:HB2 | 1:331:A:TYR:HD2 | 7        | 0.27          |
| (2,59)  | 1:332:A:HIS:O   | 1:336:A:CYS:H   | 1        | 0.27          |
| (2,50)  | 1:327:A:THR:O   | 1:331:A:TYR:N   | 4        | 0.27          |
| (2,49)  | 1:327:A:THR:O   | 1:331:A:TYR:H   | 7        | 0.27          |
| (2,44)  | 1:317:A:LEU:O   | 1:321:A:ILE:N   | 7        | 0.27          |
| (2,43)  | 1:317:A:LEU:O   | 1:321:A:ILE:H   | 6        | 0.27          |
| (2,40)  | 1:315:A:GLN:O   | 1:319:A:ASP:N   | 9        | 0.27          |
| (2,25)  | 1:296:A:GLU:O   | 1:300:A:SER:H   | 7        | 0.27          |
| (2,22)  | 1:335:A:ARG:O   | 1:339:A:SER:N   | 5        | 0.27          |
| (2,19)  | 1:332:A:HIS:O   | 1:336:A:CYS:N   | 6        | 0.27          |
| (2,8)   | 1:314:A:VAL:O   | 1:318:A:GLN:N   | 2        | 0.27          |
| (2,8)   | 1:314:A:VAL:O   | 1:318:A:GLN:N   | 4        | 0.27          |
| (2,8)   | 1:314:A:VAL:O   | 1:318:A:GLN:N   | 7        | 0.27          |
| (2,8)   | 1:314:A:VAL:O   | 1:318:A:GLN:N   | 9        | 0.27          |
| (2,8)   | 1:314:A:VAL:O   | 1:318:A:GLN:N   | 10       | 0.27          |
| (2,4)   | 1:304:A:GLU:O   | 1:308:A:CYS:N   | 8        | 0.27          |
| (3,671) | 1:331:A:TYR:HB2 | 1:331:A:TYR:HE2 | 9        | 0.26          |
| (3,671) | 1:331:A:TYR:HB2 | 1:331:A:TYR:HE2 | 10       | 0.26          |
| (3,480) | 1:312:A:LYS:H   | 1:312:A:LYS:HD2 | 7        | 0.26          |
| (3,480) | 1:312:A:LYS:H   | 1:312:A:LYS:HD3 | 7        | 0.26          |
| (3,29)  | 1:342:A:TRP:HA  | 1:342:A:TRP:HE3 | 8        | 0.26          |
| (2,47)  | 1:319:A:ASP:O   | 1:323:A:LYS:H   | 6        | 0.26          |
| (2,40)  | 1:315:A:GLN:O   | 1:319:A:ASP:N   | 2        | 0.26          |
| (2,40)  | 1:315:A:GLN:O   | 1:319:A:ASP:N   | 4        | 0.26          |
| (2,25)  | 1:296:A:GLU:O   | 1:300:A:SER:H   | 10       | 0.26          |
| (2,22)  | 1:335:A:ARG:O   | 1:339:A:SER:N   | 8        | 0.26          |
| (2,21)  | 1:334:A:GLN:O   | 1:338:A:ASP:N   | 4        | 0.26          |
| (2,19)  | 1:332:A:HIS:O   | 1:336:A:CYS:N   | 10       | 0.26          |
| (2,17)  | 1:330:A:LYS:O   | 1:334:A:GLN:N   | 4        | 0.26          |
| (2,8)   | 1:314:A:VAL:O   | 1:318:A:GLN:N   | 3        | 0.26          |
| (2,8)   | 1:314:A:VAL:O   | 1:318:A:GLN:N   | 5        | 0.26          |

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| Key     | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (2,4)   | 1:304:A:GLU:O   | 1:308:A:CYS:N    | 3        | 0.26          |
| (3,446) | 1:364:A:LEU:HA  | 1:365:A:GLU:H    | 8        | 0.25          |
| (2,57)  | 1:331:A:TYR:O   | 1:335:A:ARG:H    | 2        | 0.25          |
| (2,57)  | 1:331:A:TYR:O   | 1:335:A:ARG:H    | 3        | 0.25          |
| (2,57)  | 1:331:A:TYR:O   | 1:335:A:ARG:H    | 4        | 0.25          |
| (2,50)  | 1:327:A:THR:O   | 1:331:A:TYR:N    | 1        | 0.25          |
| (2,50)  | 1:327:A:THR:O   | 1:331:A:TYR:N    | 2        | 0.25          |
| (2,34)  | 1:306:A:GLN:O   | 1:310:A:ASP:N    | 5        | 0.25          |
| (2,34)  | 1:306:A:GLN:O   | 1:310:A:ASP:N    | 10       | 0.25          |
| (2,25)  | 1:296:A:GLU:O   | 1:300:A:SER:H    | 3        | 0.25          |
| (2,21)  | 1:334:A:GLN:O   | 1:338:A:ASP:N    | 2        | 0.25          |
| (2,21)  | 1:334:A:GLN:O   | 1:338:A:ASP:N    | 7        | 0.25          |
| (2,20)  | 1:333:A:MET:O   | 1:337:A:ILE:N    | 3        | 0.25          |
| (2,17)  | 1:330:A:LYS:O   | 1:334:A:GLN:N    | 2        | 0.25          |
| (2,17)  | 1:330:A:LYS:O   | 1:334:A:GLN:N    | 10       | 0.25          |
| (2,16)  | 1:329:A:ALA:O   | 1:333:A:MET:N    | 1        | 0.25          |
| (2,16)  | 1:329:A:ALA:O   | 1:333:A:MET:N    | 8        | 0.25          |
| (2,8)   | 1:314:A:VAL:O   | 1:318:A:GLN:N    | 8        | 0.25          |
| (2,2)   | 1:296:A:GLU:O   | 1:300:A:SER:N    | 5        | 0.25          |
| (2,64)  | 1:334:A:GLN:O   | 1:338:A:ASP:N    | 8        | 0.24          |
| (2,59)  | 1:332:A:HIS:O   | 1:336:A:CYS:H    | 9        | 0.24          |
| (2,48)  | 1:319:A:ASP:O   | 1:323:A:LYS:N    | 5        | 0.24          |
| (2,40)  | 1:315:A:GLN:O   | 1:319:A:ASP:N    | 1        | 0.24          |
| (2,34)  | 1:306:A:GLN:O   | 1:310:A:ASP:N    | 1        | 0.24          |
| (2,17)  | 1:330:A:LYS:O   | 1:334:A:GLN:N    | 1        | 0.24          |
| (2,12)  | 1:318:A:GLN:O   | 1:322:A:SER:N    | 3        | 0.24          |
| (2,12)  | 1:318:A:GLN:O   | 1:322:A:SER:N    | 8        | 0.24          |
| (2,8)   | 1:314:A:VAL:O   | 1:318:A:GLN:N    | 6        | 0.24          |
| (2,4)   | 1:304:A:GLU:O   | 1:308:A:CYS:N    | 5        | 0.24          |
| (2,4)   | 1:304:A:GLU:O   | 1:308:A:CYS:N    | 7        | 0.24          |
| (3,662) | 1:309:A:PHE:HE1 | 1:341:A:LEU:HD21 | 5        | 0.23          |
| (3,662) | 1:309:A:PHE:HE1 | 1:341:A:LEU:HD22 | 5        | 0.23          |
| (3,662) | 1:309:A:PHE:HE1 | 1:341:A:LEU:HD23 | 5        | 0.23          |
| (2,63)  | 1:334:A:GLN:O   | 1:338:A:ASP:H    | 10       | 0.23          |
| (2,59)  | 1:332:A:HIS:O   | 1:336:A:CYS:H    | 7        | 0.23          |
| (2,57)  | 1:331:A:TYR:O   | 1:335:A:ARG:H    | 1        | 0.23          |
| (2,50)  | 1:327:A:THR:O   | 1:331:A:TYR:N    | 9        | 0.23          |
| (2,50)  | 1:327:A:THR:O   | 1:331:A:TYR:N    | 10       | 0.23          |
| (2,46)  | 1:318:A:GLN:O   | 1:322:A:SER:N    | 9        | 0.23          |
| (2,42)  | 1:316:A:MET:O   | 1:320:A:ALA:N    | 2        | 0.23          |
| (2,34)  | 1:306:A:GLN:O   | 1:310:A:ASP:N    | 9        | 0.23          |
| (2,25)  | 1:296:A:GLU:O   | 1:300:A:SER:H    | 9        | 0.23          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (2,22)  | 1:335:A:ARG:O   | 1:339:A:SER:N   | 6        | 0.23          |
| (2,4)   | 1:304:A:GLU:O   | 1:308:A:CYS:N   | 6        | 0.23          |
| (2,4)   | 1:304:A:GLU:O   | 1:308:A:CYS:N   | 10       | 0.23          |
| (2,3)   | 1:303:A:GLU:O   | 1:307:A:LYS:N   | 1        | 0.23          |
| (2,2)   | 1:296:A:GLU:O   | 1:300:A:SER:N   | 6        | 0.23          |
| (2,2)   | 1:296:A:GLU:O   | 1:300:A:SER:N   | 7        | 0.23          |
| (2,2)   | 1:296:A:GLU:O   | 1:300:A:SER:N   | 8        | 0.23          |
| (3,29)  | 1:342:A:TRP:HA  | 1:342:A:TRP:HE3 | 3        | 0.22          |
| (2,64)  | 1:334:A:GLN:O   | 1:338:A:ASP:N   | 5        | 0.22          |
| (2,63)  | 1:334:A:GLN:O   | 1:338:A:ASP:H   | 6        | 0.22          |
| (2,57)  | 1:331:A:TYR:O   | 1:335:A:ARG:H   | 7        | 0.22          |
| (2,50)  | 1:327:A:THR:O   | 1:331:A:TYR:N   | 3        | 0.22          |
| (2,25)  | 1:296:A:GLU:O   | 1:300:A:SER:H   | 2        | 0.22          |
| (2,16)  | 1:329:A:ALA:O   | 1:333:A:MET:N   | 5        | 0.22          |
| (2,5)   | 1:305:A:LEU:O   | 1:309:A:PHE:N   | 7        | 0.22          |
| (2,3)   | 1:303:A:GLU:O   | 1:307:A:LYS:N   | 6        | 0.22          |
| (2,1)   | 1:295:A:VAL:O   | 1:299:A:GLU:N   | 5        | 0.22          |
| (3,641) | 1:331:A:TYR:HB2 | 1:331:A:TYR:HD2 | 9        | 0.21          |
| (2,63)  | 1:334:A:GLN:O   | 1:338:A:ASP:H   | 9        | 0.21          |
| (2,59)  | 1:332:A:HIS:O   | 1:336:A:CYS:H   | 2        | 0.21          |
| (2,51)  | 1:328:A:ASP:O   | 1:332:A:HIS:H   | 8        | 0.21          |
| (2,42)  | 1:316:A:MET:O   | 1:320:A:ALA:N   | 4        | 0.21          |
| (2,25)  | 1:296:A:GLU:O   | 1:300:A:SER:H   | 1        | 0.21          |
| (2,25)  | 1:296:A:GLU:O   | 1:300:A:SER:H   | 4        | 0.21          |
| (2,17)  | 1:330:A:LYS:O   | 1:334:A:GLN:N   | 7        | 0.21          |
| (2,17)  | 1:330:A:LYS:O   | 1:334:A:GLN:N   | 9        | 0.21          |
| (2,16)  | 1:329:A:ALA:O   | 1:333:A:MET:N   | 2        | 0.21          |
| (2,16)  | 1:329:A:ALA:O   | 1:333:A:MET:N   | 3        | 0.21          |
| (2,16)  | 1:329:A:ALA:O   | 1:333:A:MET:N   | 6        | 0.21          |
| (2,4)   | 1:304:A:GLU:O   | 1:308:A:CYS:N   | 1        | 0.21          |
| (2,4)   | 1:304:A:GLU:O   | 1:308:A:CYS:N   | 9        | 0.21          |
| (2,3)   | 1:303:A:GLU:O   | 1:307:A:LYS:N   | 7        | 0.21          |
| (2,2)   | 1:296:A:GLU:O   | 1:300:A:SER:N   | 10       | 0.21          |
| (3,641) | 1:331:A:TYR:HB2 | 1:331:A:TYR:HD2 | 10       | 0.2           |
| (3,29)  | 1:342:A:TRP:HA  | 1:342:A:TRP:HE3 | 10       | 0.2           |
| (2,60)  | 1:332:A:HIS:O   | 1:336:A:CYS:N   | 1        | 0.2           |
| (2,59)  | 1:332:A:HIS:O   | 1:336:A:CYS:H   | 4        | 0.2           |
| (2,51)  | 1:328:A:ASP:O   | 1:332:A:HIS:H   | 5        | 0.2           |
| (2,50)  | 1:327:A:THR:O   | 1:331:A:TYR:N   | 5        | 0.2           |
| (2,48)  | 1:319:A:ASP:O   | 1:323:A:LYS:N   | 10       | 0.2           |
| (2,21)  | 1:334:A:GLN:O   | 1:338:A:ASP:N   | 1        | 0.2           |
| (2,17)  | 1:330:A:LYS:O   | 1:334:A:GLN:N   | 5        | 0.2           |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (2,16)  | 1:329:A:ALA:O   | 1:333:A:MET:N   | 10       | 0.2           |
| (2,5)   | 1:305:A:LEU:O   | 1:309:A:PHE:N   | 6        | 0.2           |
| (2,2)   | 1:296:A:GLU:O   | 1:300:A:SER:N   | 3        | 0.2           |
| (2,1)   | 1:295:A:VAL:O   | 1:299:A:GLU:N   | 2        | 0.2           |
| (2,1)   | 1:295:A:VAL:O   | 1:299:A:GLU:N   | 8        | 0.2           |
| (3,807) | 1:335:A:ARG:HA  | 1:338:A:ASP:HB2 | 9        | 0.19          |
| (3,807) | 1:335:A:ARG:HA  | 1:338:A:ASP:HB3 | 9        | 0.19          |
| (3,791) | 1:323:A:LYS:HD2 | 1:324:A:MET:H   | 1        | 0.19          |
| (3,791) | 1:323:A:LYS:HD3 | 1:324:A:MET:H   | 1        | 0.19          |
| (3,791) | 1:323:A:LYS:HD2 | 1:324:A:MET:H   | 2        | 0.19          |
| (3,791) | 1:323:A:LYS:HD3 | 1:324:A:MET:H   | 2        | 0.19          |
| (3,791) | 1:323:A:LYS:HD2 | 1:324:A:MET:H   | 4        | 0.19          |
| (3,791) | 1:323:A:LYS:HD3 | 1:324:A:MET:H   | 4        | 0.19          |
| (3,791) | 1:323:A:LYS:HD2 | 1:324:A:MET:H   | 9        | 0.19          |
| (3,791) | 1:323:A:LYS:HD3 | 1:324:A:MET:H   | 9        | 0.19          |
| (3,420) | 1:342:A:TRP:HB3 | 1:342:A:TRP:HE1 | 3        | 0.19          |
| (3,420) | 1:342:A:TRP:HB3 | 1:342:A:TRP:HE1 | 5        | 0.19          |
| (3,420) | 1:342:A:TRP:HB3 | 1:342:A:TRP:HE1 | 8        | 0.19          |
| (3,420) | 1:342:A:TRP:HB3 | 1:342:A:TRP:HE1 | 10       | 0.19          |
| (3,204) | 1:305:A:LEU:HG  | 1:309:A:PHE:HE1 | 7        | 0.19          |
| (2,57)  | 1:331:A:TYR:O   | 1:335:A:ARG:H   | 9        | 0.19          |
| (2,51)  | 1:328:A:ASP:O   | 1:332:A:HIS:H   | 7        | 0.19          |
| (2,51)  | 1:328:A:ASP:O   | 1:332:A:HIS:H   | 9        | 0.19          |
| (2,42)  | 1:316:A:MET:O   | 1:320:A:ALA:N   | 1        | 0.19          |
| (2,34)  | 1:306:A:GLN:O   | 1:310:A:ASP:N   | 4        | 0.19          |
| (2,22)  | 1:335:A:ARG:O   | 1:339:A:SER:N   | 2        | 0.19          |
| (2,22)  | 1:335:A:ARG:O   | 1:339:A:SER:N   | 10       | 0.19          |
| (2,19)  | 1:332:A:HIS:O   | 1:336:A:CYS:N   | 5        | 0.19          |
| (2,19)  | 1:332:A:HIS:O   | 1:336:A:CYS:N   | 8        | 0.19          |
| (2,17)  | 1:330:A:LYS:O   | 1:334:A:GLN:N   | 8        | 0.19          |
| (2,12)  | 1:318:A:GLN:O   | 1:322:A:SER:N   | 6        | 0.19          |
| (2,4)   | 1:304:A:GLU:O   | 1:308:A:CYS:N   | 2        | 0.19          |
| (2,4)   | 1:304:A:GLU:O   | 1:308:A:CYS:N   | 4        | 0.19          |
| (2,3)   | 1:303:A:GLU:O   | 1:307:A:LYS:N   | 2        | 0.19          |
| (2,3)   | 1:303:A:GLU:O   | 1:307:A:LYS:N   | 4        | 0.19          |
| (2,1)   | 1:295:A:VAL:O   | 1:299:A:GLU:N   | 7        | 0.19          |
| (2,1)   | 1:295:A:VAL:O   | 1:299:A:GLU:N   | 10       | 0.19          |
| (3,204) | 1:305:A:LEU:HG  | 1:309:A:PHE:HE1 | 6        | 0.18          |
| (2,51)  | 1:328:A:ASP:O   | 1:332:A:HIS:H   | 6        | 0.18          |
| (2,50)  | 1:327:A:THR:O   | 1:331:A:TYR:N   | 8        | 0.18          |
| (2,34)  | 1:306:A:GLN:O   | 1:310:A:ASP:N   | 2        | 0.18          |
| (2,29)  | 1:304:A:GLU:O   | 1:308:A:CYS:H   | 3        | 0.18          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (2,29)  | 1:304:A:GLU:O   | 1:308:A:CYS:H   | 8        | 0.18          |
| (2,16)  | 1:329:A:ALA:O   | 1:333:A:MET:N   | 4        | 0.18          |
| (2,3)   | 1:303:A:GLU:O   | 1:307:A:LYS:N   | 5        | 0.18          |
| (2,3)   | 1:303:A:GLU:O   | 1:307:A:LYS:N   | 9        | 0.18          |
| (2,2)   | 1:296:A:GLU:O   | 1:300:A:SER:N   | 2        | 0.18          |
| (2,2)   | 1:296:A:GLU:O   | 1:300:A:SER:N   | 9        | 0.18          |
| (2,1)   | 1:295:A:VAL:O   | 1:299:A:GLU:N   | 1        | 0.18          |
| (2,1)   | 1:295:A:VAL:O   | 1:299:A:GLU:N   | 3        | 0.18          |
| (3,657) | 1:309:A:PHE:HB2 | 1:309:A:PHE:HD1 | 3        | 0.17          |
| (3,657) | 1:309:A:PHE:HB2 | 1:309:A:PHE:HD1 | 5        | 0.17          |
| (3,657) | 1:309:A:PHE:HB2 | 1:309:A:PHE:HD1 | 8        | 0.17          |
| (3,657) | 1:309:A:PHE:HB2 | 1:309:A:PHE:HD1 | 10       | 0.17          |
| (2,64)  | 1:334:A:GLN:O   | 1:338:A:ASP:N   | 9        | 0.17          |
| (2,64)  | 1:334:A:GLN:O   | 1:338:A:ASP:N   | 10       | 0.17          |
| (2,60)  | 1:332:A:HIS:O   | 1:336:A:CYS:N   | 9        | 0.17          |
| (2,51)  | 1:328:A:ASP:O   | 1:332:A:HIS:H   | 1        | 0.17          |
| (2,48)  | 1:319:A:ASP:O   | 1:323:A:LYS:N   | 7        | 0.17          |
| (2,47)  | 1:319:A:ASP:O   | 1:323:A:LYS:H   | 8        | 0.17          |
| (2,44)  | 1:317:A:LEU:O   | 1:321:A:ILE:N   | 6        | 0.17          |
| (2,34)  | 1:306:A:GLN:O   | 1:310:A:ASP:N   | 7        | 0.17          |
| (2,3)   | 1:303:A:GLU:O   | 1:307:A:LYS:N   | 10       | 0.17          |
| (2,2)   | 1:296:A:GLU:O   | 1:300:A:SER:N   | 1        | 0.17          |
| (2,2)   | 1:296:A:GLU:O   | 1:300:A:SER:N   | 4        | 0.17          |
| (2,1)   | 1:295:A:VAL:O   | 1:299:A:GLU:N   | 6        | 0.17          |
| (2,1)   | 1:295:A:VAL:O   | 1:299:A:GLU:N   | 9        | 0.17          |
| (3,609) | 1:308:A:CYS:HA  | 1:313:A:ASP:H   | 2        | 0.16          |
| (2,65)  | 1:335:A:ARG:O   | 1:339:A:SER:H   | 5        | 0.16          |
| (2,61)  | 1:333:A:MET:O   | 1:337:A:ILE:H   | 8        | 0.16          |
| (2,60)  | 1:332:A:HIS:O   | 1:336:A:CYS:N   | 7        | 0.16          |
| (2,57)  | 1:331:A:TYR:O   | 1:335:A:ARG:H   | 6        | 0.16          |
| (2,51)  | 1:328:A:ASP:O   | 1:332:A:HIS:H   | 2        | 0.16          |
| (2,51)  | 1:328:A:ASP:O   | 1:332:A:HIS:H   | 10       | 0.16          |
| (2,50)  | 1:327:A:THR:O   | 1:331:A:TYR:N   | 6        | 0.16          |
| (2,45)  | 1:318:A:GLN:O   | 1:322:A:SER:H   | 10       | 0.16          |
| (2,34)  | 1:306:A:GLN:O   | 1:310:A:ASP:N   | 6        | 0.16          |
| (2,31)  | 1:305:A:LEU:O   | 1:309:A:PHE:H   | 8        | 0.16          |
| (2,17)  | 1:330:A:LYS:O   | 1:334:A:GLN:N   | 6        | 0.16          |
| (2,1)   | 1:295:A:VAL:O   | 1:299:A:GLU:N   | 4        | 0.16          |
| (3,657) | 1:309:A:PHE:HB2 | 1:309:A:PHE:HD1 | 4        | 0.15          |
| (3,657) | 1:309:A:PHE:HB2 | 1:309:A:PHE:HD1 | 9        | 0.15          |
| (3,609) | 1:308:A:CYS:HA  | 1:313:A:ASP:H   | 4        | 0.15          |
| (3,609) | 1:308:A:CYS:HA  | 1:313:A:ASP:H   | 9        | 0.15          |

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| Key     | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (3,88)  | 1:334:A:GLN:HA  | 1:335:A:ARG:HD2  | 3        | 0.15          |
| (3,88)  | 1:334:A:GLN:HA  | 1:335:A:ARG:HD3  | 3        | 0.15          |
| (2,64)  | 1:334:A:GLN:O   | 1:338:A:ASP:N    | 6        | 0.15          |
| (2,60)  | 1:332:A:HIS:O   | 1:336:A:CYS:N    | 2        | 0.15          |
| (2,51)  | 1:328:A:ASP:O   | 1:332:A:HIS:H    | 3        | 0.15          |
| (2,51)  | 1:328:A:ASP:O   | 1:332:A:HIS:H    | 4        | 0.15          |
| (2,45)  | 1:318:A:GLN:O   | 1:322:A:SER:H    | 5        | 0.15          |
| (2,31)  | 1:305:A:LEU:O   | 1:309:A:PHE:H    | 1        | 0.15          |
| (2,31)  | 1:305:A:LEU:O   | 1:309:A:PHE:H    | 3        | 0.15          |
| (3,657) | 1:309:A:PHE:HB2 | 1:309:A:PHE:HD1  | 1        | 0.14          |
| (3,657) | 1:309:A:PHE:HB2 | 1:309:A:PHE:HD1  | 2        | 0.14          |
| (3,609) | 1:308:A:CYS:HA  | 1:313:A:ASP:H    | 1        | 0.14          |
| (3,547) | 1:321:A:ILE:H   | 1:323:A:LYS:HG2  | 1        | 0.14          |
| (3,547) | 1:321:A:ILE:H   | 1:323:A:LYS:HG3  | 1        | 0.14          |
| (3,547) | 1:321:A:ILE:H   | 1:323:A:LYS:HG2  | 2        | 0.14          |
| (3,547) | 1:321:A:ILE:H   | 1:323:A:LYS:HG3  | 2        | 0.14          |
| (3,547) | 1:321:A:ILE:H   | 1:323:A:LYS:HG2  | 4        | 0.14          |
| (3,547) | 1:321:A:ILE:H   | 1:323:A:LYS:HG3  | 4        | 0.14          |
| (3,547) | 1:321:A:ILE:H   | 1:323:A:LYS:HG2  | 9        | 0.14          |
| (3,547) | 1:321:A:ILE:H   | 1:323:A:LYS:HG3  | 9        | 0.14          |
| (3,366) | 1:314:A:VAL:HA  | 1:318:A:GLN:H    | 7        | 0.14          |
| (2,65)  | 1:335:A:ARG:O   | 1:339:A:SER:H    | 8        | 0.14          |
| (2,61)  | 1:333:A:MET:O   | 1:337:A:ILE:H    | 5        | 0.14          |
| (2,61)  | 1:333:A:MET:O   | 1:337:A:ILE:H    | 6        | 0.14          |
| (2,60)  | 1:332:A:HIS:O   | 1:336:A:CYS:N    | 4        | 0.14          |
| (2,57)  | 1:331:A:TYR:O   | 1:335:A:ARG:H    | 5        | 0.14          |
| (2,52)  | 1:328:A:ASP:O   | 1:332:A:HIS:N    | 5        | 0.14          |
| (2,52)  | 1:328:A:ASP:O   | 1:332:A:HIS:N    | 8        | 0.14          |
| (2,50)  | 1:327:A:THR:O   | 1:331:A:TYR:N    | 7        | 0.14          |
| (2,31)  | 1:305:A:LEU:O   | 1:309:A:PHE:H    | 2        | 0.14          |
| (2,31)  | 1:305:A:LEU:O   | 1:309:A:PHE:H    | 5        | 0.14          |
| (3,826) | 1:340:A:GLY:HA2 | 1:343:A:VAL:HG11 | 8        | 0.13          |
| (3,826) | 1:340:A:GLY:HA2 | 1:343:A:VAL:HG12 | 8        | 0.13          |
| (3,826) | 1:340:A:GLY:HA2 | 1:343:A:VAL:HG13 | 8        | 0.13          |
| (3,826) | 1:340:A:GLY:HA2 | 1:343:A:VAL:HG21 | 8        | 0.13          |
| (3,826) | 1:340:A:GLY:HA2 | 1:343:A:VAL:HG22 | 8        | 0.13          |
| (3,826) | 1:340:A:GLY:HA2 | 1:343:A:VAL:HG23 | 8        | 0.13          |
| (3,826) | 1:340:A:GLY:HA3 | 1:343:A:VAL:HG11 | 8        | 0.13          |
| (3,826) | 1:340:A:GLY:HA3 | 1:343:A:VAL:HG12 | 8        | 0.13          |
| (3,826) | 1:340:A:GLY:HA3 | 1:343:A:VAL:HG13 | 8        | 0.13          |
| (3,826) | 1:340:A:GLY:HA3 | 1:343:A:VAL:HG21 | 8        | 0.13          |
| (3,826) | 1:340:A:GLY:HA3 | 1:343:A:VAL:HG22 | 8        | 0.13          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,826) | 1:340:A:GLY:HA3  | 1:343:A:VAL:HG23 | 8        | 0.13          |
| (2,57)  | 1:331:A:TYR:O    | 1:335:A:ARG:H    | 8        | 0.13          |
| (2,57)  | 1:331:A:TYR:O    | 1:335:A:ARG:H    | 10       | 0.13          |
| (2,52)  | 1:328:A:ASP:O    | 1:332:A:HIS:N    | 7        | 0.13          |
| (2,47)  | 1:319:A:ASP:O    | 1:323:A:LYS:H    | 3        | 0.13          |
| (2,31)  | 1:305:A:LEU:O    | 1:309:A:PHE:H    | 4        | 0.13          |
| (2,22)  | 1:335:A:ARG:O    | 1:339:A:SER:N    | 3        | 0.13          |
| (2,22)  | 1:335:A:ARG:O    | 1:339:A:SER:N    | 7        | 0.13          |
| (2,3)   | 1:303:A:GLU:O    | 1:307:A:LYS:N    | 3        | 0.13          |
| (3,820) | 1:338:A:ASP:HB2  | 1:339:A:SER:H    | 9        | 0.12          |
| (3,820) | 1:338:A:ASP:HB3  | 1:339:A:SER:H    | 9        | 0.12          |
| (3,609) | 1:308:A:CYS:HA   | 1:313:A:ASP:H    | 7        | 0.12          |
| (2,65)  | 1:335:A:ARG:O    | 1:339:A:SER:H    | 6        | 0.12          |
| (2,52)  | 1:328:A:ASP:O    | 1:332:A:HIS:N    | 6        | 0.12          |
| (2,52)  | 1:328:A:ASP:O    | 1:332:A:HIS:N    | 9        | 0.12          |
| (2,48)  | 1:319:A:ASP:O    | 1:323:A:LYS:N    | 6        | 0.12          |
| (2,31)  | 1:305:A:LEU:O    | 1:309:A:PHE:H    | 9        | 0.12          |
| (2,3)   | 1:303:A:GLU:O    | 1:307:A:LYS:N    | 8        | 0.12          |
| (3,747) | 1:305:A:LEU:HD11 | 1:332:A:HIS:HA   | 10       | 0.11          |
| (3,747) | 1:305:A:LEU:HD12 | 1:332:A:HIS:HA   | 10       | 0.11          |
| (3,747) | 1:305:A:LEU:HD13 | 1:332:A:HIS:HA   | 10       | 0.11          |
| (3,747) | 1:305:A:LEU:HD21 | 1:332:A:HIS:HA   | 10       | 0.11          |
| (3,747) | 1:305:A:LEU:HD22 | 1:332:A:HIS:HA   | 10       | 0.11          |
| (3,747) | 1:305:A:LEU:HD23 | 1:332:A:HIS:HA   | 10       | 0.11          |
| (3,609) | 1:308:A:CYS:HA   | 1:313:A:ASP:H    | 5        | 0.11          |
| (3,609) | 1:308:A:CYS:HA   | 1:313:A:ASP:H    | 6        | 0.11          |
| (3,609) | 1:308:A:CYS:HA   | 1:313:A:ASP:H    | 8        | 0.11          |
| (3,347) | 1:324:A:MET:HG3  | 1:325:A:ASP:H    | 2        | 0.11          |
| (3,347) | 1:324:A:MET:HG2  | 1:325:A:ASP:H    | 2        | 0.11          |
| (3,347) | 1:324:A:MET:HG3  | 1:325:A:ASP:H    | 4        | 0.11          |
| (3,347) | 1:324:A:MET:HG2  | 1:325:A:ASP:H    | 4        | 0.11          |
| (2,63)  | 1:334:A:GLN:O    | 1:338:A:ASP:H    | 3        | 0.11          |
| (2,61)  | 1:333:A:MET:O    | 1:337:A:ILE:H    | 1        | 0.11          |
| (2,61)  | 1:333:A:MET:O    | 1:337:A:ILE:H    | 7        | 0.11          |
| (2,61)  | 1:333:A:MET:O    | 1:337:A:ILE:H    | 9        | 0.11          |
| (2,61)  | 1:333:A:MET:O    | 1:337:A:ILE:H    | 10       | 0.11          |
| (2,59)  | 1:332:A:HIS:O    | 1:336:A:CYS:H    | 3        | 0.11          |
| (2,58)  | 1:331:A:TYR:O    | 1:335:A:ARG:N    | 3        | 0.11          |
| (2,52)  | 1:328:A:ASP:O    | 1:332:A:HIS:N    | 1        | 0.11          |
| (2,52)  | 1:328:A:ASP:O    | 1:332:A:HIS:N    | 2        | 0.11          |
| (2,29)  | 1:304:A:GLU:O    | 1:308:A:CYS:H    | 5        | 0.11          |
| (2,22)  | 1:335:A:ARG:O    | 1:339:A:SER:N    | 1        | 0.11          |

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| Key    | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|--------|---------------|---------------|----------|---------------|
| (2,22) | 1:335:A:ARG:O | 1:339:A:SER:N | 4        | 0.11          |
| (2,22) | 1:335:A:ARG:O | 1:339:A:SER:N | 9        | 0.11          |
| (2,58) | 1:331:A:TYR:O | 1:335:A:ARG:N | 4        | 0.1           |
| (2,55) | 1:330:A:LYS:O | 1:334:A:GLN:H | 3        | 0.1           |
| (2,52) | 1:328:A:ASP:O | 1:332:A:HIS:N | 10       | 0.1           |

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

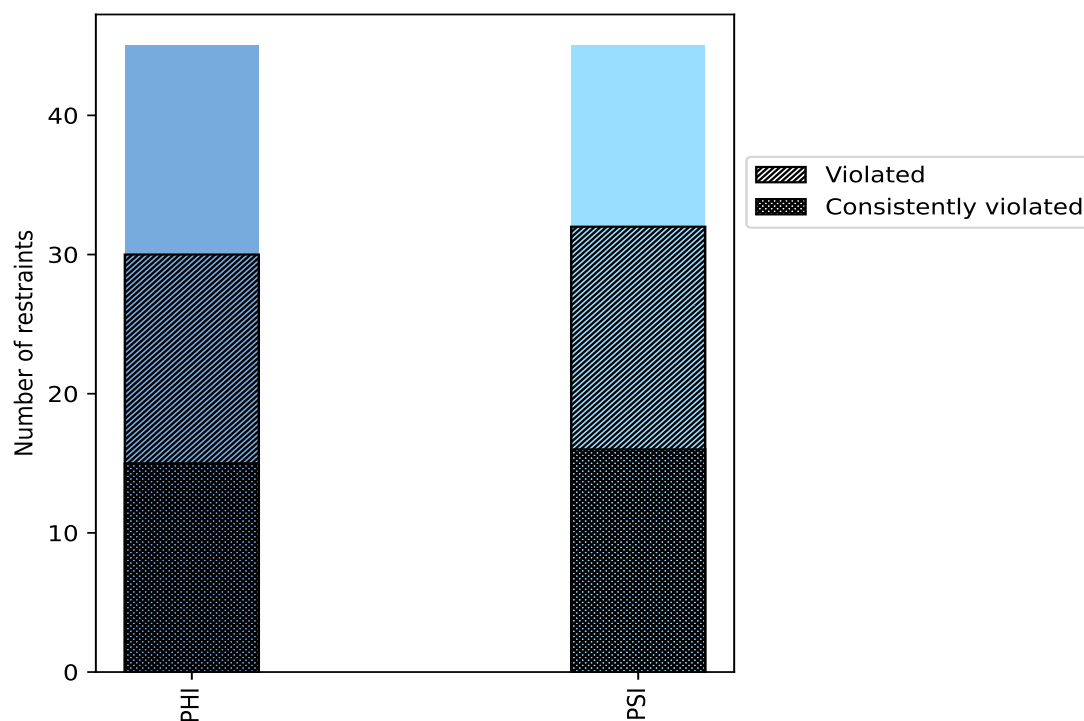
### 10.1 Summary of dihedral-angle violations [i](#)

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

| Angle type | Count | % <sup>1</sup> | Violated <sup>3</sup> |                |                | Consistently Violated <sup>4</sup> |                |                |
|------------|-------|----------------|-----------------------|----------------|----------------|------------------------------------|----------------|----------------|
|            |       |                | Count                 | % <sup>2</sup> | % <sup>1</sup> | Count                              | % <sup>2</sup> | % <sup>1</sup> |
| PHI        | 45    | 50.0           | 30                    | 66.7           | 33.3           | 15                                 | 33.3           | 16.7           |
| PSI        | 45    | 50.0           | 32                    | 71.1           | 35.6           | 16                                 | 35.6           | 17.8           |
| Total      | 90    | 100.0          | 62                    | 68.9           | 68.9           | 31                                 | 34.4           | 34.4           |

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

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



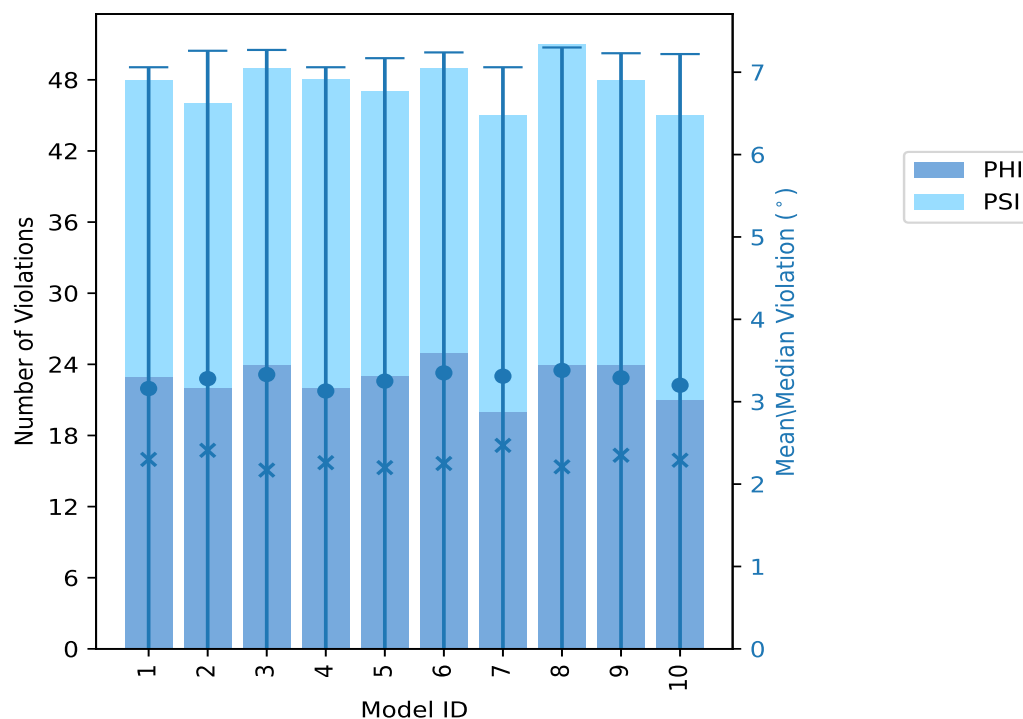
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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

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

| Model ID | Number of violations |     |       | Mean (°) | Max (°) | SD (°) | Median (°) |
|----------|----------------------|-----|-------|----------|---------|--------|------------|
|          | PHI                  | PSI | Total |          |         |        |            |
| 1        | 23                   | 25  | 48    | 3.16     | 24.12   | 3.9    | 2.3        |
| 2        | 22                   | 24  | 46    | 3.28     | 24.21   | 3.98   | 2.41       |
| 3        | 24                   | 25  | 49    | 3.33     | 23.92   | 3.94   | 2.17       |
| 4        | 22                   | 26  | 48    | 3.13     | 24.16   | 3.93   | 2.26       |
| 5        | 23                   | 24  | 47    | 3.25     | 23.39   | 3.92   | 2.2        |
| 6        | 25                   | 24  | 49    | 3.35     | 24.03   | 3.89   | 2.25       |
| 7        | 20                   | 25  | 45    | 3.31     | 20.53   | 3.75   | 2.47       |
| 8        | 24                   | 27  | 51    | 3.38     | 24.1    | 3.92   | 2.21       |
| 9        | 24                   | 24  | 48    | 3.29     | 24.14   | 3.94   | 2.35       |
| 10       | 21                   | 24  | 45    | 3.2      | 23.93   | 4.02   | 2.29       |

### 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

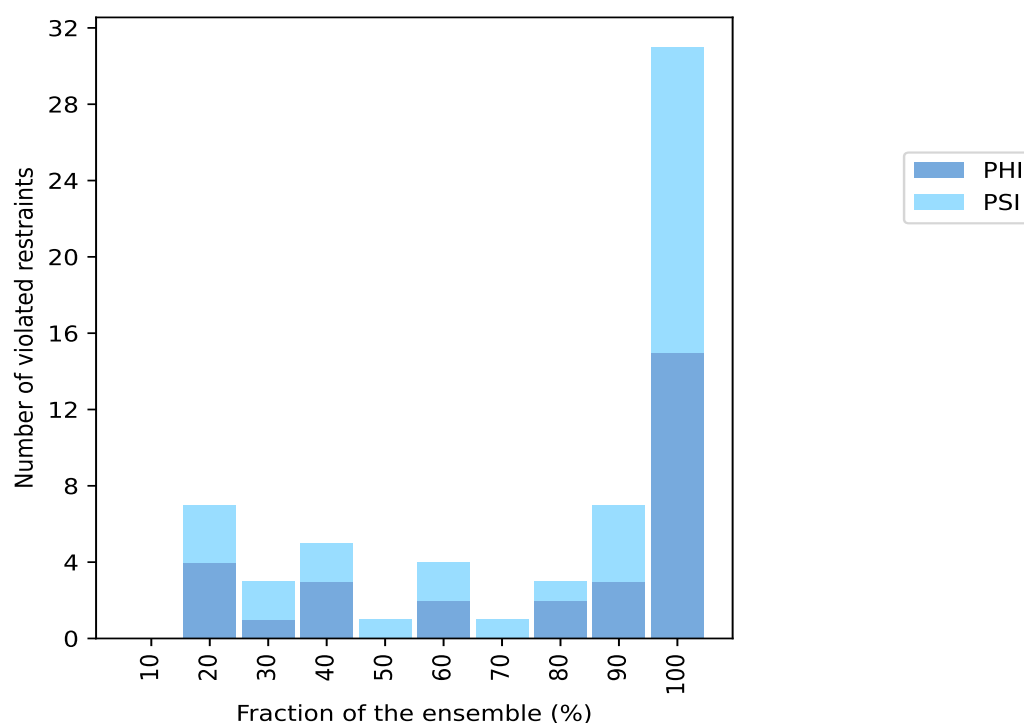
### 10.3 Dihedral-angle violation statistics for the ensemble [i](#)

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>       | %     |
| 0                             | 0   | 0     | 1                        | 10.0  |
| 4                             | 3   | 7     | 2                        | 20.0  |
| 1                             | 2   | 3     | 3                        | 30.0  |
| 3                             | 2   | 5     | 4                        | 40.0  |
| 0                             | 1   | 1     | 5                        | 50.0  |
| 2                             | 2   | 4     | 6                        | 60.0  |
| 0                             | 1   | 1     | 7                        | 70.0  |
| 2                             | 1   | 3     | 8                        | 80.0  |
| 3                             | 4   | 7     | 9                        | 90.0  |
| 15                            | 16  | 31    | 10                       | 100.0 |

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

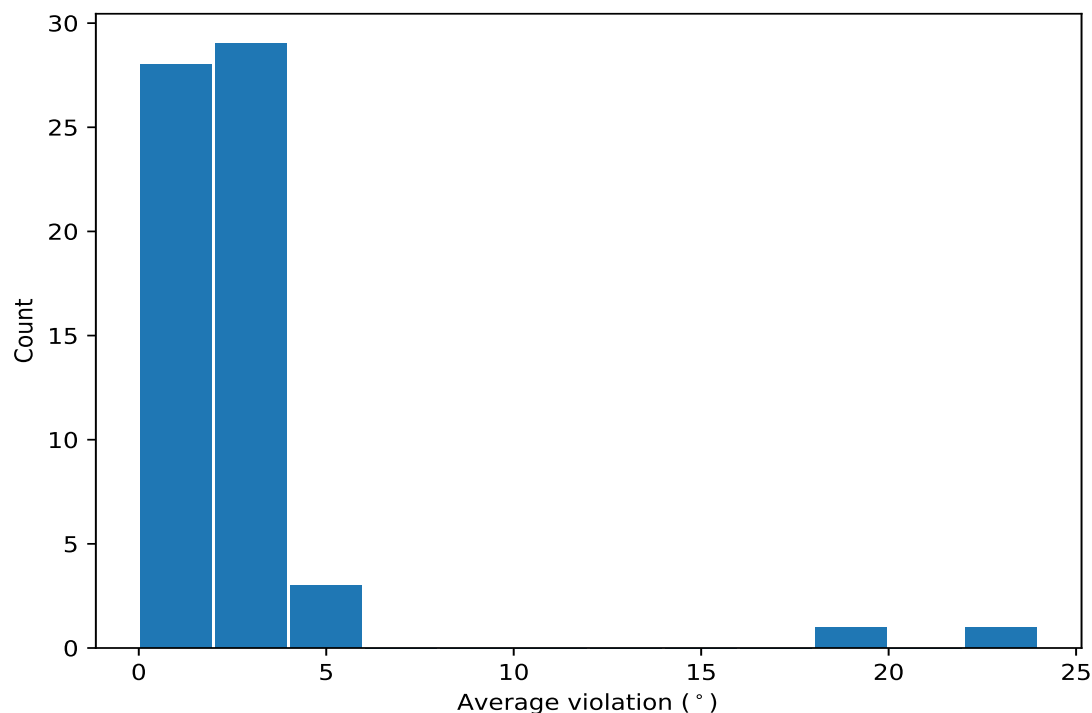
#### 10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



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

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

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



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

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

| Key    | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Models <sup>1</sup> | Mean  | SD <sup>2</sup> | Median |
|--------|---------------|----------------|----------------|---------------|---------------------|-------|-----------------|--------|
| (1,35) | 1:311:A:VAL:C | 1:312:A:LYS:N  | 1:312:A:LYS:CA | 1:312:A:LYS:C | 10                  | 23.65 | 1.06            | 24.06  |
| (1,36) | 1:312:A:LYS:N | 1:312:A:LYS:CA | 1:312:A:LYS:C  | 1:313:A:ASP:N | 10                  | 18.26 | 0.46            | 18.1   |
| (1,33) | 1:310:A:ASP:C | 1:311:A:VAL:N  | 1:311:A:VAL:CA | 1:311:A:VAL:C | 10                  | 5.66  | 0.19            | 5.68   |
| (1,29) | 1:308:A:CYS:C | 1:309:A:PHE:N  | 1:309:A:PHE:CA | 1:309:A:PHE:C | 10                  | 4.72  | 0.5             | 4.73   |
| (1,75) | 1:334:A:GLN:C | 1:335:A:ARG:N  | 1:335:A:ARG:CA | 1:335:A:ARG:C | 10                  | 3.82  | 1.45            | 3.32   |
| (1,74) | 1:334:A:GLN:N | 1:334:A:GLN:CA | 1:334:A:GLN:C  | 1:335:A:ARG:N | 10                  | 3.82  | 0.72            | 3.8    |
| (1,38) | 1:314:A:VAL:N | 1:314:A:VAL:CA | 1:314:A:VAL:C  | 1:315:A:GLN:N | 10                  | 3.68  | 0.63            | 3.54   |
| (1,24) | 1:306:A:GLN:N | 1:306:A:GLN:CA | 1:306:A:GLN:C  | 1:307:A:LYS:N | 10                  | 3.48  | 1.05            | 3.0    |
| (1,8)  | 1:296:A:GLU:N | 1:296:A:GLU:CA | 1:296:A:GLU:C  | 1:297:A:VAL:N | 10                  | 3.45  | 0.26            | 3.5    |
| (1,9)  | 1:296:A:GLU:C | 1:297:A:VAL:N  | 1:297:A:VAL:CA | 1:297:A:VAL:C | 10                  | 3.08  | 0.28            | 3.05   |
| (1,41) | 1:315:A:GLN:C | 1:316:A:MET:N  | 1:316:A:MET:CA | 1:316:A:MET:C | 10                  | 3.02  | 0.18            | 3.01   |
| (1,40) | 1:315:A:GLN:N | 1:315:A:GLN:CA | 1:315:A:GLN:C  | 1:316:A:MET:N | 10                  | 2.9   | 0.27            | 2.78   |
| (1,76) | 1:335:A:ARG:N | 1:335:A:ARG:CA | 1:335:A:ARG:C  | 1:336:A:CYS:N | 10                  | 2.82  | 0.58            | 2.8    |

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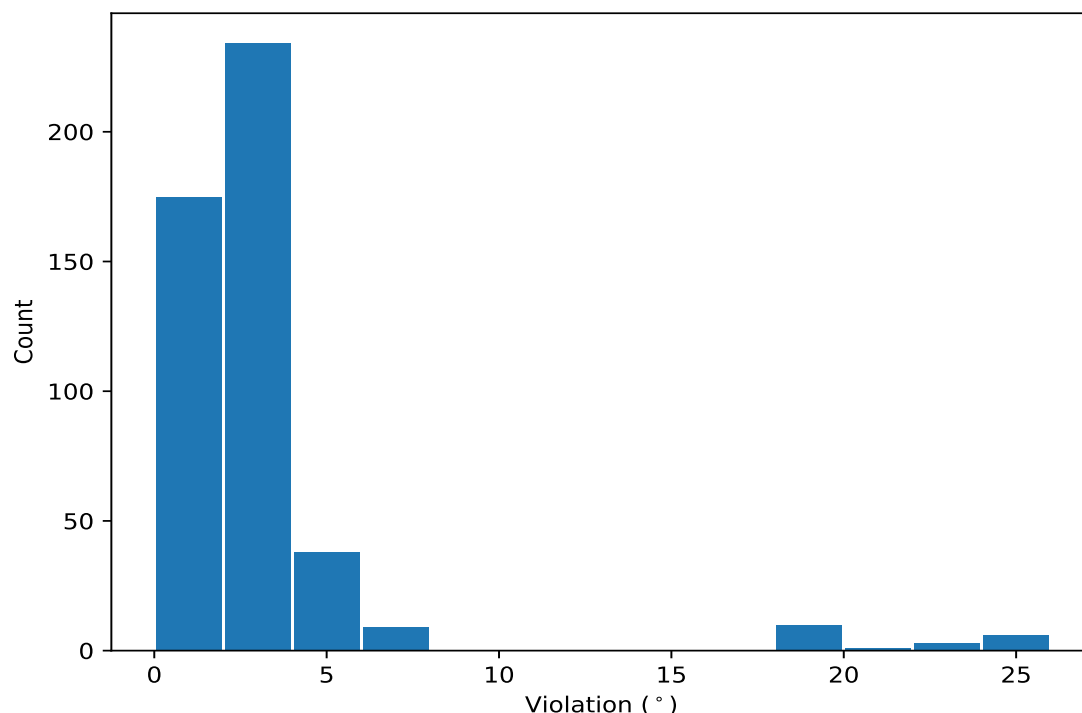
| Key    | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Models <sup>1</sup> | Mean | SD <sup>2</sup> | Median |
|--------|---------------|----------------|----------------|---------------|---------------------|------|-----------------|--------|
| (1,77) | 1:335:A:ARG:C | 1:336:A:CYS:N  | 1:336:A:CYS:CA | 1:336:A:CYS:C | 10                  | 2.78 | 0.4             | 2.65   |
| (1,62) | 1:328:A:ASP:N | 1:328:A:ASP:CA | 1:328:A:ASP:C  | 1:329:A:ALA:N | 10                  | 2.75 | 0.22            | 2.73   |
| (1,68) | 1:331:A:TYR:N | 1:331:A:TYR:CA | 1:331:A:TYR:C  | 1:332:A:HIS:N | 10                  | 2.52 | 0.26            | 2.51   |
| (1,64) | 1:329:A:ALA:N | 1:329:A:ALA:CA | 1:329:A:ALA:C  | 1:330:A:LYS:N | 10                  | 2.5  | 0.34            | 2.5    |
| (1,28) | 1:308:A:CYS:N | 1:308:A:CYS:CA | 1:308:A:CYS:C  | 1:309:A:PHE:N | 10                  | 2.4  | 0.42            | 2.38   |
| (1,71) | 1:332:A:HIS:C | 1:333:A:MET:N  | 1:333:A:MET:CA | 1:333:A:MET:C | 10                  | 2.37 | 0.43            | 2.3    |
| (1,63) | 1:328:A:ASP:C | 1:329:A:ALA:N  | 1:329:A:ALA:CA | 1:329:A:ALA:C | 10                  | 2.33 | 0.33            | 2.42   |
| (1,59) | 1:326:A:PRO:C | 1:327:A:THR:N  | 1:327:A:THR:CA | 1:327:A:THR:C | 10                  | 2.32 | 0.38            | 2.37   |
| (1,61) | 1:327:A:THR:C | 1:328:A:ASP:N  | 1:328:A:ASP:CA | 1:328:A:ASP:C | 10                  | 2.29 | 0.27            | 2.32   |
| (1,13) | 1:298:A:TYR:C | 1:299:A:GLU:N  | 1:299:A:GLU:CA | 1:299:A:GLU:C | 10                  | 2.18 | 0.36            | 2.24   |
| (1,31) | 1:309:A:PHE:C | 1:310:A:ASP:N  | 1:310:A:ASP:CA | 1:310:A:ASP:C | 10                  | 2.16 | 0.11            | 2.2    |
| (1,60) | 1:327:A:THR:N | 1:327:A:THR:CA | 1:327:A:THR:C  | 1:328:A:ASP:N | 10                  | 2.03 | 0.36            | 1.93   |
| (1,65) | 1:329:A:ALA:C | 1:330:A:LYS:N  | 1:330:A:LYS:CA | 1:330:A:LYS:C | 10                  | 1.79 | 0.37            | 1.78   |
| (1,32) | 1:310:A:ASP:N | 1:310:A:ASP:CA | 1:310:A:ASP:C  | 1:311:A:VAL:N | 10                  | 1.64 | 0.15            | 1.62   |
| (1,14) | 1:299:A:GLU:N | 1:299:A:GLU:CA | 1:299:A:GLU:C  | 1:300:A:SER:N | 10                  | 1.6  | 0.19            | 1.65   |
| (1,90) | 1:375:A:ASP:N | 1:375:A:ASP:CA | 1:375:A:ASP:C  | 1:376:A:VAL:N | 10                  | 1.54 | 0.11            | 1.59   |
| (1,25) | 1:306:A:GLN:C | 1:307:A:LYS:N  | 1:307:A:LYS:CA | 1:307:A:LYS:C | 10                  | 1.4  | 0.26            | 1.38   |
| (1,88) | 1:373:A:GLU:N | 1:373:A:GLU:CA | 1:373:A:GLU:C  | 1:374:A:LYS:N | 10                  | 1.36 | 0.05            | 1.35   |
| (1,21) | 1:304:A:GLU:C | 1:305:A:LEU:N  | 1:305:A:LEU:CA | 1:305:A:LEU:C | 9                   | 2.96 | 1.83            | 2.3    |
| (1,82) | 1:338:A:ASP:N | 1:338:A:ASP:CA | 1:338:A:ASP:C  | 1:339:A:SER:N | 9                   | 2.45 | 0.79            | 2.44   |
| (1,37) | 1:313:A:ASP:C | 1:314:A:VAL:N  | 1:314:A:VAL:CA | 1:314:A:VAL:C | 9                   | 1.97 | 0.18            | 2.0    |
| (1,70) | 1:332:A:HIS:N | 1:332:A:HIS:CA | 1:332:A:HIS:C  | 1:333:A:MET:N | 9                   | 1.89 | 0.6             | 1.68   |
| (1,55) | 1:322:A:SER:C | 1:323:A:LYS:N  | 1:323:A:LYS:CA | 1:323:A:LYS:C | 9                   | 1.54 | 0.32            | 1.44   |
| (1,12) | 1:298:A:TYR:N | 1:298:A:TYR:CA | 1:298:A:TYR:C  | 1:299:A:GLU:N | 9                   | 1.51 | 0.3             | 1.49   |
| (1,46) | 1:318:A:GLN:N | 1:318:A:GLN:CA | 1:318:A:GLN:C  | 1:319:A:ASP:N | 9                   | 1.45 | 0.38            | 1.31   |
| (1,79) | 1:336:A:CYS:C | 1:337:A:ILE:N  | 1:337:A:ILE:CA | 1:337:A:ILE:C | 8                   | 3.08 | 1.29            | 2.54   |
| (1,20) | 1:304:A:GLU:N | 1:304:A:GLU:CA | 1:304:A:GLU:C  | 1:305:A:LEU:N | 8                   | 1.99 | 0.65            | 1.88   |
| (1,23) | 1:305:A:LEU:C | 1:306:A:GLN:N  | 1:306:A:GLN:CA | 1:306:A:GLN:C | 8                   | 1.88 | 0.37            | 1.8    |
| (1,80) | 1:337:A:ILE:N | 1:337:A:ILE:CA | 1:337:A:ILE:C  | 1:338:A:ASP:N | 7                   | 2.47 | 1.7             | 2.13   |
| (1,51) | 1:320:A:ALA:C | 1:321:A:ILE:N  | 1:321:A:ILE:CA | 1:321:A:ILE:C | 6                   | 5.04 | 1.52            | 5.28   |
| (1,54) | 1:322:A:SER:N | 1:322:A:SER:CA | 1:322:A:SER:C  | 1:323:A:LYS:N | 6                   | 3.51 | 0.77            | 3.51   |
| (1,44) | 1:317:A:LEU:N | 1:317:A:LEU:CA | 1:317:A:LEU:C  | 1:318:A:GLN:N | 6                   | 1.78 | 0.45            | 1.93   |
| (1,85) | 1:341:A:LEU:C | 1:342:A:TRP:N  | 1:342:A:TRP:CA | 1:342:A:TRP:C | 6                   | 1.5  | 0.21            | 1.44   |
| (1,56) | 1:323:A:LYS:N | 1:323:A:LYS:CA | 1:323:A:LYS:C  | 1:324:A:MET:N | 5                   | 3.95 | 1.46            | 4.63   |
| (1,83) | 1:338:A:ASP:C | 1:339:A:SER:N  | 1:339:A:SER:CA | 1:339:A:SER:C | 4                   | 1.9  | 0.36            | 2.04   |
| (1,47) | 1:318:A:GLN:C | 1:319:A:ASP:N  | 1:319:A:ASP:CA | 1:319:A:ASP:C | 4                   | 1.82 | 0.49            | 2.02   |
| (1,86) | 1:342:A:TRP:N | 1:342:A:TRP:CA | 1:342:A:TRP:C  | 1:343:A:VAL:N | 4                   | 1.78 | 0.3             | 1.91   |
| (1,22) | 1:305:A:LEU:N | 1:305:A:LEU:CA | 1:305:A:LEU:C  | 1:306:A:GLN:N | 4                   | 1.27 | 0.3             | 1.18   |
| (1,43) | 1:316:A:MET:C | 1:317:A:LEU:N  | 1:317:A:LEU:CA | 1:317:A:LEU:C | 4                   | 1.08 | 0.03            | 1.09   |
| (1,78) | 1:336:A:CYS:N | 1:336:A:CYS:CA | 1:336:A:CYS:C  | 1:337:A:ILE:N | 3                   | 1.65 | 0.48            | 1.4    |
| (1,69) | 1:331:A:TYR:C | 1:332:A:HIS:N  | 1:332:A:HIS:CA | 1:332:A:HIS:C | 3                   | 1.41 | 0.14            | 1.5    |
| (1,50) | 1:320:A:ALA:N | 1:320:A:ALA:CA | 1:320:A:ALA:C  | 1:321:A:ILE:N | 3                   | 1.23 | 0.17            | 1.26   |
| (1,81) | 1:337:A:ILE:C | 1:338:A:ASP:N  | 1:338:A:ASP:CA | 1:338:A:ASP:C | 2                   | 2.34 | 1.29            | 2.34   |
| (1,27) | 1:307:A:LYS:C | 1:308:A:CYS:N  | 1:308:A:CYS:CA | 1:308:A:CYS:C | 2                   | 2.05 | 0.21            | 2.05   |
| (1,26) | 1:307:A:LYS:N | 1:307:A:LYS:CA | 1:307:A:LYS:C  | 1:308:A:CYS:N | 2                   | 1.66 | 0.47            | 1.66   |
| (1,18) | 1:303:A:GLU:N | 1:303:A:GLU:CA | 1:303:A:GLU:C  | 1:304:A:GLU:N | 2                   | 1.18 | 0.14            | 1.18   |
| (1,11) | 1:297:A:VAL:C | 1:298:A:TYR:N  | 1:298:A:TYR:CA | 1:298:A:TYR:C | 2                   | 1.09 | 0.01            | 1.09   |
| (1,53) | 1:321:A:ILE:C | 1:322:A:SER:N  | 1:322:A:SER:CA | 1:322:A:SER:C | 2                   | 1.09 | 0.0             | 1.09   |
| (1,52) | 1:321:A:ILE:N | 1:321:A:ILE:CA | 1:321:A:ILE:C  | 1:322:A:SER:N | 2                   | 1.06 | 0.02            | 1.06   |

<sup>1</sup> Number of violated models, <sup>2</sup>Standard deviation, All angle values are in degree (°)

## 10.5 All violated dihedral-angle restraints [i](#)

### 10.5.1 Histogram : Distribution of violations [i](#)

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



### 10.5.2 Table: All violated dihedral-angle restraints [i](#)

The following table lists the absolute value of the violation for each restraint in the ensemble sorted by its value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint.

| Key    | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|--------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,35) | 1:311:A:VAL:C | 1:312:A:LYS:N  | 1:312:A:LYS:CA | 1:312:A:LYS:C | 2        | 24.21         |
| (1,35) | 1:311:A:VAL:C | 1:312:A:LYS:N  | 1:312:A:LYS:CA | 1:312:A:LYS:C | 4        | 24.16         |
| (1,35) | 1:311:A:VAL:C | 1:312:A:LYS:N  | 1:312:A:LYS:CA | 1:312:A:LYS:C | 9        | 24.14         |
| (1,35) | 1:311:A:VAL:C | 1:312:A:LYS:N  | 1:312:A:LYS:CA | 1:312:A:LYS:C | 1        | 24.12         |
| (1,35) | 1:311:A:VAL:C | 1:312:A:LYS:N  | 1:312:A:LYS:CA | 1:312:A:LYS:C | 8        | 24.1          |
| (1,35) | 1:311:A:VAL:C | 1:312:A:LYS:N  | 1:312:A:LYS:CA | 1:312:A:LYS:C | 6        | 24.03         |
| (1,35) | 1:311:A:VAL:C | 1:312:A:LYS:N  | 1:312:A:LYS:CA | 1:312:A:LYS:C | 10       | 23.93         |
| (1,35) | 1:311:A:VAL:C | 1:312:A:LYS:N  | 1:312:A:LYS:CA | 1:312:A:LYS:C | 3        | 23.92         |
| (1,35) | 1:311:A:VAL:C | 1:312:A:LYS:N  | 1:312:A:LYS:CA | 1:312:A:LYS:C | 5        | 23.39         |
| (1,35) | 1:311:A:VAL:C | 1:312:A:LYS:N  | 1:312:A:LYS:CA | 1:312:A:LYS:C | 7        | 20.53         |
| (1,36) | 1:312:A:LYS:N | 1:312:A:LYS:CA | 1:312:A:LYS:C  | 1:313:A:ASP:N | 7        | 19.61         |
| (1,36) | 1:312:A:LYS:N | 1:312:A:LYS:CA | 1:312:A:LYS:C  | 1:313:A:ASP:N | 5        | 18.4          |
| (1,36) | 1:312:A:LYS:N | 1:312:A:LYS:CA | 1:312:A:LYS:C  | 1:313:A:ASP:N | 3        | 18.14         |
| (1,36) | 1:312:A:LYS:N | 1:312:A:LYS:CA | 1:312:A:LYS:C  | 1:313:A:ASP:N | 10       | 18.12         |

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| Key    | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|--------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,36) | 1:312:A:LYS:N | 1:312:A:LYS:CA | 1:312:A:LYS:C  | 1:313:A:ASP:N | 8        | 18.11         |
| (1,36) | 1:312:A:LYS:N | 1:312:A:LYS:CA | 1:312:A:LYS:C  | 1:313:A:ASP:N | 6        | 18.1          |
| (1,36) | 1:312:A:LYS:N | 1:312:A:LYS:CA | 1:312:A:LYS:C  | 1:313:A:ASP:N | 4        | 18.08         |
| (1,36) | 1:312:A:LYS:N | 1:312:A:LYS:CA | 1:312:A:LYS:C  | 1:313:A:ASP:N | 1        | 18.03         |
| (1,36) | 1:312:A:LYS:N | 1:312:A:LYS:CA | 1:312:A:LYS:C  | 1:313:A:ASP:N | 2        | 18.02         |
| (1,36) | 1:312:A:LYS:N | 1:312:A:LYS:CA | 1:312:A:LYS:C  | 1:313:A:ASP:N | 9        | 18.0          |
| (1,51) | 1:320:A:ALA:C | 1:321:A:ILE:N  | 1:321:A:ILE:CA | 1:321:A:ILE:C | 3        | 6.78          |
| (1,51) | 1:320:A:ALA:C | 1:321:A:ILE:N  | 1:321:A:ILE:CA | 1:321:A:ILE:C | 8        | 6.54          |
| (1,80) | 1:337:A:ILE:N | 1:337:A:ILE:CA | 1:337:A:ILE:C  | 1:338:A:ASP:N | 9        | 6.49          |
| (1,21) | 1:304:A:GLU:C | 1:305:A:LEU:N  | 1:305:A:LEU:CA | 1:305:A:LEU:C | 8        | 6.41          |
| (1,51) | 1:320:A:ALA:C | 1:321:A:ILE:N  | 1:321:A:ILE:CA | 1:321:A:ILE:C | 6        | 6.17          |
| (1,75) | 1:334:A:GLN:C | 1:335:A:ARG:N  | 1:335:A:ARG:CA | 1:335:A:ARG:C | 5        | 6.16          |
| (1,21) | 1:304:A:GLU:C | 1:305:A:LEU:N  | 1:305:A:LEU:CA | 1:305:A:LEU:C | 3        | 6.08          |
| (1,75) | 1:334:A:GLN:C | 1:335:A:ARG:N  | 1:335:A:ARG:CA | 1:335:A:ARG:C | 8        | 6.07          |
| (1,33) | 1:310:A:ASP:C | 1:311:A:VAL:N  | 1:311:A:VAL:CA | 1:311:A:VAL:C | 7        | 6.03          |
| (1,33) | 1:310:A:ASP:C | 1:311:A:VAL:N  | 1:311:A:VAL:CA | 1:311:A:VAL:C | 2        | 5.85          |
| (1,33) | 1:310:A:ASP:C | 1:311:A:VAL:N  | 1:311:A:VAL:CA | 1:311:A:VAL:C | 9        | 5.73          |
| (1,33) | 1:310:A:ASP:C | 1:311:A:VAL:N  | 1:311:A:VAL:CA | 1:311:A:VAL:C | 4        | 5.72          |
| (1,33) | 1:310:A:ASP:C | 1:311:A:VAL:N  | 1:311:A:VAL:CA | 1:311:A:VAL:C | 1        | 5.7           |
| (1,33) | 1:310:A:ASP:C | 1:311:A:VAL:N  | 1:311:A:VAL:CA | 1:311:A:VAL:C | 3        | 5.65          |
| (1,33) | 1:310:A:ASP:C | 1:311:A:VAL:N  | 1:311:A:VAL:CA | 1:311:A:VAL:C | 6        | 5.65          |
| (1,24) | 1:306:A:GLN:N | 1:306:A:GLN:CA | 1:306:A:GLN:C  | 1:307:A:LYS:N | 3        | 5.57          |
| (1,24) | 1:306:A:GLN:N | 1:306:A:GLN:CA | 1:306:A:GLN:C  | 1:307:A:LYS:N | 8        | 5.48          |
| (1,38) | 1:314:A:VAL:N | 1:314:A:VAL:CA | 1:314:A:VAL:C  | 1:315:A:GLN:N | 7        | 5.46          |
| (1,29) | 1:308:A:CYS:C | 1:309:A:PHE:N  | 1:309:A:PHE:CA | 1:309:A:PHE:C | 4        | 5.46          |
| (1,33) | 1:310:A:ASP:C | 1:311:A:VAL:N  | 1:311:A:VAL:CA | 1:311:A:VAL:C | 5        | 5.45          |
| (1,33) | 1:310:A:ASP:C | 1:311:A:VAL:N  | 1:311:A:VAL:CA | 1:311:A:VAL:C | 8        | 5.45          |
| (1,29) | 1:308:A:CYS:C | 1:309:A:PHE:N  | 1:309:A:PHE:CA | 1:309:A:PHE:C | 2        | 5.43          |
| (1,33) | 1:310:A:ASP:C | 1:311:A:VAL:N  | 1:311:A:VAL:CA | 1:311:A:VAL:C | 10       | 5.36          |
| (1,75) | 1:334:A:GLN:C | 1:335:A:ARG:N  | 1:335:A:ARG:CA | 1:335:A:ARG:C | 6        | 5.19          |
| (1,74) | 1:334:A:GLN:N | 1:334:A:GLN:CA | 1:334:A:GLN:C  | 1:335:A:ARG:N | 10       | 5.14          |
| (1,29) | 1:308:A:CYS:C | 1:309:A:PHE:N  | 1:309:A:PHE:CA | 1:309:A:PHE:C | 1        | 5.07          |
| (1,29) | 1:308:A:CYS:C | 1:309:A:PHE:N  | 1:309:A:PHE:CA | 1:309:A:PHE:C | 9        | 4.94          |
| (1,79) | 1:336:A:CYS:C | 1:337:A:ILE:N  | 1:337:A:ILE:CA | 1:337:A:ILE:C | 6        | 4.91          |
| (1,56) | 1:323:A:LYS:N | 1:323:A:LYS:CA | 1:323:A:LYS:C  | 1:324:A:MET:N | 1        | 4.87          |
| (1,29) | 1:308:A:CYS:C | 1:309:A:PHE:N  | 1:309:A:PHE:CA | 1:309:A:PHE:C | 8        | 4.85          |
| (1,79) | 1:336:A:CYS:C | 1:337:A:ILE:N  | 1:337:A:ILE:CA | 1:337:A:ILE:C | 8        | 4.77          |
| (1,56) | 1:323:A:LYS:N | 1:323:A:LYS:CA | 1:323:A:LYS:C  | 1:324:A:MET:N | 9        | 4.68          |
| (1,56) | 1:323:A:LYS:N | 1:323:A:LYS:CA | 1:323:A:LYS:C  | 1:324:A:MET:N | 2        | 4.63          |
| (1,29) | 1:308:A:CYS:C | 1:309:A:PHE:N  | 1:309:A:PHE:CA | 1:309:A:PHE:C | 3        | 4.62          |
| (1,74) | 1:334:A:GLN:N | 1:334:A:GLN:CA | 1:334:A:GLN:C  | 1:335:A:ARG:N | 8        | 4.54          |
| (1,56) | 1:323:A:LYS:N | 1:323:A:LYS:CA | 1:323:A:LYS:C  | 1:324:A:MET:N | 4        | 4.54          |
| (1,29) | 1:308:A:CYS:C | 1:309:A:PHE:N  | 1:309:A:PHE:CA | 1:309:A:PHE:C | 5        | 4.47          |
| (1,74) | 1:334:A:GLN:N | 1:334:A:GLN:CA | 1:334:A:GLN:C  | 1:335:A:ARG:N | 5        | 4.43          |
| (1,51) | 1:320:A:ALA:C | 1:321:A:ILE:N  | 1:321:A:ILE:CA | 1:321:A:ILE:C | 7        | 4.39          |
| (1,79) | 1:336:A:CYS:C | 1:337:A:ILE:N  | 1:337:A:ILE:CA | 1:337:A:ILE:C | 5        | 4.34          |
| (1,54) | 1:322:A:SER:N | 1:322:A:SER:CA | 1:322:A:SER:C  | 1:323:A:LYS:N | 6        | 4.33          |
| (1,54) | 1:322:A:SER:N | 1:322:A:SER:CA | 1:322:A:SER:C  | 1:323:A:LYS:N | 8        | 4.33          |
| (1,29) | 1:308:A:CYS:C | 1:309:A:PHE:N  | 1:309:A:PHE:CA | 1:309:A:PHE:C | 10       | 4.26          |
| (1,75) | 1:334:A:GLN:C | 1:335:A:ARG:N  | 1:335:A:ARG:CA | 1:335:A:ARG:C | 10       | 4.2           |
| (1,29) | 1:308:A:CYS:C | 1:309:A:PHE:N  | 1:309:A:PHE:CA | 1:309:A:PHE:C | 6        | 4.18          |

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| Key    | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|--------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,54) | 1:322:A:SER:N | 1:322:A:SER:CA | 1:322:A:SER:C  | 1:323:A:LYS:N | 3        | 4.17          |
| (1,74) | 1:334:A:GLN:N | 1:334:A:GLN:CA | 1:334:A:GLN:C  | 1:335:A:ARG:N | 3        | 4.06          |
| (1,82) | 1:338:A:ASP:N | 1:338:A:ASP:CA | 1:338:A:ASP:C  | 1:339:A:SER:N | 2        | 3.93          |
| (1,75) | 1:334:A:GLN:C | 1:335:A:ARG:N  | 1:335:A:ARG:CA | 1:335:A:ARG:C | 3        | 3.91          |
| (1,8)  | 1:296:A:GLU:N | 1:296:A:GLU:CA | 1:296:A:GLU:C  | 1:297:A:VAL:N | 3        | 3.91          |
| (1,29) | 1:308:A:CYS:C | 1:309:A:PHE:N  | 1:309:A:PHE:CA | 1:309:A:PHE:C | 7        | 3.88          |
| (1,38) | 1:314:A:VAL:N | 1:314:A:VAL:CA | 1:314:A:VAL:C  | 1:315:A:GLN:N | 5        | 3.86          |
| (1,74) | 1:334:A:GLN:N | 1:334:A:GLN:CA | 1:334:A:GLN:C  | 1:335:A:ARG:N | 6        | 3.83          |
| (1,74) | 1:334:A:GLN:N | 1:334:A:GLN:CA | 1:334:A:GLN:C  | 1:335:A:ARG:N | 9        | 3.78          |
| (1,77) | 1:335:A:ARG:C | 1:336:A:CYS:N  | 1:336:A:CYS:CA | 1:336:A:CYS:C | 9        | 3.74          |
| (1,76) | 1:335:A:ARG:N | 1:335:A:ARG:CA | 1:335:A:ARG:C  | 1:336:A:CYS:N | 5        | 3.74          |
| (1,38) | 1:314:A:VAL:N | 1:314:A:VAL:CA | 1:314:A:VAL:C  | 1:315:A:GLN:N | 8        | 3.73          |
| (1,38) | 1:314:A:VAL:N | 1:314:A:VAL:CA | 1:314:A:VAL:C  | 1:315:A:GLN:N | 4        | 3.66          |
| (1,8)  | 1:296:A:GLU:N | 1:296:A:GLU:CA | 1:296:A:GLU:C  | 1:297:A:VAL:N | 6        | 3.66          |
| (1,9)  | 1:296:A:GLU:C | 1:297:A:VAL:N  | 1:297:A:VAL:CA | 1:297:A:VAL:C | 3        | 3.64          |
| (1,8)  | 1:296:A:GLU:N | 1:296:A:GLU:CA | 1:296:A:GLU:C  | 1:297:A:VAL:N | 7        | 3.64          |
| (1,81) | 1:337:A:ILE:C | 1:338:A:ASP:N  | 1:338:A:ASP:CA | 1:338:A:ASP:C | 9        | 3.63          |
| (1,8)  | 1:296:A:GLU:N | 1:296:A:GLU:CA | 1:296:A:GLU:C  | 1:297:A:VAL:N | 8        | 3.62          |
| (1,38) | 1:314:A:VAL:N | 1:314:A:VAL:CA | 1:314:A:VAL:C  | 1:315:A:GLN:N | 1        | 3.59          |
| (1,8)  | 1:296:A:GLU:N | 1:296:A:GLU:CA | 1:296:A:GLU:C  | 1:297:A:VAL:N | 10       | 3.53          |
| (1,38) | 1:314:A:VAL:N | 1:314:A:VAL:CA | 1:314:A:VAL:C  | 1:315:A:GLN:N | 9        | 3.5           |
| (1,76) | 1:335:A:ARG:N | 1:335:A:ARG:CA | 1:335:A:ARG:C  | 1:336:A:CYS:N | 6        | 3.49          |
| (1,8)  | 1:296:A:GLU:N | 1:296:A:GLU:CA | 1:296:A:GLU:C  | 1:297:A:VAL:N | 4        | 3.47          |
| (1,24) | 1:306:A:GLN:N | 1:306:A:GLN:CA | 1:306:A:GLN:C  | 1:307:A:LYS:N | 10       | 3.45          |
| (1,38) | 1:314:A:VAL:N | 1:314:A:VAL:CA | 1:314:A:VAL:C  | 1:315:A:GLN:N | 2        | 3.43          |
| (1,40) | 1:315:A:GLN:N | 1:315:A:GLN:CA | 1:315:A:GLN:C  | 1:316:A:MET:N | 6        | 3.4           |
| (1,74) | 1:334:A:GLN:N | 1:334:A:GLN:CA | 1:334:A:GLN:C  | 1:335:A:ARG:N | 4        | 3.38          |
| (1,76) | 1:335:A:ARG:N | 1:335:A:ARG:CA | 1:335:A:ARG:C  | 1:336:A:CYS:N | 8        | 3.36          |
| (1,41) | 1:315:A:GLN:C | 1:316:A:MET:N  | 1:316:A:MET:CA | 1:316:A:MET:C | 8        | 3.34          |
| (1,9)  | 1:296:A:GLU:C | 1:297:A:VAL:N  | 1:297:A:VAL:CA | 1:297:A:VAL:C | 7        | 3.32          |
| (1,8)  | 1:296:A:GLU:N | 1:296:A:GLU:CA | 1:296:A:GLU:C  | 1:297:A:VAL:N | 1        | 3.31          |
| (1,74) | 1:334:A:GLN:N | 1:334:A:GLN:CA | 1:334:A:GLN:C  | 1:335:A:ARG:N | 2        | 3.3           |
| (1,38) | 1:314:A:VAL:N | 1:314:A:VAL:CA | 1:314:A:VAL:C  | 1:315:A:GLN:N | 3        | 3.29          |
| (1,9)  | 1:296:A:GLU:C | 1:297:A:VAL:N  | 1:297:A:VAL:CA | 1:297:A:VAL:C | 6        | 3.28          |
| (1,9)  | 1:296:A:GLU:C | 1:297:A:VAL:N  | 1:297:A:VAL:CA | 1:297:A:VAL:C | 10       | 3.28          |
| (1,41) | 1:315:A:GLN:C | 1:316:A:MET:N  | 1:316:A:MET:CA | 1:316:A:MET:C | 6        | 3.27          |
| (1,38) | 1:314:A:VAL:N | 1:314:A:VAL:CA | 1:314:A:VAL:C  | 1:315:A:GLN:N | 10       | 3.25          |
| (1,24) | 1:306:A:GLN:N | 1:306:A:GLN:CA | 1:306:A:GLN:C  | 1:307:A:LYS:N | 5        | 3.25          |
| (1,71) | 1:332:A:HIS:C | 1:333:A:MET:N  | 1:333:A:MET:CA | 1:333:A:MET:C | 9        | 3.23          |
| (1,77) | 1:335:A:ARG:C | 1:336:A:CYS:N  | 1:336:A:CYS:CA | 1:336:A:CYS:C | 3        | 3.22          |
| (1,51) | 1:320:A:ALA:C | 1:321:A:ILE:N  | 1:321:A:ILE:CA | 1:321:A:ILE:C | 5        | 3.22          |
| (1,40) | 1:315:A:GLN:N | 1:315:A:GLN:CA | 1:315:A:GLN:C  | 1:316:A:MET:N | 7        | 3.22          |
| (1,62) | 1:328:A:ASP:N | 1:328:A:ASP:CA | 1:328:A:ASP:C  | 1:329:A:ALA:N | 7        | 3.19          |
| (1,82) | 1:338:A:ASP:N | 1:338:A:ASP:CA | 1:338:A:ASP:C  | 1:339:A:SER:N | 3        | 3.17          |
| (1,40) | 1:315:A:GLN:N | 1:315:A:GLN:CA | 1:315:A:GLN:C  | 1:316:A:MET:N | 8        | 3.17          |
| (1,8)  | 1:296:A:GLU:N | 1:296:A:GLU:CA | 1:296:A:GLU:C  | 1:297:A:VAL:N | 9        | 3.15          |
| (1,51) | 1:320:A:ALA:C | 1:321:A:ILE:N  | 1:321:A:ILE:CA | 1:321:A:ILE:C | 10       | 3.13          |
| (1,21) | 1:304:A:GLU:C | 1:305:A:LEU:N  | 1:305:A:LEU:CA | 1:305:A:LEU:C | 5        | 3.13          |
| (1,74) | 1:334:A:GLN:N | 1:334:A:GLN:CA | 1:334:A:GLN:C  | 1:335:A:ARG:N | 7        | 3.12          |
| (1,8)  | 1:296:A:GLU:N | 1:296:A:GLU:CA | 1:296:A:GLU:C  | 1:297:A:VAL:N | 5        | 3.12          |
| (1,70) | 1:332:A:HIS:N | 1:332:A:HIS:CA | 1:332:A:HIS:C  | 1:333:A:MET:N | 9        | 3.11          |

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| Key    | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|--------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,8)  | 1:296:A:GLU:N | 1:296:A:GLU:CA | 1:296:A:GLU:C  | 1:297:A:VAL:N | 2        | 3.1           |
| (1,9)  | 1:296:A:GLU:C | 1:297:A:VAL:N  | 1:297:A:VAL:CA | 1:297:A:VAL:C | 8        | 3.08          |
| (1,41) | 1:315:A:GLN:C | 1:316:A:MET:N  | 1:316:A:MET:CA | 1:316:A:MET:C | 10       | 3.07          |
| (1,38) | 1:314:A:VAL:N | 1:314:A:VAL:CA | 1:314:A:VAL:C  | 1:315:A:GLN:N | 6        | 3.07          |
| (1,41) | 1:315:A:GLN:C | 1:316:A:MET:N  | 1:316:A:MET:CA | 1:316:A:MET:C | 5        | 3.05          |
| (1,28) | 1:308:A:CYS:N | 1:308:A:CYS:CA | 1:308:A:CYS:C  | 1:309:A:PHE:N | 2        | 3.05          |
| (1,64) | 1:329:A:ALA:N | 1:329:A:ALA:CA | 1:329:A:ALA:C  | 1:330:A:LYS:N | 7        | 3.04          |
| (1,41) | 1:315:A:GLN:C | 1:316:A:MET:N  | 1:316:A:MET:CA | 1:316:A:MET:C | 3        | 3.02          |
| (1,24) | 1:306:A:GLN:N | 1:306:A:GLN:CA | 1:306:A:GLN:C  | 1:307:A:LYS:N | 7        | 3.02          |
| (1,9)  | 1:296:A:GLU:C | 1:297:A:VAL:N  | 1:297:A:VAL:CA | 1:297:A:VAL:C | 4        | 3.02          |
| (1,41) | 1:315:A:GLN:C | 1:316:A:MET:N  | 1:316:A:MET:CA | 1:316:A:MET:C | 7        | 3.01          |
| (1,40) | 1:315:A:GLN:N | 1:315:A:GLN:CA | 1:315:A:GLN:C  | 1:316:A:MET:N | 3        | 3.0           |
| (1,82) | 1:338:A:ASP:N | 1:338:A:ASP:CA | 1:338:A:ASP:C  | 1:339:A:SER:N | 10       | 2.99          |
| (1,41) | 1:315:A:GLN:C | 1:316:A:MET:N  | 1:316:A:MET:CA | 1:316:A:MET:C | 9        | 2.99          |
| (1,24) | 1:306:A:GLN:N | 1:306:A:GLN:CA | 1:306:A:GLN:C  | 1:307:A:LYS:N | 6        | 2.97          |
| (1,62) | 1:328:A:ASP:N | 1:328:A:ASP:CA | 1:328:A:ASP:C  | 1:329:A:ALA:N | 6        | 2.95          |
| (1,64) | 1:329:A:ALA:N | 1:329:A:ALA:CA | 1:329:A:ALA:C  | 1:330:A:LYS:N | 6        | 2.93          |
| (1,9)  | 1:296:A:GLU:C | 1:297:A:VAL:N  | 1:297:A:VAL:CA | 1:297:A:VAL:C | 1        | 2.93          |
| (1,76) | 1:335:A:ARG:N | 1:335:A:ARG:CA | 1:335:A:ARG:C  | 1:336:A:CYS:N | 2        | 2.92          |
| (1,28) | 1:308:A:CYS:N | 1:308:A:CYS:CA | 1:308:A:CYS:C  | 1:309:A:PHE:N | 7        | 2.91          |
| (1,24) | 1:306:A:GLN:N | 1:306:A:GLN:CA | 1:306:A:GLN:C  | 1:307:A:LYS:N | 9        | 2.91          |
| (1,62) | 1:328:A:ASP:N | 1:328:A:ASP:CA | 1:328:A:ASP:C  | 1:329:A:ALA:N | 5        | 2.88          |
| (1,62) | 1:328:A:ASP:N | 1:328:A:ASP:CA | 1:328:A:ASP:C  | 1:329:A:ALA:N | 8        | 2.87          |
| (1,20) | 1:304:A:GLU:N | 1:304:A:GLU:CA | 1:304:A:GLU:C  | 1:305:A:LEU:N | 6        | 2.87          |
| (1,76) | 1:335:A:ARG:N | 1:335:A:ARG:CA | 1:335:A:ARG:C  | 1:336:A:CYS:N | 9        | 2.86          |
| (1,41) | 1:315:A:GLN:C | 1:316:A:MET:N  | 1:316:A:MET:CA | 1:316:A:MET:C | 1        | 2.86          |
| (1,54) | 1:322:A:SER:N | 1:322:A:SER:CA | 1:322:A:SER:C  | 1:323:A:LYS:N | 7        | 2.85          |
| (1,24) | 1:306:A:GLN:N | 1:306:A:GLN:CA | 1:306:A:GLN:C  | 1:307:A:LYS:N | 1        | 2.85          |
| (1,77) | 1:335:A:ARG:C | 1:336:A:CYS:N  | 1:336:A:CYS:CA | 1:336:A:CYS:C | 6        | 2.83          |
| (1,68) | 1:331:A:TYR:N | 1:331:A:TYR:CA | 1:331:A:TYR:C  | 1:332:A:HIS:N | 6        | 2.83          |
| (1,64) | 1:329:A:ALA:N | 1:329:A:ALA:CA | 1:329:A:ALA:C  | 1:330:A:LYS:N | 8        | 2.83          |
| (1,40) | 1:315:A:GLN:N | 1:315:A:GLN:CA | 1:315:A:GLN:C  | 1:316:A:MET:N | 5        | 2.82          |
| (1,9)  | 1:296:A:GLU:C | 1:297:A:VAL:N  | 1:297:A:VAL:CA | 1:297:A:VAL:C | 9        | 2.82          |
| (1,79) | 1:336:A:CYS:C | 1:337:A:ILE:N  | 1:337:A:ILE:CA | 1:337:A:ILE:C | 2        | 2.81          |
| (1,59) | 1:326:A:PRO:C | 1:327:A:THR:N  | 1:327:A:THR:CA | 1:327:A:THR:C | 1        | 2.81          |
| (1,82) | 1:338:A:ASP:N | 1:338:A:ASP:CA | 1:338:A:ASP:C  | 1:339:A:SER:N | 4        | 2.79          |
| (1,68) | 1:331:A:TYR:N | 1:331:A:TYR:CA | 1:331:A:TYR:C  | 1:332:A:HIS:N | 2        | 2.79          |
| (1,68) | 1:331:A:TYR:N | 1:331:A:TYR:CA | 1:331:A:TYR:C  | 1:332:A:HIS:N | 5        | 2.79          |
| (1,63) | 1:328:A:ASP:C | 1:329:A:ALA:N  | 1:329:A:ALA:CA | 1:329:A:ALA:C | 7        | 2.79          |
| (1,41) | 1:315:A:GLN:C | 1:316:A:MET:N  | 1:316:A:MET:CA | 1:316:A:MET:C | 2        | 2.79          |
| (1,20) | 1:304:A:GLU:N | 1:304:A:GLU:CA | 1:304:A:GLU:C  | 1:305:A:LEU:N | 7        | 2.79          |
| (1,9)  | 1:296:A:GLU:C | 1:297:A:VAL:N  | 1:297:A:VAL:CA | 1:297:A:VAL:C | 2        | 2.79          |
| (1,68) | 1:331:A:TYR:N | 1:331:A:TYR:CA | 1:331:A:TYR:C  | 1:332:A:HIS:N | 4        | 2.78          |
| (1,62) | 1:328:A:ASP:N | 1:328:A:ASP:CA | 1:328:A:ASP:C  | 1:329:A:ALA:N | 3        | 2.77          |
| (1,41) | 1:315:A:GLN:C | 1:316:A:MET:N  | 1:316:A:MET:CA | 1:316:A:MET:C | 4        | 2.77          |
| (1,63) | 1:328:A:ASP:C | 1:329:A:ALA:N  | 1:329:A:ALA:CA | 1:329:A:ALA:C | 6        | 2.75          |
| (1,40) | 1:315:A:GLN:N | 1:315:A:GLN:CA | 1:315:A:GLN:C  | 1:316:A:MET:N | 9        | 2.75          |
| (1,54) | 1:322:A:SER:N | 1:322:A:SER:CA | 1:322:A:SER:C  | 1:323:A:LYS:N | 5        | 2.74          |
| (1,40) | 1:315:A:GLN:N | 1:315:A:GLN:CA | 1:315:A:GLN:C  | 1:316:A:MET:N | 10       | 2.74          |
| (1,76) | 1:335:A:ARG:N | 1:335:A:ARG:CA | 1:335:A:ARG:C  | 1:336:A:CYS:N | 1        | 2.73          |
| (1,75) | 1:334:A:GLN:C | 1:335:A:ARG:N  | 1:335:A:ARG:CA | 1:335:A:ARG:C | 9        | 2.73          |

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| Key    | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|--------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,75) | 1:334:A:GLN:C | 1:335:A:ARG:N  | 1:335:A:ARG:CA | 1:335:A:ARG:C | 4        | 2.71          |
| (1,28) | 1:308:A:CYS:N | 1:308:A:CYS:CA | 1:308:A:CYS:C  | 1:309:A:PHE:N | 4        | 2.71          |
| (1,75) | 1:334:A:GLN:C | 1:335:A:ARG:N  | 1:335:A:ARG:CA | 1:335:A:ARG:C | 2        | 2.7           |
| (1,77) | 1:335:A:ARG:C | 1:336:A:CYS:N  | 1:336:A:CYS:CA | 1:336:A:CYS:C | 2        | 2.69          |
| (1,62) | 1:328:A:ASP:N | 1:328:A:ASP:CA | 1:328:A:ASP:C  | 1:329:A:ALA:N | 10       | 2.69          |
| (1,59) | 1:326:A:PRO:C | 1:327:A:THR:N  | 1:327:A:THR:CA | 1:327:A:THR:C | 4        | 2.69          |
| (1,40) | 1:315:A:GLN:N | 1:315:A:GLN:CA | 1:315:A:GLN:C  | 1:316:A:MET:N | 1        | 2.69          |
| (1,9)  | 1:296:A:GLU:C | 1:297:A:VAL:N  | 1:297:A:VAL:CA | 1:297:A:VAL:C | 5        | 2.69          |
| (1,71) | 1:332:A:HIS:C | 1:333:A:MET:N  | 1:333:A:MET:CA | 1:333:A:MET:C | 1        | 2.68          |
| (1,24) | 1:306:A:GLN:N | 1:306:A:GLN:CA | 1:306:A:GLN:C  | 1:307:A:LYS:N | 4        | 2.67          |
| (1,59) | 1:326:A:PRO:C | 1:327:A:THR:N  | 1:327:A:THR:CA | 1:327:A:THR:C | 2        | 2.66          |
| (1,77) | 1:335:A:ARG:C | 1:336:A:CYS:N  | 1:336:A:CYS:CA | 1:336:A:CYS:C | 4        | 2.65          |
| (1,77) | 1:335:A:ARG:C | 1:336:A:CYS:N  | 1:336:A:CYS:CA | 1:336:A:CYS:C | 5        | 2.65          |
| (1,40) | 1:315:A:GLN:N | 1:315:A:GLN:CA | 1:315:A:GLN:C  | 1:316:A:MET:N | 4        | 2.65          |
| (1,13) | 1:298:A:TYR:C | 1:299:A:GLU:N  | 1:299:A:GLU:CA | 1:299:A:GLU:C | 1        | 2.65          |
| (1,77) | 1:335:A:ARG:C | 1:336:A:CYS:N  | 1:336:A:CYS:CA | 1:336:A:CYS:C | 1        | 2.64          |
| (1,62) | 1:328:A:ASP:N | 1:328:A:ASP:CA | 1:328:A:ASP:C  | 1:329:A:ALA:N | 2        | 2.64          |
| (1,23) | 1:305:A:LEU:C | 1:306:A:GLN:N  | 1:306:A:GLN:CA | 1:306:A:GLN:C | 2        | 2.63          |
| (1,59) | 1:326:A:PRO:C | 1:327:A:THR:N  | 1:327:A:THR:CA | 1:327:A:THR:C | 9        | 2.62          |
| (1,54) | 1:322:A:SER:N | 1:322:A:SER:CA | 1:322:A:SER:C  | 1:323:A:LYS:N | 10       | 2.62          |
| (1,24) | 1:306:A:GLN:N | 1:306:A:GLN:CA | 1:306:A:GLN:C  | 1:307:A:LYS:N | 2        | 2.62          |
| (1,63) | 1:328:A:ASP:C | 1:329:A:ALA:N  | 1:329:A:ALA:CA | 1:329:A:ALA:C | 10       | 2.61          |
| (1,28) | 1:308:A:CYS:N | 1:308:A:CYS:CA | 1:308:A:CYS:C  | 1:309:A:PHE:N | 6        | 2.61          |
| (1,20) | 1:304:A:GLU:N | 1:304:A:GLU:CA | 1:304:A:GLU:C  | 1:305:A:LEU:N | 10       | 2.61          |
| (1,77) | 1:335:A:ARG:C | 1:336:A:CYS:N  | 1:336:A:CYS:CA | 1:336:A:CYS:C | 8        | 2.6           |
| (1,61) | 1:327:A:THR:C | 1:328:A:ASP:N  | 1:328:A:ASP:CA | 1:328:A:ASP:C | 1        | 2.6           |
| (1,59) | 1:326:A:PRO:C | 1:327:A:THR:N  | 1:327:A:THR:CA | 1:327:A:THR:C | 7        | 2.59          |
| (1,61) | 1:327:A:THR:C | 1:328:A:ASP:N  | 1:328:A:ASP:CA | 1:328:A:ASP:C | 9        | 2.58          |
| (1,74) | 1:334:A:GLN:N | 1:334:A:GLN:CA | 1:334:A:GLN:C  | 1:335:A:ARG:N | 1        | 2.57          |
| (1,71) | 1:332:A:HIS:C | 1:333:A:MET:N  | 1:333:A:MET:CA | 1:333:A:MET:C | 7        | 2.57          |
| (1,61) | 1:327:A:THR:C | 1:328:A:ASP:N  | 1:328:A:ASP:CA | 1:328:A:ASP:C | 4        | 2.57          |
| (1,68) | 1:331:A:TYR:N | 1:331:A:TYR:CA | 1:331:A:TYR:C  | 1:332:A:HIS:N | 8        | 2.56          |
| (1,64) | 1:329:A:ALA:N | 1:329:A:ALA:CA | 1:329:A:ALA:C  | 1:330:A:LYS:N | 9        | 2.56          |
| (1,13) | 1:298:A:TYR:C | 1:299:A:GLU:N  | 1:299:A:GLU:CA | 1:299:A:GLU:C | 3        | 2.56          |
| (1,71) | 1:332:A:HIS:C | 1:333:A:MET:N  | 1:333:A:MET:CA | 1:333:A:MET:C | 6        | 2.55          |
| (1,60) | 1:327:A:THR:N | 1:327:A:THR:CA | 1:327:A:THR:C  | 1:328:A:ASP:N | 4        | 2.55          |
| (1,64) | 1:329:A:ALA:N | 1:329:A:ALA:CA | 1:329:A:ALA:C  | 1:330:A:LYS:N | 5        | 2.53          |
| (1,76) | 1:335:A:ARG:N | 1:335:A:ARG:CA | 1:335:A:ARG:C  | 1:336:A:CYS:N | 3        | 2.52          |
| (1,62) | 1:328:A:ASP:N | 1:328:A:ASP:CA | 1:328:A:ASP:C  | 1:329:A:ALA:N | 1        | 2.51          |
| (1,40) | 1:315:A:GLN:N | 1:315:A:GLN:CA | 1:315:A:GLN:C  | 1:316:A:MET:N | 2        | 2.51          |
| (1,76) | 1:335:A:ARG:N | 1:335:A:ARG:CA | 1:335:A:ARG:C  | 1:336:A:CYS:N | 7        | 2.5           |
| (1,62) | 1:328:A:ASP:N | 1:328:A:ASP:CA | 1:328:A:ASP:C  | 1:329:A:ALA:N | 4        | 2.5           |
| (1,76) | 1:335:A:ARG:N | 1:335:A:ARG:CA | 1:335:A:ARG:C  | 1:336:A:CYS:N | 4        | 2.49          |
| (1,75) | 1:334:A:GLN:C | 1:335:A:ARG:N  | 1:335:A:ARG:CA | 1:335:A:ARG:C | 7        | 2.48          |
| (1,77) | 1:335:A:ARG:C | 1:336:A:CYS:N  | 1:336:A:CYS:CA | 1:336:A:CYS:C | 7        | 2.47          |
| (1,63) | 1:328:A:ASP:C | 1:329:A:ALA:N  | 1:329:A:ALA:CA | 1:329:A:ALA:C | 8        | 2.47          |
| (1,70) | 1:332:A:HIS:N | 1:332:A:HIS:CA | 1:332:A:HIS:C  | 1:333:A:MET:N | 1        | 2.46          |
| (1,68) | 1:331:A:TYR:N | 1:331:A:TYR:CA | 1:331:A:TYR:C  | 1:332:A:HIS:N | 10       | 2.46          |
| (1,64) | 1:329:A:ALA:N | 1:329:A:ALA:CA | 1:329:A:ALA:C  | 1:330:A:LYS:N | 3        | 2.46          |
| (1,62) | 1:328:A:ASP:N | 1:328:A:ASP:CA | 1:328:A:ASP:C  | 1:329:A:ALA:N | 9        | 2.46          |
| (1,13) | 1:298:A:TYR:C | 1:299:A:GLU:N  | 1:299:A:GLU:CA | 1:299:A:GLU:C | 4        | 2.46          |

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| Key    | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|--------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,63) | 1:328:A:ASP:C | 1:329:A:ALA:N  | 1:329:A:ALA:CA | 1:329:A:ALA:C | 3        | 2.45          |
| (1,61) | 1:327:A:THR:C | 1:328:A:ASP:N  | 1:328:A:ASP:CA | 1:328:A:ASP:C | 2        | 2.45          |
| (1,13) | 1:298:A:TYR:C | 1:299:A:GLU:N  | 1:299:A:GLU:CA | 1:299:A:GLU:C | 10       | 2.45          |
| (1,82) | 1:338:A:ASP:N | 1:338:A:ASP:CA | 1:338:A:ASP:C  | 1:339:A:SER:N | 7        | 2.44          |
| (1,68) | 1:331:A:TYR:N | 1:331:A:TYR:CA | 1:331:A:TYR:C  | 1:332:A:HIS:N | 3        | 2.44          |
| (1,61) | 1:327:A:THR:C | 1:328:A:ASP:N  | 1:328:A:ASP:CA | 1:328:A:ASP:C | 10       | 2.44          |
| (1,60) | 1:327:A:THR:N | 1:327:A:THR:CA | 1:327:A:THR:C  | 1:328:A:ASP:N | 1        | 2.44          |
| (1,65) | 1:329:A:ALA:C | 1:330:A:LYS:N  | 1:330:A:LYS:CA | 1:330:A:LYS:C | 7        | 2.42          |
| (1,60) | 1:327:A:THR:N | 1:327:A:THR:CA | 1:327:A:THR:C  | 1:328:A:ASP:N | 9        | 2.42          |
| (1,28) | 1:308:A:CYS:N | 1:308:A:CYS:CA | 1:308:A:CYS:C  | 1:309:A:PHE:N | 8        | 2.4           |
| (1,63) | 1:328:A:ASP:C | 1:329:A:ALA:N  | 1:329:A:ALA:CA | 1:329:A:ALA:C | 5        | 2.39          |
| (1,64) | 1:329:A:ALA:N | 1:329:A:ALA:CA | 1:329:A:ALA:C  | 1:330:A:LYS:N | 1        | 2.37          |
| (1,60) | 1:327:A:THR:N | 1:327:A:THR:CA | 1:327:A:THR:C  | 1:328:A:ASP:N | 2        | 2.37          |
| (1,28) | 1:308:A:CYS:N | 1:308:A:CYS:CA | 1:308:A:CYS:C  | 1:309:A:PHE:N | 3        | 2.37          |
| (1,13) | 1:298:A:TYR:C | 1:299:A:GLU:N  | 1:299:A:GLU:CA | 1:299:A:GLU:C | 2        | 2.34          |
| (1,78) | 1:336:A:CYS:N | 1:336:A:CYS:CA | 1:336:A:CYS:C  | 1:337:A:ILE:N | 1        | 2.33          |
| (1,28) | 1:308:A:CYS:N | 1:308:A:CYS:CA | 1:308:A:CYS:C  | 1:309:A:PHE:N | 1        | 2.33          |
| (1,21) | 1:304:A:GLU:C | 1:305:A:LEU:N  | 1:305:A:LEU:CA | 1:305:A:LEU:C | 7        | 2.33          |
| (1,71) | 1:332:A:HIS:C | 1:333:A:MET:N  | 1:333:A:MET:CA | 1:333:A:MET:C | 2        | 2.32          |
| (1,21) | 1:304:A:GLU:C | 1:305:A:LEU:N  | 1:305:A:LEU:CA | 1:305:A:LEU:C | 10       | 2.3           |
| (1,71) | 1:332:A:HIS:C | 1:333:A:MET:N  | 1:333:A:MET:CA | 1:333:A:MET:C | 4        | 2.29          |
| (1,71) | 1:332:A:HIS:C | 1:333:A:MET:N  | 1:333:A:MET:CA | 1:333:A:MET:C | 10       | 2.29          |
| (1,31) | 1:309:A:PHE:C | 1:310:A:ASP:N  | 1:310:A:ASP:CA | 1:310:A:ASP:C | 5        | 2.29          |
| (1,80) | 1:337:A:ILE:N | 1:337:A:ILE:CA | 1:337:A:ILE:C  | 1:338:A:ASP:N | 8        | 2.28          |
| (1,79) | 1:336:A:CYS:C | 1:337:A:ILE:N  | 1:337:A:ILE:CA | 1:337:A:ILE:C | 1        | 2.28          |
| (1,44) | 1:317:A:LEU:N | 1:317:A:LEU:CA | 1:317:A:LEU:C  | 1:318:A:GLN:N | 9        | 2.28          |
| (1,31) | 1:309:A:PHE:C | 1:310:A:ASP:N  | 1:310:A:ASP:CA | 1:310:A:ASP:C | 10       | 2.28          |
| (1,77) | 1:335:A:ARG:C | 1:336:A:CYS:N  | 1:336:A:CYS:CA | 1:336:A:CYS:C | 10       | 2.26          |
| (1,27) | 1:307:A:LYS:C | 1:308:A:CYS:N  | 1:308:A:CYS:CA | 1:308:A:CYS:C | 7        | 2.26          |
| (1,80) | 1:337:A:ILE:N | 1:337:A:ILE:CA | 1:337:A:ILE:C  | 1:338:A:ASP:N | 6        | 2.25          |
| (1,65) | 1:329:A:ALA:C | 1:330:A:LYS:N  | 1:330:A:LYS:CA | 1:330:A:LYS:C | 8        | 2.25          |
| (1,47) | 1:318:A:GLN:C | 1:319:A:ASP:N  | 1:319:A:ASP:CA | 1:319:A:ASP:C | 1        | 2.24          |
| (1,37) | 1:313:A:ASP:C | 1:314:A:VAL:N  | 1:314:A:VAL:CA | 1:314:A:VAL:C | 4        | 2.24          |
| (1,31) | 1:309:A:PHE:C | 1:310:A:ASP:N  | 1:310:A:ASP:CA | 1:310:A:ASP:C | 7        | 2.24          |
| (1,83) | 1:338:A:ASP:C | 1:339:A:SER:N  | 1:339:A:SER:CA | 1:339:A:SER:C | 10       | 2.23          |
| (1,70) | 1:332:A:HIS:N | 1:332:A:HIS:CA | 1:332:A:HIS:C  | 1:333:A:MET:N | 7        | 2.22          |
| (1,68) | 1:331:A:TYR:N | 1:331:A:TYR:CA | 1:331:A:TYR:C  | 1:332:A:HIS:N | 7        | 2.22          |
| (1,31) | 1:309:A:PHE:C | 1:310:A:ASP:N  | 1:310:A:ASP:CA | 1:310:A:ASP:C | 1        | 2.22          |
| (1,31) | 1:309:A:PHE:C | 1:310:A:ASP:N  | 1:310:A:ASP:CA | 1:310:A:ASP:C | 8        | 2.21          |
| (1,71) | 1:332:A:HIS:C | 1:333:A:MET:N  | 1:333:A:MET:CA | 1:333:A:MET:C | 5        | 2.2           |
| (1,64) | 1:329:A:ALA:N | 1:329:A:ALA:CA | 1:329:A:ALA:C  | 1:330:A:LYS:N | 2        | 2.2           |
| (1,61) | 1:327:A:THR:C | 1:328:A:ASP:N  | 1:328:A:ASP:CA | 1:328:A:ASP:C | 8        | 2.2           |
| (1,44) | 1:317:A:LEU:N | 1:317:A:LEU:CA | 1:317:A:LEU:C  | 1:318:A:GLN:N | 1        | 2.2           |
| (1,64) | 1:329:A:ALA:N | 1:329:A:ALA:CA | 1:329:A:ALA:C  | 1:330:A:LYS:N | 10       | 2.19          |
| (1,31) | 1:309:A:PHE:C | 1:310:A:ASP:N  | 1:310:A:ASP:CA | 1:310:A:ASP:C | 4        | 2.19          |
| (1,61) | 1:327:A:THR:C | 1:328:A:ASP:N  | 1:328:A:ASP:CA | 1:328:A:ASP:C | 5        | 2.18          |
| (1,23) | 1:305:A:LEU:C | 1:306:A:GLN:N  | 1:306:A:GLN:CA | 1:306:A:GLN:C | 4        | 2.18          |
| (1,68) | 1:331:A:TYR:N | 1:331:A:TYR:CA | 1:331:A:TYR:C  | 1:332:A:HIS:N | 1        | 2.17          |
| (1,61) | 1:327:A:THR:C | 1:328:A:ASP:N  | 1:328:A:ASP:CA | 1:328:A:ASP:C | 3        | 2.17          |
| (1,47) | 1:318:A:GLN:C | 1:319:A:ASP:N  | 1:319:A:ASP:CA | 1:319:A:ASP:C | 4        | 2.17          |
| (1,46) | 1:318:A:GLN:N | 1:318:A:GLN:CA | 1:318:A:GLN:C  | 1:319:A:ASP:N | 1        | 2.17          |

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| Key    | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|--------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,71) | 1:332:A:HIS:C | 1:333:A:MET:N  | 1:333:A:MET:CA | 1:333:A:MET:C | 8        | 2.15          |
| (1,59) | 1:326:A:PRO:C | 1:327:A:THR:N  | 1:327:A:THR:CA | 1:327:A:THR:C | 8        | 2.15          |
| (1,13) | 1:298:A:TYR:C | 1:299:A:GLU:N  | 1:299:A:GLU:CA | 1:299:A:GLU:C | 9        | 2.15          |
| (1,80) | 1:337:A:ILE:N | 1:337:A:ILE:CA | 1:337:A:ILE:C  | 1:338:A:ASP:N | 5        | 2.13          |
| (1,68) | 1:331:A:TYR:N | 1:331:A:TYR:CA | 1:331:A:TYR:C  | 1:332:A:HIS:N | 9        | 2.13          |
| (1,31) | 1:309:A:PHE:C | 1:310:A:ASP:N  | 1:310:A:ASP:CA | 1:310:A:ASP:C | 6        | 2.13          |
| (1,26) | 1:307:A:LYS:N | 1:307:A:LYS:CA | 1:307:A:LYS:C  | 1:308:A:CYS:N | 6        | 2.12          |
| (1,70) | 1:332:A:HIS:N | 1:332:A:HIS:CA | 1:332:A:HIS:C  | 1:333:A:MET:N | 6        | 2.11          |
| (1,37) | 1:313:A:ASP:C | 1:314:A:VAL:N  | 1:314:A:VAL:CA | 1:314:A:VAL:C | 2        | 2.11          |
| (1,75) | 1:334:A:GLN:C | 1:335:A:ARG:N  | 1:335:A:ARG:CA | 1:335:A:ARG:C | 1        | 2.09          |
| (1,37) | 1:313:A:ASP:C | 1:314:A:VAL:N  | 1:314:A:VAL:CA | 1:314:A:VAL:C | 8        | 2.09          |
| (1,31) | 1:309:A:PHE:C | 1:310:A:ASP:N  | 1:310:A:ASP:CA | 1:310:A:ASP:C | 3        | 2.09          |
| (1,28) | 1:308:A:CYS:N | 1:308:A:CYS:CA | 1:308:A:CYS:C  | 1:309:A:PHE:N | 5        | 2.09          |
| (1,59) | 1:326:A:PRO:C | 1:327:A:THR:N  | 1:327:A:THR:CA | 1:327:A:THR:C | 6        | 2.07          |
| (1,37) | 1:313:A:ASP:C | 1:314:A:VAL:N  | 1:314:A:VAL:CA | 1:314:A:VAL:C | 1        | 2.07          |
| (1,31) | 1:309:A:PHE:C | 1:310:A:ASP:N  | 1:310:A:ASP:CA | 1:310:A:ASP:C | 9        | 2.07          |
| (1,79) | 1:336:A:CYS:C | 1:337:A:ILE:N  | 1:337:A:ILE:CA | 1:337:A:ILE:C | 4        | 2.06          |
| (1,63) | 1:328:A:ASP:C | 1:329:A:ALA:N  | 1:329:A:ALA:CA | 1:329:A:ALA:C | 2        | 2.06          |
| (1,65) | 1:329:A:ALA:C | 1:330:A:LYS:N  | 1:330:A:LYS:CA | 1:330:A:LYS:C | 6        | 2.05          |
| (1,83) | 1:338:A:ASP:C | 1:339:A:SER:N  | 1:339:A:SER:CA | 1:339:A:SER:C | 3        | 2.04          |
| (1,59) | 1:326:A:PRO:C | 1:327:A:THR:N  | 1:327:A:THR:CA | 1:327:A:THR:C | 5        | 2.04          |
| (1,83) | 1:338:A:ASP:C | 1:339:A:SER:N  | 1:339:A:SER:CA | 1:339:A:SER:C | 2        | 2.03          |
| (1,13) | 1:298:A:TYR:C | 1:299:A:GLU:N  | 1:299:A:GLU:CA | 1:299:A:GLU:C | 7        | 2.03          |
| (1,65) | 1:329:A:ALA:C | 1:330:A:LYS:N  | 1:330:A:LYS:CA | 1:330:A:LYS:C | 5        | 2.02          |
| (1,86) | 1:342:A:TRP:N | 1:342:A:TRP:CA | 1:342:A:TRP:C  | 1:343:A:VAL:N | 5        | 2.01          |
| (1,86) | 1:342:A:TRP:N | 1:342:A:TRP:CA | 1:342:A:TRP:C  | 1:343:A:VAL:N | 8        | 2.01          |
| (1,32) | 1:310:A:ASP:N | 1:310:A:ASP:CA | 1:310:A:ASP:C  | 1:311:A:VAL:N | 6        | 2.01          |
| (1,82) | 1:338:A:ASP:N | 1:338:A:ASP:CA | 1:338:A:ASP:C  | 1:339:A:SER:N | 1        | 2.0           |
| (1,60) | 1:327:A:THR:N | 1:327:A:THR:CA | 1:327:A:THR:C  | 1:328:A:ASP:N | 5        | 2.0           |
| (1,44) | 1:317:A:LEU:N | 1:317:A:LEU:CA | 1:317:A:LEU:C  | 1:318:A:GLN:N | 2        | 2.0           |
| (1,37) | 1:313:A:ASP:C | 1:314:A:VAL:N  | 1:314:A:VAL:CA | 1:314:A:VAL:C | 5        | 2.0           |
| (1,23) | 1:305:A:LEU:C | 1:306:A:GLN:N  | 1:306:A:GLN:CA | 1:306:A:GLN:C | 8        | 2.0           |
| (1,21) | 1:304:A:GLU:C | 1:305:A:LEU:N  | 1:305:A:LEU:CA | 1:305:A:LEU:C | 6        | 1.98          |
| (1,28) | 1:308:A:CYS:N | 1:308:A:CYS:CA | 1:308:A:CYS:C  | 1:309:A:PHE:N | 9        | 1.97          |
| (1,55) | 1:322:A:SER:C | 1:323:A:LYS:N  | 1:323:A:LYS:CA | 1:323:A:LYS:C | 1        | 1.95          |
| (1,20) | 1:304:A:GLU:N | 1:304:A:GLU:CA | 1:304:A:GLU:C  | 1:305:A:LEU:N | 3        | 1.95          |
| (1,65) | 1:329:A:ALA:C | 1:330:A:LYS:N  | 1:330:A:LYS:CA | 1:330:A:LYS:C | 9        | 1.94          |
| (1,46) | 1:318:A:GLN:N | 1:318:A:GLN:CA | 1:318:A:GLN:C  | 1:319:A:ASP:N | 4        | 1.94          |
| (1,37) | 1:313:A:ASP:C | 1:314:A:VAL:N  | 1:314:A:VAL:CA | 1:314:A:VAL:C | 9        | 1.94          |
| (1,13) | 1:298:A:TYR:C | 1:299:A:GLU:N  | 1:299:A:GLU:CA | 1:299:A:GLU:C | 8        | 1.94          |
| (1,12) | 1:298:A:TYR:N | 1:298:A:TYR:CA | 1:298:A:TYR:C  | 1:299:A:GLU:N | 2        | 1.94          |
| (1,55) | 1:322:A:SER:C | 1:323:A:LYS:N  | 1:323:A:LYS:CA | 1:323:A:LYS:C | 9        | 1.93          |
| (1,63) | 1:328:A:ASP:C | 1:329:A:ALA:N  | 1:329:A:ALA:CA | 1:329:A:ALA:C | 1        | 1.91          |
| (1,63) | 1:328:A:ASP:C | 1:329:A:ALA:N  | 1:329:A:ALA:CA | 1:329:A:ALA:C | 4        | 1.91          |
| (1,63) | 1:328:A:ASP:C | 1:329:A:ALA:N  | 1:329:A:ALA:CA | 1:329:A:ALA:C | 9        | 1.91          |
| (1,61) | 1:327:A:THR:C | 1:328:A:ASP:N  | 1:328:A:ASP:CA | 1:328:A:ASP:C | 6        | 1.91          |
| (1,37) | 1:313:A:ASP:C | 1:314:A:VAL:N  | 1:314:A:VAL:CA | 1:314:A:VAL:C | 6        | 1.9           |
| (1,31) | 1:309:A:PHE:C | 1:310:A:ASP:N  | 1:310:A:ASP:CA | 1:310:A:ASP:C | 2        | 1.9           |
| (1,79) | 1:336:A:CYS:C | 1:337:A:ILE:N  | 1:337:A:ILE:CA | 1:337:A:ILE:C | 7        | 1.89          |
| (1,64) | 1:329:A:ALA:N | 1:329:A:ALA:CA | 1:329:A:ALA:C  | 1:330:A:LYS:N | 4        | 1.89          |
| (1,12) | 1:298:A:TYR:N | 1:298:A:TYR:CA | 1:298:A:TYR:C  | 1:299:A:GLU:N | 1        | 1.89          |

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| Key    | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|--------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,59) | 1:326:A:PRO:C | 1:327:A:THR:N  | 1:327:A:THR:CA | 1:327:A:THR:C | 3        | 1.88          |
| (1,85) | 1:341:A:LEU:C | 1:342:A:TRP:N  | 1:342:A:TRP:CA | 1:342:A:TRP:C | 8        | 1.87          |
| (1,47) | 1:318:A:GLN:C | 1:319:A:ASP:N  | 1:319:A:ASP:CA | 1:319:A:ASP:C | 2        | 1.87          |
| (1,60) | 1:327:A:THR:N | 1:327:A:THR:CA | 1:327:A:THR:C  | 1:328:A:ASP:N | 10       | 1.86          |
| (1,44) | 1:317:A:LEU:N | 1:317:A:LEU:CA | 1:317:A:LEU:C  | 1:318:A:GLN:N | 4        | 1.86          |
| (1,27) | 1:307:A:LYS:C | 1:308:A:CYS:N  | 1:308:A:CYS:CA | 1:308:A:CYS:C | 6        | 1.84          |
| (1,23) | 1:305:A:LEU:C | 1:306:A:GLN:N  | 1:306:A:GLN:CA | 1:306:A:GLN:C | 3        | 1.84          |
| (1,14) | 1:299:A:GLU:N | 1:299:A:GLU:CA | 1:299:A:GLU:C  | 1:300:A:SER:N | 6        | 1.83          |
| (1,86) | 1:342:A:TRP:N | 1:342:A:TRP:CA | 1:342:A:TRP:C  | 1:343:A:VAL:N | 3        | 1.81          |
| (1,61) | 1:327:A:THR:C | 1:328:A:ASP:N  | 1:328:A:ASP:CA | 1:328:A:ASP:C | 7        | 1.81          |
| (1,55) | 1:322:A:SER:C | 1:323:A:LYS:N  | 1:323:A:LYS:CA | 1:323:A:LYS:C | 2        | 1.81          |
| (1,37) | 1:313:A:ASP:C | 1:314:A:VAL:N  | 1:314:A:VAL:CA | 1:314:A:VAL:C | 3        | 1.81          |
| (1,20) | 1:304:A:GLU:N | 1:304:A:GLU:CA | 1:304:A:GLU:C  | 1:305:A:LEU:N | 9        | 1.81          |
| (1,60) | 1:327:A:THR:N | 1:327:A:THR:CA | 1:327:A:THR:C  | 1:328:A:ASP:N | 3        | 1.8           |
| (1,12) | 1:298:A:TYR:N | 1:298:A:TYR:CA | 1:298:A:TYR:C  | 1:299:A:GLU:N | 4        | 1.78          |
| (1,25) | 1:306:A:GLN:C | 1:307:A:LYS:N  | 1:307:A:LYS:CA | 1:307:A:LYS:C | 6        | 1.77          |
| (1,32) | 1:310:A:ASP:N | 1:310:A:ASP:CA | 1:310:A:ASP:C  | 1:311:A:VAL:N | 10       | 1.76          |
| (1,23) | 1:305:A:LEU:C | 1:306:A:GLN:N  | 1:306:A:GLN:CA | 1:306:A:GLN:C | 5        | 1.76          |
| (1,14) | 1:299:A:GLU:N | 1:299:A:GLU:CA | 1:299:A:GLU:C  | 1:300:A:SER:N | 3        | 1.76          |
| (1,55) | 1:322:A:SER:C | 1:323:A:LYS:N  | 1:323:A:LYS:CA | 1:323:A:LYS:C | 4        | 1.75          |
| (1,14) | 1:299:A:GLU:N | 1:299:A:GLU:CA | 1:299:A:GLU:C  | 1:300:A:SER:N | 7        | 1.73          |
| (1,46) | 1:318:A:GLN:N | 1:318:A:GLN:CA | 1:318:A:GLN:C  | 1:319:A:ASP:N | 2        | 1.72          |
| (1,22) | 1:305:A:LEU:N | 1:305:A:LEU:CA | 1:305:A:LEU:C  | 1:306:A:GLN:N | 2        | 1.72          |
| (1,60) | 1:327:A:THR:N | 1:327:A:THR:CA | 1:327:A:THR:C  | 1:328:A:ASP:N | 8        | 1.71          |
| (1,25) | 1:306:A:GLN:C | 1:307:A:LYS:N  | 1:307:A:LYS:CA | 1:307:A:LYS:C | 3        | 1.71          |
| (1,90) | 1:375:A:ASP:N | 1:375:A:ASP:CA | 1:375:A:ASP:C  | 1:376:A:VAL:N | 1        | 1.69          |
| (1,23) | 1:305:A:LEU:C | 1:306:A:GLN:N  | 1:306:A:GLN:CA | 1:306:A:GLN:C | 9        | 1.69          |
| (1,82) | 1:338:A:ASP:N | 1:338:A:ASP:CA | 1:338:A:ASP:C  | 1:339:A:SER:N | 6        | 1.68          |
| (1,70) | 1:332:A:HIS:N | 1:332:A:HIS:CA | 1:332:A:HIS:C  | 1:333:A:MET:N | 2        | 1.68          |
| (1,32) | 1:310:A:ASP:N | 1:310:A:ASP:CA | 1:310:A:ASP:C  | 1:311:A:VAL:N | 7        | 1.68          |
| (1,21) | 1:304:A:GLU:C | 1:305:A:LEU:N  | 1:305:A:LEU:CA | 1:305:A:LEU:C | 2        | 1.68          |
| (1,14) | 1:299:A:GLU:N | 1:299:A:GLU:CA | 1:299:A:GLU:C  | 1:300:A:SER:N | 4        | 1.68          |
| (1,32) | 1:310:A:ASP:N | 1:310:A:ASP:CA | 1:310:A:ASP:C  | 1:311:A:VAL:N | 5        | 1.67          |
| (1,14) | 1:299:A:GLU:N | 1:299:A:GLU:CA | 1:299:A:GLU:C  | 1:300:A:SER:N | 1        | 1.67          |
| (1,13) | 1:298:A:TYR:C | 1:299:A:GLU:N  | 1:299:A:GLU:CA | 1:299:A:GLU:C | 5        | 1.67          |
| (1,59) | 1:326:A:PRO:C | 1:327:A:THR:N  | 1:327:A:THR:CA | 1:327:A:THR:C | 10       | 1.65          |
| (1,25) | 1:306:A:GLN:C | 1:307:A:LYS:N  | 1:307:A:LYS:CA | 1:307:A:LYS:C | 7        | 1.65          |
| (1,32) | 1:310:A:ASP:N | 1:310:A:ASP:CA | 1:310:A:ASP:C  | 1:311:A:VAL:N | 9        | 1.64          |
| (1,14) | 1:299:A:GLU:N | 1:299:A:GLU:CA | 1:299:A:GLU:C  | 1:300:A:SER:N | 2        | 1.64          |
| (1,90) | 1:375:A:ASP:N | 1:375:A:ASP:CA | 1:375:A:ASP:C  | 1:376:A:VAL:N | 3        | 1.63          |
| (1,85) | 1:341:A:LEU:C | 1:342:A:TRP:N  | 1:342:A:TRP:CA | 1:342:A:TRP:C | 9        | 1.63          |
| (1,82) | 1:338:A:ASP:N | 1:338:A:ASP:CA | 1:338:A:ASP:C  | 1:339:A:SER:N | 8        | 1.63          |
| (1,14) | 1:299:A:GLU:N | 1:299:A:GLU:CA | 1:299:A:GLU:C  | 1:300:A:SER:N | 10       | 1.63          |
| (1,12) | 1:298:A:TYR:N | 1:298:A:TYR:CA | 1:298:A:TYR:C  | 1:299:A:GLU:N | 9        | 1.63          |
| (1,90) | 1:375:A:ASP:N | 1:375:A:ASP:CA | 1:375:A:ASP:C  | 1:376:A:VAL:N | 6        | 1.62          |
| (1,90) | 1:375:A:ASP:N | 1:375:A:ASP:CA | 1:375:A:ASP:C  | 1:376:A:VAL:N | 9        | 1.62          |
| (1,80) | 1:337:A:ILE:N | 1:337:A:ILE:CA | 1:337:A:ILE:C  | 1:338:A:ASP:N | 3        | 1.62          |
| (1,65) | 1:329:A:ALA:C | 1:330:A:LYS:N  | 1:330:A:LYS:CA | 1:330:A:LYS:C | 1        | 1.62          |
| (1,25) | 1:306:A:GLN:C | 1:307:A:LYS:N  | 1:307:A:LYS:CA | 1:307:A:LYS:C | 8        | 1.62          |
| (1,23) | 1:305:A:LEU:C | 1:306:A:GLN:N  | 1:306:A:GLN:CA | 1:306:A:GLN:C | 1        | 1.62          |
| (1,60) | 1:327:A:THR:N | 1:327:A:THR:CA | 1:327:A:THR:C  | 1:328:A:ASP:N | 6        | 1.61          |

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| Key    | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|--------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,37) | 1:313:A:ASP:C | 1:314:A:VAL:N  | 1:314:A:VAL:CA | 1:314:A:VAL:C | 10       | 1.61          |
| (1,32) | 1:310:A:ASP:N | 1:310:A:ASP:CA | 1:310:A:ASP:C  | 1:311:A:VAL:N | 8        | 1.61          |
| (1,90) | 1:375:A:ASP:N | 1:375:A:ASP:CA | 1:375:A:ASP:C  | 1:376:A:VAL:N | 4        | 1.6           |
| (1,76) | 1:335:A:ARG:N | 1:335:A:ARG:CA | 1:335:A:ARG:C  | 1:336:A:CYS:N | 10       | 1.59          |
| (1,28) | 1:308:A:CYS:N | 1:308:A:CYS:CA | 1:308:A:CYS:C  | 1:309:A:PHE:N | 10       | 1.59          |
| (1,90) | 1:375:A:ASP:N | 1:375:A:ASP:CA | 1:375:A:ASP:C  | 1:376:A:VAL:N | 10       | 1.58          |
| (1,32) | 1:310:A:ASP:N | 1:310:A:ASP:CA | 1:310:A:ASP:C  | 1:311:A:VAL:N | 1        | 1.58          |
| (1,79) | 1:336:A:CYS:C | 1:337:A:ILE:N  | 1:337:A:ILE:CA | 1:337:A:ILE:C | 9        | 1.57          |
| (1,13) | 1:298:A:TYR:C | 1:299:A:GLU:N  | 1:299:A:GLU:CA | 1:299:A:GLU:C | 6        | 1.56          |
| (1,32) | 1:310:A:ASP:N | 1:310:A:ASP:CA | 1:310:A:ASP:C  | 1:311:A:VAL:N | 3        | 1.55          |
| (1,60) | 1:327:A:THR:N | 1:327:A:THR:CA | 1:327:A:THR:C  | 1:328:A:ASP:N | 7        | 1.53          |
| (1,90) | 1:375:A:ASP:N | 1:375:A:ASP:CA | 1:375:A:ASP:C  | 1:376:A:VAL:N | 8        | 1.52          |
| (1,70) | 1:332:A:HIS:N | 1:332:A:HIS:CA | 1:332:A:HIS:C  | 1:333:A:MET:N | 8        | 1.52          |
| (1,20) | 1:304:A:GLU:N | 1:304:A:GLU:CA | 1:304:A:GLU:C  | 1:305:A:LEU:N | 1        | 1.52          |
| (1,69) | 1:331:A:TYR:C | 1:332:A:HIS:N  | 1:332:A:HIS:CA | 1:332:A:HIS:C | 6        | 1.51          |
| (1,69) | 1:331:A:TYR:C | 1:332:A:HIS:N  | 1:332:A:HIS:CA | 1:332:A:HIS:C | 5        | 1.5           |
| (1,21) | 1:304:A:GLU:C | 1:305:A:LEU:N  | 1:305:A:LEU:CA | 1:305:A:LEU:C | 9        | 1.49          |
| (1,12) | 1:298:A:TYR:N | 1:298:A:TYR:CA | 1:298:A:TYR:C  | 1:299:A:GLU:N | 3        | 1.49          |
| (1,90) | 1:375:A:ASP:N | 1:375:A:ASP:CA | 1:375:A:ASP:C  | 1:376:A:VAL:N | 7        | 1.48          |
| (1,70) | 1:332:A:HIS:N | 1:332:A:HIS:CA | 1:332:A:HIS:C  | 1:333:A:MET:N | 4        | 1.48          |
| (1,14) | 1:299:A:GLU:N | 1:299:A:GLU:CA | 1:299:A:GLU:C  | 1:300:A:SER:N | 5        | 1.48          |
| (1,85) | 1:341:A:LEU:C | 1:342:A:TRP:N  | 1:342:A:TRP:CA | 1:342:A:TRP:C | 3        | 1.47          |
| (1,32) | 1:310:A:ASP:N | 1:310:A:ASP:CA | 1:310:A:ASP:C  | 1:311:A:VAL:N | 2        | 1.47          |
| (1,32) | 1:310:A:ASP:N | 1:310:A:ASP:CA | 1:310:A:ASP:C  | 1:311:A:VAL:N | 4        | 1.47          |
| (1,88) | 1:373:A:GLU:N | 1:373:A:GLU:CA | 1:373:A:GLU:C  | 1:374:A:LYS:N | 1        | 1.45          |
| (1,88) | 1:373:A:GLU:N | 1:373:A:GLU:CA | 1:373:A:GLU:C  | 1:374:A:LYS:N | 3        | 1.44          |
| (1,82) | 1:338:A:ASP:N | 1:338:A:ASP:CA | 1:338:A:ASP:C  | 1:339:A:SER:N | 5        | 1.44          |
| (1,71) | 1:332:A:HIS:C | 1:333:A:MET:N  | 1:333:A:MET:CA | 1:333:A:MET:C | 3        | 1.44          |
| (1,55) | 1:322:A:SER:C | 1:323:A:LYS:N  | 1:323:A:LYS:CA | 1:323:A:LYS:C | 8        | 1.44          |
| (1,80) | 1:337:A:ILE:N | 1:337:A:ILE:CA | 1:337:A:ILE:C  | 1:338:A:ASP:N | 10       | 1.43          |
| (1,65) | 1:329:A:ALA:C | 1:330:A:LYS:N  | 1:330:A:LYS:CA | 1:330:A:LYS:C | 2        | 1.43          |
| (1,55) | 1:322:A:SER:C | 1:323:A:LYS:N  | 1:323:A:LYS:CA | 1:323:A:LYS:C | 6        | 1.43          |
| (1,50) | 1:320:A:ALA:N | 1:320:A:ALA:CA | 1:320:A:ALA:C  | 1:321:A:ILE:N | 7        | 1.43          |
| (1,85) | 1:341:A:LEU:C | 1:342:A:TRP:N  | 1:342:A:TRP:CA | 1:342:A:TRP:C | 10       | 1.42          |
| (1,65) | 1:329:A:ALA:C | 1:330:A:LYS:N  | 1:330:A:LYS:CA | 1:330:A:LYS:C | 3        | 1.42          |
| (1,65) | 1:329:A:ALA:C | 1:330:A:LYS:N  | 1:330:A:LYS:CA | 1:330:A:LYS:C | 10       | 1.42          |
| (1,55) | 1:322:A:SER:C | 1:323:A:LYS:N  | 1:323:A:LYS:CA | 1:323:A:LYS:C | 7        | 1.42          |
| (1,88) | 1:373:A:GLU:N | 1:373:A:GLU:CA | 1:373:A:GLU:C  | 1:374:A:LYS:N | 7        | 1.41          |
| (1,14) | 1:299:A:GLU:N | 1:299:A:GLU:CA | 1:299:A:GLU:C  | 1:300:A:SER:N | 9        | 1.41          |
| (1,78) | 1:336:A:CYS:N | 1:336:A:CYS:CA | 1:336:A:CYS:C  | 1:337:A:ILE:N | 7        | 1.4           |
| (1,85) | 1:341:A:LEU:C | 1:342:A:TRP:N  | 1:342:A:TRP:CA | 1:342:A:TRP:C | 1        | 1.39          |
| (1,25) | 1:306:A:GLN:C | 1:307:A:LYS:N  | 1:307:A:LYS:CA | 1:307:A:LYS:C | 1        | 1.38          |
| (1,25) | 1:306:A:GLN:C | 1:307:A:LYS:N  | 1:307:A:LYS:CA | 1:307:A:LYS:C | 9        | 1.38          |
| (1,22) | 1:305:A:LEU:N | 1:305:A:LEU:CA | 1:305:A:LEU:C  | 1:306:A:GLN:N | 4        | 1.37          |
| (1,90) | 1:375:A:ASP:N | 1:375:A:ASP:CA | 1:375:A:ASP:C  | 1:376:A:VAL:N | 5        | 1.36          |
| (1,88) | 1:373:A:GLU:N | 1:373:A:GLU:CA | 1:373:A:GLU:C  | 1:374:A:LYS:N | 2        | 1.36          |
| (1,20) | 1:304:A:GLU:N | 1:304:A:GLU:CA | 1:304:A:GLU:C  | 1:305:A:LEU:N | 4        | 1.36          |
| (1,88) | 1:373:A:GLU:N | 1:373:A:GLU:CA | 1:373:A:GLU:C  | 1:374:A:LYS:N | 5        | 1.35          |
| (1,88) | 1:373:A:GLU:N | 1:373:A:GLU:CA | 1:373:A:GLU:C  | 1:374:A:LYS:N | 8        | 1.35          |
| (1,46) | 1:318:A:GLN:N | 1:318:A:GLN:CA | 1:318:A:GLN:C  | 1:319:A:ASP:N | 7        | 1.35          |
| (1,88) | 1:373:A:GLU:N | 1:373:A:GLU:CA | 1:373:A:GLU:C  | 1:374:A:LYS:N | 10       | 1.34          |

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| Key    | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|--------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,90) | 1:375:A:ASP:N | 1:375:A:ASP:CA | 1:375:A:ASP:C  | 1:376:A:VAL:N | 2        | 1.33          |
| (1,88) | 1:373:A:GLU:N | 1:373:A:GLU:CA | 1:373:A:GLU:C  | 1:374:A:LYS:N | 9        | 1.33          |
| (1,12) | 1:298:A:TYR:N | 1:298:A:TYR:CA | 1:298:A:TYR:C  | 1:299:A:GLU:N | 7        | 1.33          |
| (1,12) | 1:298:A:TYR:N | 1:298:A:TYR:CA | 1:298:A:TYR:C  | 1:299:A:GLU:N | 8        | 1.33          |
| (1,65) | 1:329:A:ALA:C | 1:330:A:LYS:N  | 1:330:A:LYS:CA | 1:330:A:LYS:C | 4        | 1.32          |
| (1,23) | 1:305:A:LEU:C | 1:306:A:GLN:N  | 1:306:A:GLN:CA | 1:306:A:GLN:C | 10       | 1.32          |
| (1,88) | 1:373:A:GLU:N | 1:373:A:GLU:CA | 1:373:A:GLU:C  | 1:374:A:LYS:N | 6        | 1.31          |
| (1,46) | 1:318:A:GLN:N | 1:318:A:GLN:CA | 1:318:A:GLN:C  | 1:319:A:ASP:N | 6        | 1.31          |
| (1,18) | 1:303:A:GLU:N | 1:303:A:GLU:CA | 1:303:A:GLU:C  | 1:304:A:GLU:N | 5        | 1.31          |
| (1,88) | 1:373:A:GLU:N | 1:373:A:GLU:CA | 1:373:A:GLU:C  | 1:374:A:LYS:N | 4        | 1.3           |
| (1,83) | 1:338:A:ASP:C | 1:339:A:SER:N  | 1:339:A:SER:CA | 1:339:A:SER:C | 4        | 1.3           |
| (1,46) | 1:318:A:GLN:N | 1:318:A:GLN:CA | 1:318:A:GLN:C  | 1:319:A:ASP:N | 9        | 1.29          |
| (1,86) | 1:342:A:TRP:N | 1:342:A:TRP:CA | 1:342:A:TRP:C  | 1:343:A:VAL:N | 10       | 1.27          |
| (1,50) | 1:320:A:ALA:N | 1:320:A:ALA:CA | 1:320:A:ALA:C  | 1:321:A:ILE:N | 3        | 1.26          |
| (1,25) | 1:306:A:GLN:C | 1:307:A:LYS:N  | 1:307:A:LYS:CA | 1:307:A:LYS:C | 10       | 1.24          |
| (1,78) | 1:336:A:CYS:N | 1:336:A:CYS:CA | 1:336:A:CYS:C  | 1:337:A:ILE:N | 4        | 1.23          |
| (1,70) | 1:332:A:HIS:N | 1:332:A:HIS:CA | 1:332:A:HIS:C  | 1:333:A:MET:N | 5        | 1.23          |
| (1,21) | 1:304:A:GLU:C | 1:305:A:LEU:N  | 1:305:A:LEU:CA | 1:305:A:LEU:C | 1        | 1.23          |
| (1,70) | 1:332:A:HIS:N | 1:332:A:HIS:CA | 1:332:A:HIS:C  | 1:333:A:MET:N | 10       | 1.22          |
| (1,69) | 1:331:A:TYR:C | 1:332:A:HIS:N  | 1:332:A:HIS:CA | 1:332:A:HIS:C | 8        | 1.21          |
| (1,25) | 1:306:A:GLN:C | 1:307:A:LYS:N  | 1:307:A:LYS:CA | 1:307:A:LYS:C | 5        | 1.21          |
| (1,85) | 1:341:A:LEU:C | 1:342:A:TRP:N  | 1:342:A:TRP:CA | 1:342:A:TRP:C | 6        | 1.2           |
| (1,44) | 1:317:A:LEU:N | 1:317:A:LEU:CA | 1:317:A:LEU:C  | 1:318:A:GLN:N | 8        | 1.2           |
| (1,26) | 1:307:A:LYS:N | 1:307:A:LYS:CA | 1:307:A:LYS:C  | 1:308:A:CYS:N | 7        | 1.19          |
| (1,44) | 1:317:A:LEU:N | 1:317:A:LEU:CA | 1:317:A:LEU:C  | 1:318:A:GLN:N | 3        | 1.16          |
| (1,14) | 1:299:A:GLU:N | 1:299:A:GLU:CA | 1:299:A:GLU:C  | 1:300:A:SER:N | 8        | 1.15          |
| (1,46) | 1:318:A:GLN:N | 1:318:A:GLN:CA | 1:318:A:GLN:C  | 1:319:A:ASP:N | 8        | 1.14          |
| (1,55) | 1:322:A:SER:C | 1:323:A:LYS:N  | 1:323:A:LYS:CA | 1:323:A:LYS:C | 5        | 1.13          |
| (1,43) | 1:316:A:MET:C | 1:317:A:LEU:N  | 1:317:A:LEU:CA | 1:317:A:LEU:C | 5        | 1.12          |
| (1,12) | 1:298:A:TYR:N | 1:298:A:TYR:CA | 1:298:A:TYR:C  | 1:299:A:GLU:N | 10       | 1.11          |
| (1,46) | 1:318:A:GLN:N | 1:318:A:GLN:CA | 1:318:A:GLN:C  | 1:319:A:ASP:N | 5        | 1.1           |
| (1,43) | 1:316:A:MET:C | 1:317:A:LEU:N  | 1:317:A:LEU:CA | 1:317:A:LEU:C | 6        | 1.1           |
| (1,12) | 1:298:A:TYR:N | 1:298:A:TYR:CA | 1:298:A:TYR:C  | 1:299:A:GLU:N | 6        | 1.1           |
| (1,11) | 1:297:A:VAL:C | 1:298:A:TYR:N  | 1:298:A:TYR:CA | 1:298:A:TYR:C | 4        | 1.1           |
| (1,53) | 1:321:A:ILE:C | 1:322:A:SER:N  | 1:322:A:SER:CA | 1:322:A:SER:C | 3        | 1.09          |
| (1,53) | 1:321:A:ILE:C | 1:322:A:SER:N  | 1:322:A:SER:CA | 1:322:A:SER:C | 6        | 1.09          |
| (1,43) | 1:316:A:MET:C | 1:317:A:LEU:N  | 1:317:A:LEU:CA | 1:317:A:LEU:C | 8        | 1.08          |
| (1,11) | 1:297:A:VAL:C | 1:298:A:TYR:N  | 1:298:A:TYR:CA | 1:298:A:TYR:C | 9        | 1.08          |
| (1,80) | 1:337:A:ILE:N | 1:337:A:ILE:CA | 1:337:A:ILE:C  | 1:338:A:ASP:N | 4        | 1.07          |
| (1,52) | 1:321:A:ILE:N | 1:321:A:ILE:CA | 1:321:A:ILE:C  | 1:322:A:SER:N | 3        | 1.07          |
| (1,81) | 1:337:A:ILE:C | 1:338:A:ASP:N  | 1:338:A:ASP:CA | 1:338:A:ASP:C | 3        | 1.05          |
| (1,52) | 1:321:A:ILE:N | 1:321:A:ILE:CA | 1:321:A:ILE:C  | 1:322:A:SER:N | 8        | 1.04          |
| (1,43) | 1:316:A:MET:C | 1:317:A:LEU:N  | 1:317:A:LEU:CA | 1:317:A:LEU:C | 1        | 1.04          |
| (1,25) | 1:306:A:GLN:C | 1:307:A:LYS:N  | 1:307:A:LYS:CA | 1:307:A:LYS:C | 4        | 1.04          |
| (1,18) | 1:303:A:GLU:N | 1:303:A:GLU:CA | 1:303:A:GLU:C  | 1:304:A:GLU:N | 2        | 1.04          |
| (1,56) | 1:323:A:LYS:N | 1:323:A:LYS:CA | 1:323:A:LYS:C  | 1:324:A:MET:N | 5        | 1.03          |
| (1,55) | 1:322:A:SER:C | 1:323:A:LYS:N  | 1:323:A:LYS:CA | 1:323:A:LYS:C | 3        | 1.02          |
| (1,46) | 1:318:A:GLN:N | 1:318:A:GLN:CA | 1:318:A:GLN:C  | 1:319:A:ASP:N | 10       | 1.02          |
| (1,50) | 1:320:A:ALA:N | 1:320:A:ALA:CA | 1:320:A:ALA:C  | 1:321:A:ILE:N | 8        | 1.01          |
| (1,47) | 1:318:A:GLN:C | 1:319:A:ASP:N  | 1:319:A:ASP:CA | 1:319:A:ASP:C | 9        | 1.01          |
| (1,20) | 1:304:A:GLU:N | 1:304:A:GLU:CA | 1:304:A:GLU:C  | 1:305:A:LEU:N | 8        | 1.01          |

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*Continued from previous page...*

| Key    | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|--------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,25) | 1:306:A:GLN:C | 1:307:A:LYS:N  | 1:307:A:LYS:CA | 1:307:A:LYS:C | 2        | 1.0           |
| (1,22) | 1:305:A:LEU:N | 1:305:A:LEU:CA | 1:305:A:LEU:C  | 1:306:A:GLN:N | 1        | 1.0           |
| (1,22) | 1:305:A:LEU:N | 1:305:A:LEU:CA | 1:305:A:LEU:C  | 1:306:A:GLN:N | 9        | 1.0           |