



# Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2026 – 11:42 PM UTC

PDB ID : 6HQ1 / pdb\_00006hq1  
BMRB ID : 34318  
Title : Solution structure of the globular domain from human histone H1.0  
Authors : Martinsen, J.H.; Bugge, K.; Kragelund, B.B.  
Deposited on : 2018-09-23

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

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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

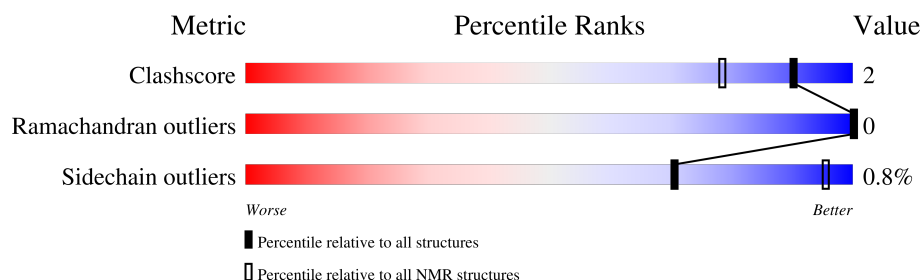
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 86%.

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     | 75     | <br>89% . 8%     |

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 6 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:5-A:73 (69)         | 0.36              | 6            |

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

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

The models can be grouped into 4 clusters and 1 single-model cluster was found.

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

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1170 atoms, of which 598 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Histone H1.0.

| Mol | Chain | Residues | Atoms |     |     |     |     |   | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|-------|
| 1   | A     | 75       | Total | C   | H   | N   | O   | S | 0     |
|     |       |          | 1170  | 356 | 598 | 108 | 107 | 1 |       |

There is a discrepancy between the modelled and reference sequences:

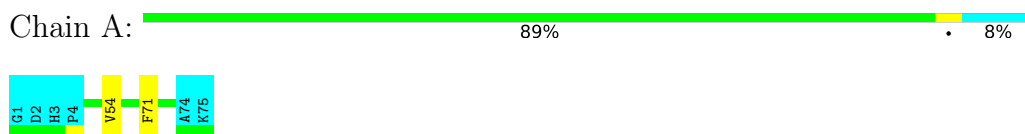
| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | 1       | GLY      | -      | expression tag | UNP P07305 |

## 4 Residue-property plots

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

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

- Molecule 1: Histone H1.0

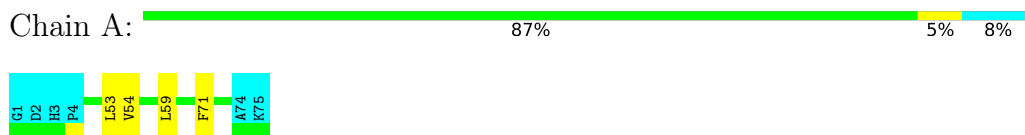


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

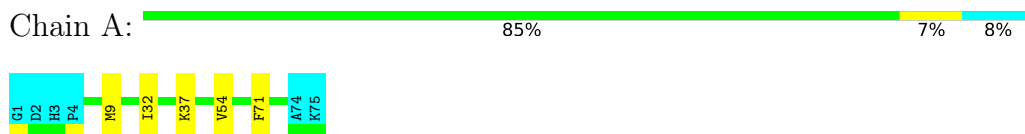
#### 4.2.1 Score per residue for model 1

- Molecule 1: Histone H1.0



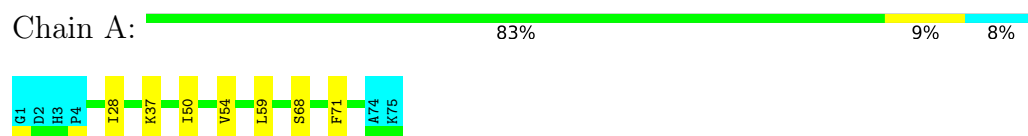
#### 4.2.2 Score per residue for model 2

- Molecule 1: Histone H1.0



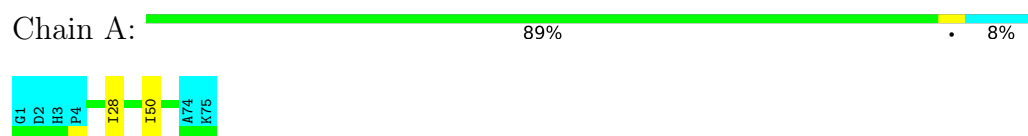
### 4.2.3 Score per residue for model 3

- Molecule 1: Histone H1.0



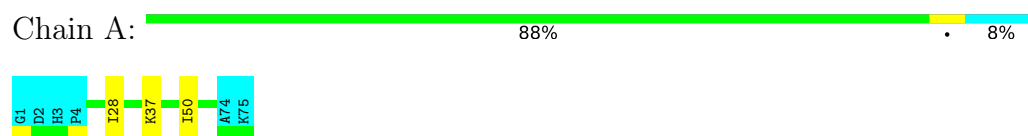
### 4.2.4 Score per residue for model 4

- Molecule 1: Histone H1.0



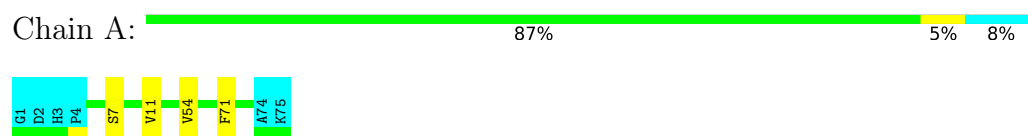
### 4.2.5 Score per residue for model 5

- Molecule 1: Histone H1.0



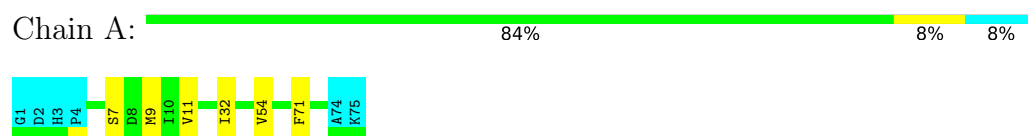
### 4.2.6 Score per residue for model 6 (medoid)

- Molecule 1: Histone H1.0



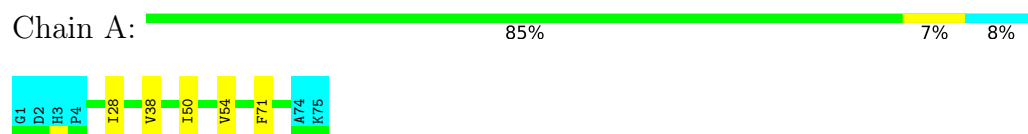
### 4.2.7 Score per residue for model 7

- Molecule 1: Histone H1.0



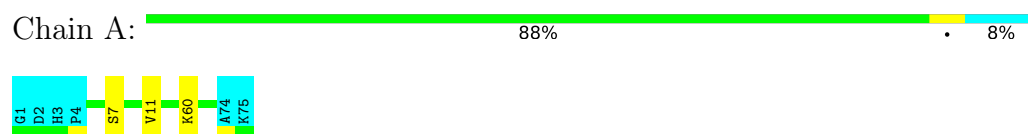
### 4.2.8 Score per residue for model 8

- Molecule 1: Histone H1.0



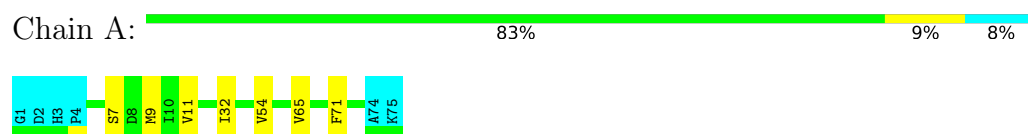
### 4.2.9 Score per residue for model 9

- Molecule 1: Histone H1.0



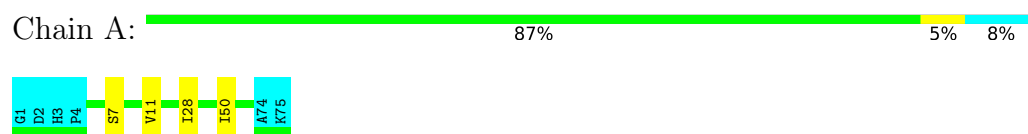
### 4.2.10 Score per residue for model 10

- Molecule 1: Histone H1.0



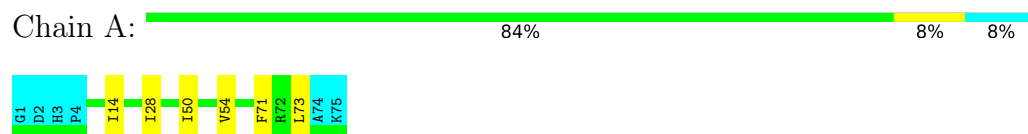
### 4.2.11 Score per residue for model 11

- Molecule 1: Histone H1.0



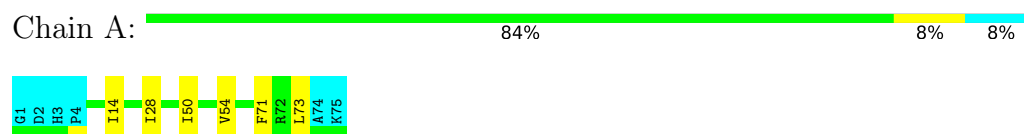
### 4.2.12 Score per residue for model 12

- Molecule 1: Histone H1.0



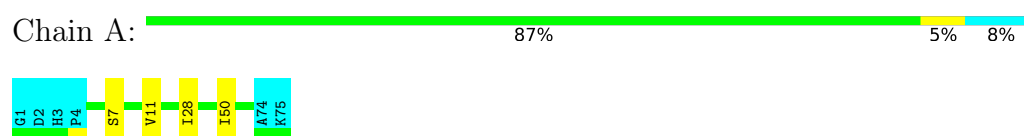
#### 4.2.13 Score per residue for model 13

- Molecule 1: Histone H1.0



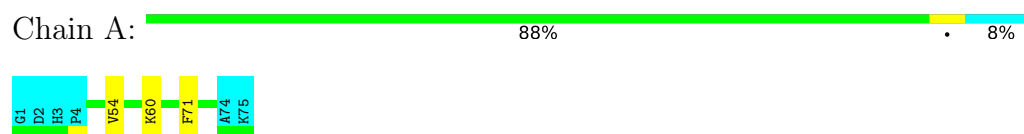
#### 4.2.14 Score per residue for model 14

- Molecule 1: Histone H1.0



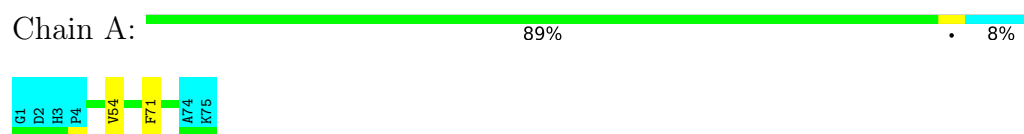
#### 4.2.15 Score per residue for model 15

- Molecule 1: Histone H1.0



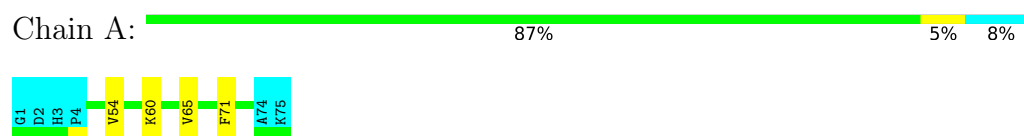
#### 4.2.16 Score per residue for model 16

- Molecule 1: Histone H1.0



#### 4.2.17 Score per residue for model 17

- Molecule 1: Histone H1.0



#### 4.2.18 Score per residue for model 18

- Molecule 1: Histone H1.0

Chain A:  85% 7% 8%



#### 4.2.19 Score per residue for model 19

- Molecule 1: Histone H1.0

Chain A:  83% 9% 8%



#### 4.2.20 Score per residue for model 20

- Molecule 1: Histone H1.0

Chain A:  84% 8% 8%



## 5 Refinement protocol and experimental data overview

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

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

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

| Software name | Classification        | Version |
|---------------|-----------------------|---------|
| TALOS         | geometry optimization |         |
| CYANA         | structure calculation |         |
| Xplor-NIH     | structure calculation |         |

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                       | 857            |
| Number of shifts mapped to atoms             | 857            |
| Number of unparsed shifts                    | 0              |
| Number of shifts with mapping errors         | 0              |
| Number of shifts with mapping warnings       | 0              |
| Assignment completeness (well-defined parts) | 86%            |

## 6 Model quality [i](#)

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

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

| Mol | Chain | Bond lengths |                      | Bond angles |                      |
|-----|-------|--------------|----------------------|-------------|----------------------|
|     |       | RMSZ         | #Z>5                 | RMSZ        | #Z>5                 |
| 1   | A     | 1.14±0.01    | 0±0/534 ( 0.0± 0.0%) | 1.17±0.01   | 0±0/712 ( 0.0± 0.1%) |
| All | All   | 1.14         | 0/10680 ( 0.0%)      | 1.17        | 3/14240 ( 0.0%)      |

There are no bond-length outliers.

All unique angle outliers are listed below.

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) | Models |       |
|-----|-------|-----|------|--------|-------|-------------|----------|--------|-------|
|     |       |     |      |        |       |             |          | Worst  | Total |
| 1   | A     | 68  | SER  | N-CA-C | -5.16 | 107.53      | 113.88   | 18     | 3     |

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     | 529   | 561      | 562      | 2±1     |
| All | All   | 10580 | 11220    | 11240    | 37      |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

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

| Atom-1          | Atom-2         | Clash(Å) | Distance(Å) | Models |       |
|-----------------|----------------|----------|-------------|--------|-------|
|                 |                |          |             | Worst  | Total |
| 1:A:54:VAL:HG21 | 1:A:71:PHE:CE2 | 0.57     | 2.35        | 8      | 14    |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:28:ILE:HG21 | 1:A:50:ILE:HD11 | 0.50     | 1.83        | 13     | 8     |
| 1:A:14:ILE:HG21 | 1:A:73:LEU:HB2  | 0.45     | 1.89        | 12     | 1     |
| 1:A:7:SER:O     | 1:A:11:VAL:HG23 | 0.44     | 2.13        | 19     | 8     |
| 1:A:14:ILE:HG21 | 1:A:73:LEU:HG   | 0.43     | 1.91        | 13     | 1     |
| 1:A:9:MET:HE2   | 1:A:32:ILE:HG23 | 0.42     | 1.91        | 7      | 3     |
| 1:A:53:LEU:HB3  | 1:A:59:LEU:HD13 | 0.42     | 1.92        | 1      | 1     |
| 1:A:65:VAL:O    | 1:A:65:VAL:HG13 | 0.40     | 2.16        | 19     | 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     | 69/75 (92%)     | 66±0 (96±1%) | 3±0 (4±1%) | 0±0 (0±0%) | 100         | 100 |
| All | All   | 1380/1500 (92%) | 1319 (96%)   | 61 (4%)    | 0 (0%)     | 100         | 100 |

There are no Ramachandran outliers.

### 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     | 57/61 (93%)     | 57±1 (99±1%) | 0±1 (1±1%) | 70          | 95 |
| All | All   | 1140/1220 (93%) | 1131 (99%)   | 9 (1%)     | 70          | 95 |

All 4 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     | 65  | VAL  | 3              |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 73  | LEU  | 3              |
| 1   | A     | 60  | LYS  | 2              |
| 1   | A     | 59  | LEU  | 1              |

### 6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 6.7 Other polymers [i](#)

There are no such molecules in this entry.

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

There are no chain breaks in this entry.

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

The completeness of assignment taking into account all chemical shift lists is 86% for the well-defined parts and 85% for the entire structure.

### 7.1 Chemical shift list 1

File name: `working_cs.cif`

Chemical shift list name: *starch\_output*

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

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

|                                         |     |
|-----------------------------------------|-----|
| Total number of shifts                  | 857 |
| Number of shifts mapped to atoms        | 857 |
| Number of unparsed shifts               | 0   |
| Number of shifts with mapping errors    | 0   |
| Number of shifts with mapping warnings  | 0   |
| Number of shift outliers (ShiftChecker) | 0   |

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

The following table shows the suggested chemical shift referencing corrections.

| Nucleus                | # values | Correction $\pm$ precision, ppm | Suggested action           |
|------------------------|----------|---------------------------------|----------------------------|
| $^{13}\text{C}_\alpha$ | 75       | $-0.68 \pm 0.18$                | Should be checked          |
| $^{13}\text{C}_\beta$  | 68       | $0.12 \pm 0.12$                 | None needed ( $< 0.5$ ppm) |
| $^{13}\text{C}'$       | 71       | $-0.62 \pm 0.26$                | Should be applied          |
| $^{15}\text{N}$        | 71       | $0.29 \pm 0.36$                 | None needed ( $< 0.5$ ppm) |

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

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 86%, i.e. 807 atoms were assigned a chemical shift out of a possible 943. 0 out of 9 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total         | $^1\text{H}$  | $^{13}\text{C}$ | $^{15}\text{N}$ |
|-----------|---------------|---------------|-----------------|-----------------|
| Backbone  | 348/351 (99%) | 143/144 (99%) | 137/138 (99%)   | 68/69 (99%)     |
| Sidechain | 423/549 (77%) | 278/356 (78%) | 138/165 (84%)   | 7/28 (25%)      |

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|          | Total         | <sup>1</sup> H | <sup>13</sup> C | <sup>15</sup> N |
|----------|---------------|----------------|-----------------|-----------------|
| Aromatic | 36/43 (84%)   | 18/21 (86%)    | 18/22 (82%)     | 0/0 (—%)        |
| Overall  | 807/943 (86%) | 439/521 (84%)  | 293/325 (90%)   | 75/97 (77%)     |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 85%, i.e. 857 atoms were assigned a chemical shift out of a possible 1011. 0 out of 9 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total          | <sup>1</sup> H | <sup>13</sup> C | <sup>15</sup> N |
|-----------|----------------|----------------|-----------------|-----------------|
| Backbone  | 370/380 (97%)  | 153/156 (98%)  | 146/150 (97%)   | 71/74 (96%)     |
| Sidechain | 449/582 (77%)  | 294/377 (78%)  | 148/176 (84%)   | 7/29 (24%)      |
| Aromatic  | 38/49 (78%)    | 19/25 (76%)    | 19/24 (79%)     | 0/0 (—%)        |
| Overall   | 857/1011 (85%) | 466/558 (84%)  | 313/350 (89%)   | 78/103 (76%)    |

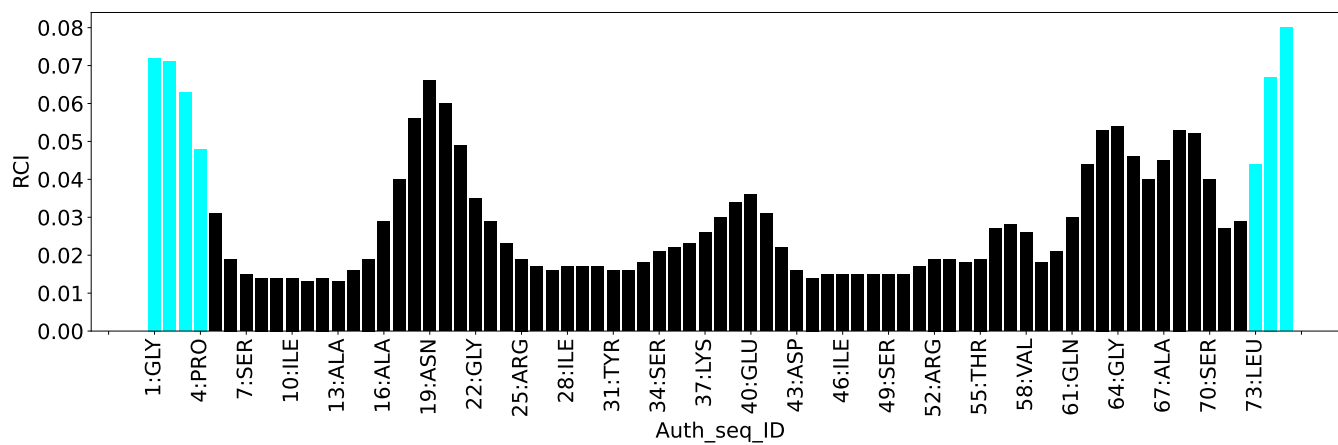
#### 7.1.4 Statistically unusual chemical shifts [i](#)

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                                | 845   |
| Intra-residue ( $ i-j =0$ )                              | 246   |
| Sequential ( $ i-j =1$ )                                 | 230   |
| Medium range ( $ i-j >1$ and $ i-j <5$ )                 | 175   |
| Long range ( $ i-j \geq 5$ )                             | 194   |
| Inter-chain                                              | 0     |
| Hydrogen bond restraints                                 | 0     |
| Disulfide bond restraints                                | 0     |
| Total dihedral-angle restraints                          | 140   |
| Number of unmapped restraints                            | 0     |
| Number of restraints per residue                         | 13.1  |
| Number of long range restraints per residue <sup>1</sup> | 2.6   |

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

### 8.2 Residual restraint violations

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

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

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

| Bins (Å)         | Average number of violations per model | Max (Å) |
|------------------|----------------------------------------|---------|
| 0.1-0.2 (Small)  | 16.6                                   | 0.2     |
| 0.2-0.5 (Medium) | 4.7                                    | 0.31    |
| >0.5 (Large)     | None                                   | None    |

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

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

| Bins (°)           | Average number of violations per model | Max (°) |
|--------------------|----------------------------------------|---------|
| 1.0-10.0 (Small)   | 11.2                                   | 4.66    |
| 10.0-20.0 (Medium) | None                                   | None    |
| >20.0 (Large)      | None                                   | None    |

## 9 Distance violation analysis ⓘ

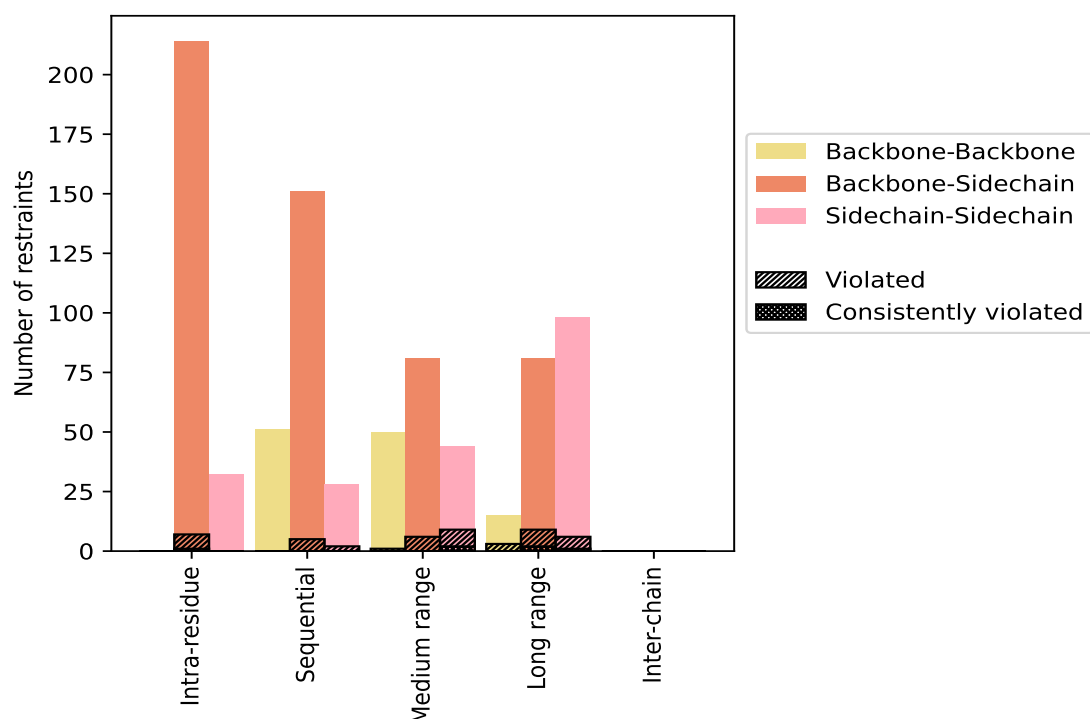
### 9.1 Summary of distance violations ⓘ

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

| Restrains type                                                              | Count      | % <sup>1</sup> | Violated <sup>3</sup> |                |                | Consistently Violated <sup>4</sup> |                |                |
|-----------------------------------------------------------------------------|------------|----------------|-----------------------|----------------|----------------|------------------------------------|----------------|----------------|
|                                                                             |            |                | Count                 | % <sup>2</sup> | % <sup>1</sup> | Count                              | % <sup>2</sup> | % <sup>1</sup> |
| <b>Intra-residue (<math> i-j =0</math>)</b>                                 | <b>246</b> | <b>29.1</b>    | <b>7</b>              | <b>2.8</b>     | <b>0.8</b>     | <b>1</b>                           | <b>0.4</b>     | <b>0.1</b>     |
| Backbone-Backbone                                                           | 0          | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 214        | 25.3           | 7                     | 3.3            | 0.8            | 1                                  | 0.5            | 0.1            |
| Sidechain-Sidechain                                                         | 32         | 3.8            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| <b>Sequential (<math> i-j =1</math>)</b>                                    | <b>230</b> | <b>27.2</b>    | <b>7</b>              | <b>3.0</b>     | <b>0.8</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| Backbone-Backbone                                                           | 51         | 6.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 151        | 17.9           | 5                     | 3.3            | 0.6            | 0                                  | 0.0            | 0.0            |
| Sidechain-Sidechain                                                         | 28         | 3.3            | 2                     | 7.1            | 0.2            | 0                                  | 0.0            | 0.0            |
| <b>Medium range (<math> i-j &gt;1</math> &amp; <math> i-j &lt;5</math>)</b> | <b>175</b> | <b>20.7</b>    | <b>16</b>             | <b>9.1</b>     | <b>1.9</b>     | <b>2</b>                           | <b>1.1</b>     | <b>0.2</b>     |
| Backbone-Backbone                                                           | 50         | 5.9            | 1                     | 2.0            | 0.1            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 81         | 9.6            | 6                     | 7.4            | 0.7            | 0                                  | 0.0            | 0.0            |
| Sidechain-Sidechain                                                         | 44         | 5.2            | 9                     | 20.5           | 1.1            | 2                                  | 4.5            | 0.2            |
| <b>Long range (<math> i-j \geq 5</math>)</b>                                | <b>194</b> | <b>23.0</b>    | <b>18</b>             | <b>9.3</b>     | <b>2.1</b>     | <b>3</b>                           | <b>1.5</b>     | <b>0.4</b>     |
| Backbone-Backbone                                                           | 15         | 1.8            | 3                     | 20.0           | 0.4            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 81         | 9.6            | 9                     | 11.1           | 1.1            | 2                                  | 2.5            | 0.2            |
| Sidechain-Sidechain                                                         | 98         | 11.6           | 6                     | 6.1            | 0.7            | 1                                  | 1.0            | 0.1            |
| <b>Inter-chain</b>                                                          | <b>0</b>   | <b>0.0</b>     | <b>0</b>              | <b>0.0</b>     | <b>0.0</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| Backbone-Backbone                                                           | 0          | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 0          | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Sidechain-Sidechain                                                         | 0          | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| <b>Hydrogen bond</b>                                                        | <b>0</b>   | <b>0.0</b>     | <b>0</b>              | <b>0.0</b>     | <b>0.0</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| <b>Disulfide bond</b>                                                       | <b>0</b>   | <b>0.0</b>     | <b>0</b>              | <b>0.0</b>     | <b>0.0</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| <b>Total</b>                                                                | <b>845</b> | <b>100.0</b>   | <b>48</b>             | <b>5.7</b>     | <b>5.7</b>     | <b>6</b>                           | <b>0.7</b>     | <b>0.7</b>     |
| Backbone-Backbone                                                           | 116        | 13.7           | 4                     | 3.4            | 0.5            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 527        | 62.4           | 27                    | 5.1            | 3.2            | 3                                  | 0.6            | 0.4            |
| Sidechain-Sidechain                                                         | 202        | 23.9           | 17                    | 8.4            | 2.0            | 3                                  | 1.5            | 0.4            |

<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        | 3                    | 2               | 7               | 11              | 0               | 23    | 0.16     | 0.26    | 0.05                | 0.15       |
| 2        | 2                    | 1               | 7               | 13              | 0               | 23    | 0.16     | 0.26    | 0.04                | 0.15       |
| 3        | 2                    | 1               | 9               | 12              | 0               | 24    | 0.16     | 0.29    | 0.06                | 0.14       |
| 4        | 1                    | 2               | 7               | 10              | 0               | 20    | 0.19     | 0.29    | 0.05                | 0.17       |
| 5        | 1                    | 1               | 7               | 10              | 0               | 19    | 0.16     | 0.29    | 0.05                | 0.13       |
| 6        | 2                    | 1               | 9               | 12              | 0               | 24    | 0.17     | 0.3     | 0.05                | 0.16       |
| 7        | 2                    | 1               | 8               | 13              | 0               | 24    | 0.16     | 0.27    | 0.05                | 0.15       |
| 8        | 1                    | 0               | 9               | 13              | 0               | 23    | 0.17     | 0.31    | 0.05                | 0.16       |
| 9        | 1                    | 4               | 6               | 10              | 0               | 21    | 0.17     | 0.28    | 0.05                | 0.17       |
| 10       | 1                    | 1               | 7               | 12              | 0               | 21    | 0.16     | 0.26    | 0.04                | 0.16       |

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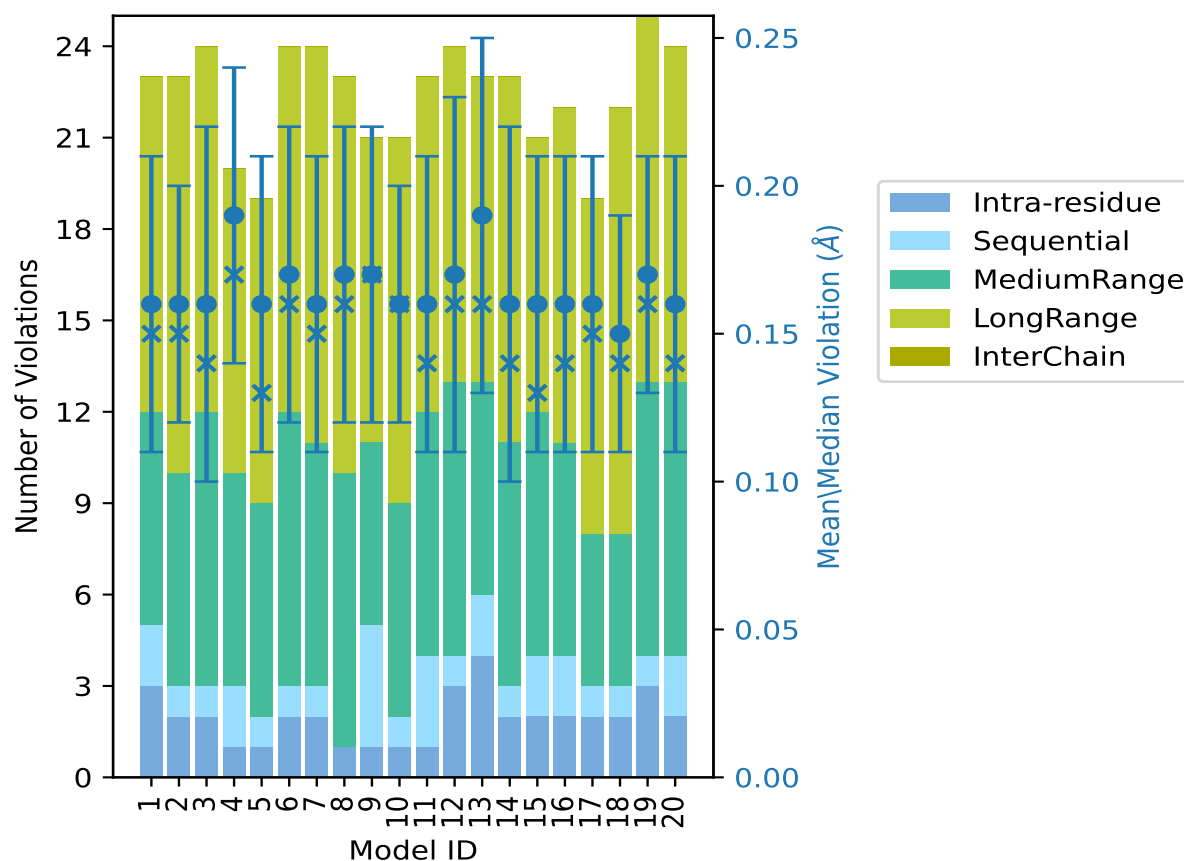
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| Model ID | Number of violations |                 |                 |                 |                 |       | Mean (Å) | Max (Å) | SD <sup>6</sup> (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
|          | IR <sup>1</sup>      | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total |          |         |                     |            |
| 11       | 1                    | 3               | 8               | 11              | 0               | 23    | 0.16     | 0.27    | 0.05                | 0.14       |
| 12       | 3                    | 1               | 9               | 11              | 0               | 24    | 0.17     | 0.3     | 0.06                | 0.16       |
| 13       | 4                    | 2               | 7               | 10              | 0               | 23    | 0.19     | 0.31    | 0.06                | 0.16       |
| 14       | 2                    | 1               | 8               | 12              | 0               | 23    | 0.16     | 0.31    | 0.06                | 0.14       |
| 15       | 2                    | 2               | 8               | 9               | 0               | 21    | 0.16     | 0.26    | 0.05                | 0.13       |
| 16       | 2                    | 2               | 7               | 11              | 0               | 22    | 0.16     | 0.28    | 0.05                | 0.14       |
| 17       | 2                    | 1               | 5               | 11              | 0               | 19    | 0.16     | 0.26    | 0.05                | 0.15       |
| 18       | 2                    | 1               | 5               | 14              | 0               | 22    | 0.15     | 0.26    | 0.04                | 0.14       |
| 19       | 3                    | 1               | 9               | 12              | 0               | 25    | 0.17     | 0.26    | 0.04                | 0.16       |
| 20       | 2                    | 2               | 9               | 11              | 0               | 24    | 0.16     | 0.26    | 0.05                | 0.14       |

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

<sup>5</sup>Inter-chain restraints, <sup>6</sup>Standard deviation

### 9.2.1 Bar graph : Distance Violation statistics for each model ⓘ



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

### 9.3 Distance violation statistics for the ensemble

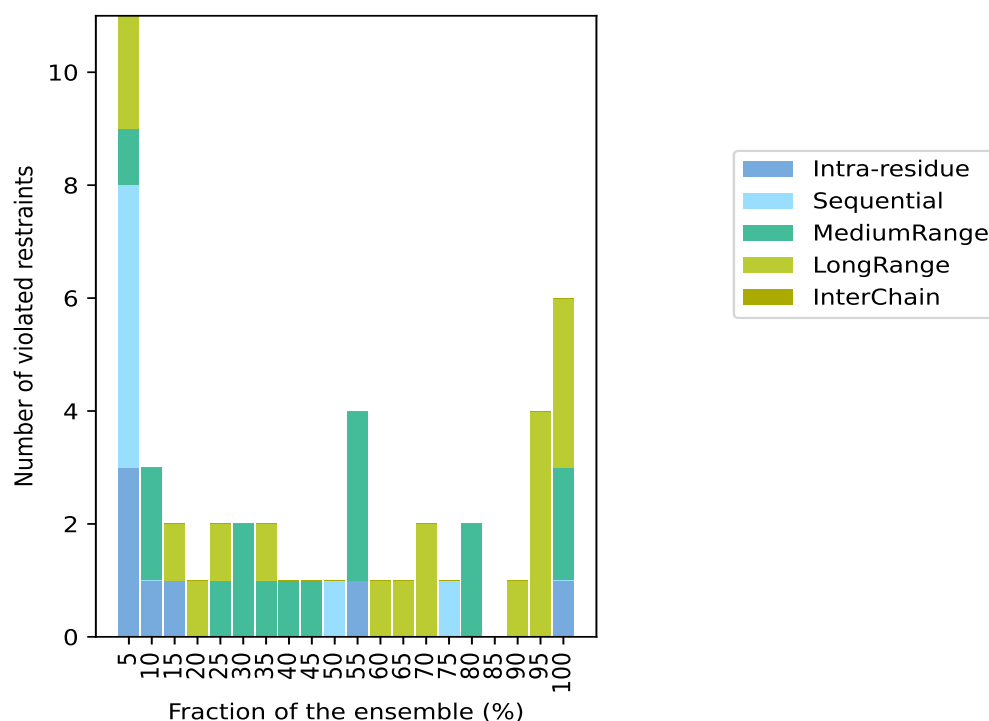
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 797(IR:239, SQ:223, MR:159, LR:176, IC:0) restraints are 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                             | 5               | 1               | 2               | 0               | 11    | 1                        | 5.0   |
| 1                             | 0               | 2               | 0               | 0               | 3     | 2                        | 10.0  |
| 1                             | 0               | 0               | 1               | 0               | 2     | 3                        | 15.0  |
| 0                             | 0               | 0               | 1               | 0               | 1     | 4                        | 20.0  |
| 0                             | 0               | 1               | 1               | 0               | 2     | 5                        | 25.0  |
| 0                             | 0               | 2               | 0               | 0               | 2     | 6                        | 30.0  |
| 0                             | 0               | 1               | 1               | 0               | 2     | 7                        | 35.0  |
| 0                             | 0               | 1               | 0               | 0               | 1     | 8                        | 40.0  |
| 0                             | 0               | 1               | 0               | 0               | 1     | 9                        | 45.0  |
| 0                             | 1               | 0               | 0               | 0               | 1     | 10                       | 50.0  |
| 1                             | 0               | 3               | 0               | 0               | 4     | 11                       | 55.0  |
| 0                             | 0               | 0               | 1               | 0               | 1     | 12                       | 60.0  |
| 0                             | 0               | 0               | 1               | 0               | 1     | 13                       | 65.0  |
| 0                             | 0               | 0               | 2               | 0               | 2     | 14                       | 70.0  |
| 0                             | 1               | 0               | 0               | 0               | 1     | 15                       | 75.0  |
| 0                             | 0               | 2               | 0               | 0               | 2     | 16                       | 80.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 17                       | 85.0  |
| 0                             | 0               | 0               | 1               | 0               | 1     | 18                       | 90.0  |
| 0                             | 0               | 0               | 4               | 0               | 4     | 19                       | 95.0  |
| 1                             | 0               | 2               | 3               | 0               | 6     | 20                       | 100.0 |

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

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

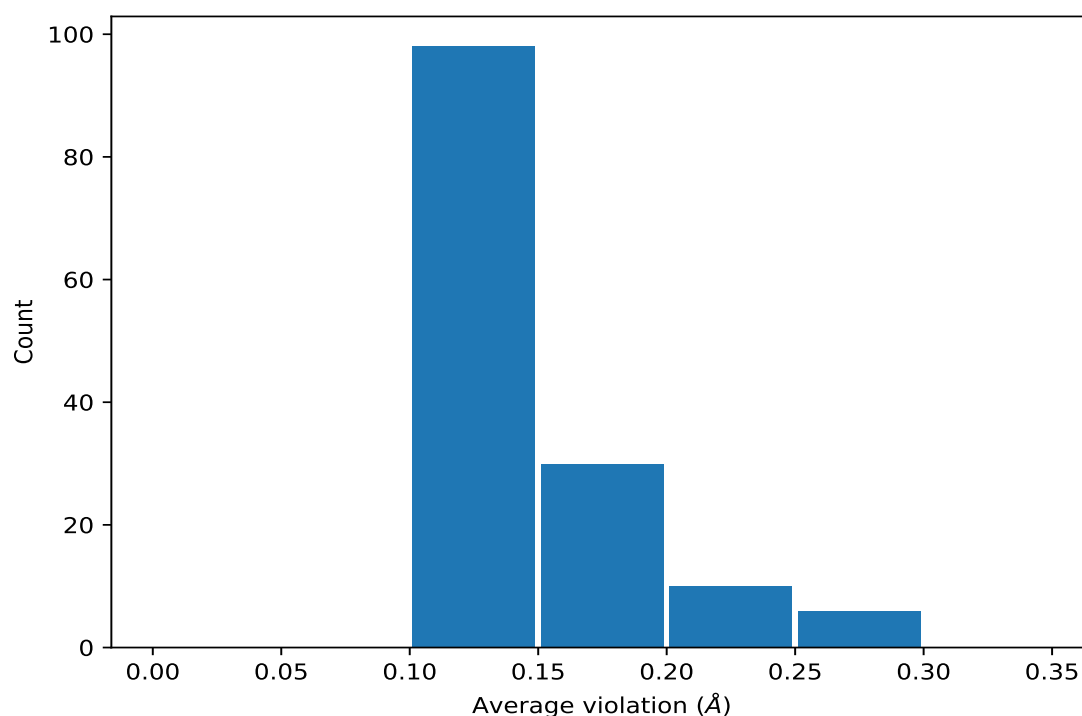
### 9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

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

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



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

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

| Key     | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,820) | 1:63:A:LYS:HG2  | 1:70:A:SER:H    | 20                  | 0.24     | 0.02                | 0.24       |
| (1,820) | 1:63:A:LYS:HG3  | 1:70:A:SER:H    | 20                  | 0.24     | 0.02                | 0.24       |
| (1,688) | 1:25:A:ARG:HB2  | 1:68:A:SER:HB2  | 20                  | 0.23     | 0.03                | 0.24       |
| (1,688) | 1:25:A:ARG:HB2  | 1:68:A:SER:HB3  | 20                  | 0.23     | 0.03                | 0.24       |
| (1,688) | 1:25:A:ARG:HB3  | 1:68:A:SER:HB2  | 20                  | 0.23     | 0.03                | 0.24       |
| (1,688) | 1:25:A:ARG:HB3  | 1:68:A:SER:HB3  | 20                  | 0.23     | 0.03                | 0.24       |
| (1,819) | 1:63:A:LYS:HB2  | 1:70:A:SER:H    | 20                  | 0.2      | 0.02                | 0.2        |
| (1,819) | 1:63:A:LYS:HB3  | 1:70:A:SER:H    | 20                  | 0.2      | 0.02                | 0.2        |
| (1,644) | 1:10:A:ILE:HG12 | 1:14:A:ILE:HD11 | 20                  | 0.19     | 0.06                | 0.17       |
| (1,644) | 1:10:A:ILE:HG12 | 1:14:A:ILE:HD12 | 20                  | 0.19     | 0.06                | 0.17       |
| (1,644) | 1:10:A:ILE:HG12 | 1:14:A:ILE:HD13 | 20                  | 0.19     | 0.06                | 0.17       |
| (1,644) | 1:10:A:ILE:HG13 | 1:14:A:ILE:HD11 | 20                  | 0.19     | 0.06                | 0.17       |
| (1,644) | 1:10:A:ILE:HG13 | 1:14:A:ILE:HD12 | 20                  | 0.19     | 0.06                | 0.17       |
| (1,644) | 1:10:A:ILE:HG13 | 1:14:A:ILE:HD13 | 20                  | 0.19     | 0.06                | 0.17       |
| (1,573) | 1:32:A:ILE:HD11 | 1:36:A:TYR:HD1  | 20                  | 0.15     | 0.02                | 0.16       |
| (1,573) | 1:32:A:ILE:HD11 | 1:36:A:TYR:HD2  | 20                  | 0.15     | 0.02                | 0.16       |

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| Key     | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,573) | 1:32:A:ILE:HD12 | 1:36:A:TYR:HD1  | 20                  | 0.15     | 0.02                | 0.16       |
| (1,573) | 1:32:A:ILE:HD12 | 1:36:A:TYR:HD2  | 20                  | 0.15     | 0.02                | 0.16       |
| (1,573) | 1:32:A:ILE:HD13 | 1:36:A:TYR:HD1  | 20                  | 0.15     | 0.02                | 0.16       |
| (1,573) | 1:32:A:ILE:HD13 | 1:36:A:TYR:HD2  | 20                  | 0.15     | 0.02                | 0.16       |
| (1,35)  | 1:10:A:ILE:HA   | 1:10:A:ILE:HD11 | 20                  | 0.13     | 0.01                | 0.13       |
| (1,35)  | 1:10:A:ILE:HA   | 1:10:A:ILE:HD12 | 20                  | 0.13     | 0.01                | 0.13       |
| (1,35)  | 1:10:A:ILE:HA   | 1:10:A:ILE:HD13 | 20                  | 0.13     | 0.01                | 0.13       |
| (1,6)   | 1:28:A:ILE:HG21 | 1:50:A:ILE:HB   | 19                  | 0.25     | 0.04                | 0.25       |
| (1,6)   | 1:28:A:ILE:HG22 | 1:50:A:ILE:HB   | 19                  | 0.25     | 0.04                | 0.25       |
| (1,6)   | 1:28:A:ILE:HG23 | 1:50:A:ILE:HB   | 19                  | 0.25     | 0.04                | 0.25       |
| (1,531) | 1:61:A:GLN:H    | 1:72:A:ARG:HB2  | 19                  | 0.17     | 0.03                | 0.17       |
| (1,531) | 1:61:A:GLN:H    | 1:72:A:ARG:HB3  | 19                  | 0.17     | 0.03                | 0.17       |
| (1,262) | 1:14:A:ILE:HD11 | 1:71:A:PHE:HA   | 19                  | 0.17     | 0.04                | 0.15       |
| (1,262) | 1:14:A:ILE:HD12 | 1:71:A:PHE:HA   | 19                  | 0.17     | 0.04                | 0.15       |
| (1,262) | 1:14:A:ILE:HD13 | 1:71:A:PHE:HA   | 19                  | 0.17     | 0.04                | 0.15       |
| (1,388) | 1:63:A:LYS:HA   | 1:70:A:SER:H    | 19                  | 0.14     | 0.02                | 0.13       |
| (1,457) | 1:61:A:GLN:H    | 1:72:A:ARG:H    | 18                  | 0.15     | 0.03                | 0.15       |
| (1,290) | 1:6:A:TYR:HE1   | 1:10:A:ILE:HD11 | 16                  | 0.13     | 0.02                | 0.14       |
| (1,290) | 1:6:A:TYR:HE1   | 1:10:A:ILE:HD12 | 16                  | 0.13     | 0.02                | 0.14       |
| (1,290) | 1:6:A:TYR:HE1   | 1:10:A:ILE:HD13 | 16                  | 0.13     | 0.02                | 0.14       |
| (1,290) | 1:6:A:TYR:HE2   | 1:10:A:ILE:HD11 | 16                  | 0.13     | 0.02                | 0.14       |
| (1,290) | 1:6:A:TYR:HE2   | 1:10:A:ILE:HD12 | 16                  | 0.13     | 0.02                | 0.14       |
| (1,290) | 1:6:A:TYR:HE2   | 1:10:A:ILE:HD13 | 16                  | 0.13     | 0.02                | 0.14       |
| (1,636) | 1:9:A:MET:HA    | 1:11:A:VAL:HG11 | 16                  | 0.12     | 0.01                | 0.12       |
| (1,636) | 1:9:A:MET:HA    | 1:11:A:VAL:HG12 | 16                  | 0.12     | 0.01                | 0.12       |
| (1,636) | 1:9:A:MET:HA    | 1:11:A:VAL:HG13 | 16                  | 0.12     | 0.01                | 0.12       |
| (1,636) | 1:9:A:MET:HA    | 1:11:A:VAL:HG21 | 16                  | 0.12     | 0.01                | 0.12       |
| (1,636) | 1:9:A:MET:HA    | 1:11:A:VAL:HG22 | 16                  | 0.12     | 0.01                | 0.12       |
| (1,636) | 1:9:A:MET:HA    | 1:11:A:VAL:HG23 | 16                  | 0.12     | 0.01                | 0.12       |
| (1,788) | 1:52:A:ARG:HD2  | 1:53:A:LEU:HB2  | 15                  | 0.17     | 0.01                | 0.17       |
| (1,788) | 1:52:A:ARG:HD2  | 1:53:A:LEU:HB3  | 15                  | 0.17     | 0.01                | 0.17       |
| (1,788) | 1:52:A:ARG:HD3  | 1:53:A:LEU:HB2  | 15                  | 0.17     | 0.01                | 0.17       |
| (1,788) | 1:52:A:ARG:HD3  | 1:53:A:LEU:HB3  | 15                  | 0.17     | 0.01                | 0.17       |
| (1,4)   | 1:14:A:ILE:HD11 | 1:28:A:ILE:HB   | 14                  | 0.15     | 0.02                | 0.16       |
| (1,4)   | 1:14:A:ILE:HD12 | 1:28:A:ILE:HB   | 14                  | 0.15     | 0.02                | 0.16       |
| (1,4)   | 1:14:A:ILE:HD13 | 1:28:A:ILE:HB   | 14                  | 0.15     | 0.02                | 0.16       |
| (1,13)  | 1:60:A:LYS:HA   | 1:72:A:ARG:HB2  | 14                  | 0.14     | 0.04                | 0.12       |
| (1,13)  | 1:60:A:LYS:HA   | 1:72:A:ARG:HB3  | 14                  | 0.14     | 0.04                | 0.12       |
| (1,803) | 1:60:A:LYS:HD2  | 1:74:A:ALA:H    | 13                  | 0.17     | 0.04                | 0.17       |
| (1,803) | 1:60:A:LYS:HD3  | 1:74:A:ALA:H    | 13                  | 0.17     | 0.04                | 0.17       |
| (1,8)   | 1:60:A:LYS:HB2  | 1:74:A:ALA:HB1  | 12                  | 0.14     | 0.02                | 0.14       |
| (1,8)   | 1:60:A:LYS:HB2  | 1:74:A:ALA:HB2  | 12                  | 0.14     | 0.02                | 0.14       |

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| Key     | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,8)   | 1:60:A:LYS:HB2  | 1:74:A:ALA:HB3  | 12                  | 0.14     | 0.02                | 0.14       |
| (1,8)   | 1:60:A:LYS:HB3  | 1:74:A:ALA:HB1  | 12                  | 0.14     | 0.02                | 0.14       |
| (1,8)   | 1:60:A:LYS:HB3  | 1:74:A:ALA:HB2  | 12                  | 0.14     | 0.02                | 0.14       |
| (1,8)   | 1:60:A:LYS:HB3  | 1:74:A:ALA:HB3  | 12                  | 0.14     | 0.02                | 0.14       |
| (1,661) | 1:15:A:GLN:H    | 1:15:A:GLN:HG2  | 11                  | 0.26     | 0.0                 | 0.26       |
| (1,661) | 1:15:A:GLN:H    | 1:15:A:GLN:HG3  | 11                  | 0.26     | 0.0                 | 0.26       |
| (1,363) | 1:55:A:THR:HG21 | 1:57:A:GLY:H    | 11                  | 0.17     | 0.01                | 0.17       |
| (1,363) | 1:55:A:THR:HG22 | 1:57:A:GLY:H    | 11                  | 0.17     | 0.01                | 0.17       |
| (1,363) | 1:55:A:THR:HG23 | 1:57:A:GLY:H    | 11                  | 0.17     | 0.01                | 0.17       |
| (1,343) | 1:52:A:ARG:HD2  | 1:55:A:THR:HG21 | 11                  | 0.12     | 0.01                | 0.12       |
| (1,343) | 1:52:A:ARG:HD2  | 1:55:A:THR:HG22 | 11                  | 0.12     | 0.01                | 0.12       |
| (1,343) | 1:52:A:ARG:HD2  | 1:55:A:THR:HG23 | 11                  | 0.12     | 0.01                | 0.12       |
| (1,343) | 1:52:A:ARG:HD3  | 1:55:A:THR:HG21 | 11                  | 0.12     | 0.01                | 0.12       |
| (1,343) | 1:52:A:ARG:HD3  | 1:55:A:THR:HG22 | 11                  | 0.12     | 0.01                | 0.12       |
| (1,343) | 1:52:A:ARG:HD3  | 1:55:A:THR:HG23 | 11                  | 0.12     | 0.01                | 0.12       |
| (1,344) | 1:52:A:ARG:HD2  | 1:55:A:THR:HG21 | 11                  | 0.12     | 0.01                | 0.12       |
| (1,344) | 1:52:A:ARG:HD2  | 1:55:A:THR:HG22 | 11                  | 0.12     | 0.01                | 0.12       |
| (1,344) | 1:52:A:ARG:HD2  | 1:55:A:THR:HG23 | 11                  | 0.12     | 0.01                | 0.12       |
| (1,344) | 1:52:A:ARG:HD3  | 1:55:A:THR:HG21 | 11                  | 0.12     | 0.01                | 0.12       |
| (1,344) | 1:52:A:ARG:HD3  | 1:55:A:THR:HG22 | 11                  | 0.12     | 0.01                | 0.12       |
| (1,344) | 1:52:A:ARG:HD3  | 1:55:A:THR:HG23 | 11                  | 0.12     | 0.01                | 0.12       |
| (1,821) | 1:64:A:GLY:HA2  | 1:65:A:VAL:HG11 | 10                  | 0.11     | 0.01                | 0.11       |
| (1,821) | 1:64:A:GLY:HA2  | 1:65:A:VAL:HG12 | 10                  | 0.11     | 0.01                | 0.11       |
| (1,821) | 1:64:A:GLY:HA2  | 1:65:A:VAL:HG13 | 10                  | 0.11     | 0.01                | 0.11       |
| (1,821) | 1:64:A:GLY:HA2  | 1:65:A:VAL:HG21 | 10                  | 0.11     | 0.01                | 0.11       |
| (1,821) | 1:64:A:GLY:HA2  | 1:65:A:VAL:HG22 | 10                  | 0.11     | 0.01                | 0.11       |
| (1,821) | 1:64:A:GLY:HA2  | 1:65:A:VAL:HG23 | 10                  | 0.11     | 0.01                | 0.11       |
| (1,821) | 1:64:A:GLY:HA3  | 1:65:A:VAL:HG11 | 10                  | 0.11     | 0.01                | 0.11       |
| (1,821) | 1:64:A:GLY:HA3  | 1:65:A:VAL:HG12 | 10                  | 0.11     | 0.01                | 0.11       |
| (1,821) | 1:64:A:GLY:HA3  | 1:65:A:VAL:HG13 | 10                  | 0.11     | 0.01                | 0.11       |
| (1,821) | 1:64:A:GLY:HA3  | 1:65:A:VAL:HG21 | 10                  | 0.11     | 0.01                | 0.11       |
| (1,821) | 1:64:A:GLY:HA3  | 1:65:A:VAL:HG22 | 10                  | 0.11     | 0.01                | 0.11       |
| (1,821) | 1:64:A:GLY:HA3  | 1:65:A:VAL:HG23 | 10                  | 0.11     | 0.01                | 0.11       |
| (1,628) | 1:7:A:SER:HB2   | 1:10:A:ILE:HG21 | 9                   | 0.14     | 0.06                | 0.12       |
| (1,628) | 1:7:A:SER:HB2   | 1:10:A:ILE:HG22 | 9                   | 0.14     | 0.06                | 0.12       |
| (1,628) | 1:7:A:SER:HB2   | 1:10:A:ILE:HG23 | 9                   | 0.14     | 0.06                | 0.12       |
| (1,628) | 1:7:A:SER:HB3   | 1:10:A:ILE:HG21 | 9                   | 0.14     | 0.06                | 0.12       |
| (1,628) | 1:7:A:SER:HB3   | 1:10:A:ILE:HG22 | 9                   | 0.14     | 0.06                | 0.12       |
| (1,628) | 1:7:A:SER:HB3   | 1:10:A:ILE:HG23 | 9                   | 0.14     | 0.06                | 0.12       |
| (1,322) | 1:15:A:GLN:HA   | 1:18:A:LYS:H    | 8                   | 0.13     | 0.02                | 0.12       |
| (1,668) | 1:17:A:GLU:HG2  | 1:19:A:ASN:H    | 7                   | 0.2      | 0.07                | 0.2        |
| (1,668) | 1:17:A:GLU:HG3  | 1:19:A:ASN:H    | 7                   | 0.2      | 0.07                | 0.2        |

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| Key     | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,398) | 1:46:A:ILE:HG21 | 1:51:A:LYS:H    | 7                   | 0.11     | 0.02                | 0.11       |
| (1,398) | 1:46:A:ILE:HG22 | 1:51:A:LYS:H    | 7                   | 0.11     | 0.02                | 0.11       |
| (1,398) | 1:46:A:ILE:HG23 | 1:51:A:LYS:H    | 7                   | 0.11     | 0.02                | 0.11       |
| (1,230) | 1:11:A:VAL:HA   | 1:14:A:ILE:HD11 | 6                   | 0.14     | 0.02                | 0.14       |
| (1,230) | 1:11:A:VAL:HA   | 1:14:A:ILE:HD12 | 6                   | 0.14     | 0.02                | 0.14       |
| (1,230) | 1:11:A:VAL:HA   | 1:14:A:ILE:HD13 | 6                   | 0.14     | 0.02                | 0.14       |
| (1,274) | 1:52:A:ARG:HA   | 1:55:A:THR:HG21 | 6                   | 0.14     | 0.01                | 0.14       |
| (1,274) | 1:52:A:ARG:HA   | 1:55:A:THR:HG22 | 6                   | 0.14     | 0.01                | 0.14       |
| (1,274) | 1:52:A:ARG:HA   | 1:55:A:THR:HG23 | 6                   | 0.14     | 0.01                | 0.14       |
| (1,38)  | 1:12:A:ALA:HB1  | 1:32:A:ILE:HG21 | 5                   | 0.12     | 0.02                | 0.11       |
| (1,38)  | 1:12:A:ALA:HB1  | 1:32:A:ILE:HG22 | 5                   | 0.12     | 0.02                | 0.11       |
| (1,38)  | 1:12:A:ALA:HB1  | 1:32:A:ILE:HG23 | 5                   | 0.12     | 0.02                | 0.11       |
| (1,38)  | 1:12:A:ALA:HB2  | 1:32:A:ILE:HG21 | 5                   | 0.12     | 0.02                | 0.11       |
| (1,38)  | 1:12:A:ALA:HB2  | 1:32:A:ILE:HG22 | 5                   | 0.12     | 0.02                | 0.11       |
| (1,38)  | 1:12:A:ALA:HB2  | 1:32:A:ILE:HG23 | 5                   | 0.12     | 0.02                | 0.11       |
| (1,38)  | 1:12:A:ALA:HB3  | 1:32:A:ILE:HG21 | 5                   | 0.12     | 0.02                | 0.11       |
| (1,38)  | 1:12:A:ALA:HB3  | 1:32:A:ILE:HG22 | 5                   | 0.12     | 0.02                | 0.11       |
| (1,38)  | 1:12:A:ALA:HB3  | 1:32:A:ILE:HG23 | 5                   | 0.12     | 0.02                | 0.11       |
| (1,754) | 1:45:A:GLN:HE21 | 1:48:A:LEU:HD11 | 5                   | 0.11     | 0.01                | 0.11       |
| (1,754) | 1:45:A:GLN:HE21 | 1:48:A:LEU:HD12 | 5                   | 0.11     | 0.01                | 0.11       |
| (1,754) | 1:45:A:GLN:HE21 | 1:48:A:LEU:HD13 | 5                   | 0.11     | 0.01                | 0.11       |
| (1,754) | 1:45:A:GLN:HE21 | 1:48:A:LEU:HD21 | 5                   | 0.11     | 0.01                | 0.11       |
| (1,754) | 1:45:A:GLN:HE21 | 1:48:A:LEU:HD22 | 5                   | 0.11     | 0.01                | 0.11       |
| (1,754) | 1:45:A:GLN:HE21 | 1:48:A:LEU:HD23 | 5                   | 0.11     | 0.01                | 0.11       |
| (1,754) | 1:45:A:GLN:HE22 | 1:48:A:LEU:HD11 | 5                   | 0.11     | 0.01                | 0.11       |
| (1,754) | 1:45:A:GLN:HE22 | 1:48:A:LEU:HD12 | 5                   | 0.11     | 0.01                | 0.11       |
| (1,754) | 1:45:A:GLN:HE22 | 1:48:A:LEU:HD13 | 5                   | 0.11     | 0.01                | 0.11       |
| (1,754) | 1:45:A:GLN:HE22 | 1:48:A:LEU:HD21 | 5                   | 0.11     | 0.01                | 0.11       |
| (1,754) | 1:45:A:GLN:HE22 | 1:48:A:LEU:HD22 | 5                   | 0.11     | 0.01                | 0.11       |
| (1,754) | 1:45:A:GLN:HE22 | 1:48:A:LEU:HD23 | 5                   | 0.11     | 0.01                | 0.11       |
| (1,575) | 1:12:A:ALA:HB1  | 1:36:A:TYR:HD1  | 4                   | 0.12     | 0.01                | 0.11       |
| (1,575) | 1:12:A:ALA:HB1  | 1:36:A:TYR:HD2  | 4                   | 0.12     | 0.01                | 0.11       |
| (1,575) | 1:12:A:ALA:HB2  | 1:36:A:TYR:HD1  | 4                   | 0.12     | 0.01                | 0.11       |
| (1,575) | 1:12:A:ALA:HB2  | 1:36:A:TYR:HD2  | 4                   | 0.12     | 0.01                | 0.11       |
| (1,575) | 1:12:A:ALA:HB3  | 1:36:A:TYR:HD1  | 4                   | 0.12     | 0.01                | 0.11       |
| (1,575) | 1:12:A:ALA:HB3  | 1:36:A:TYR:HD2  | 4                   | 0.12     | 0.01                | 0.11       |
| (1,381) | 1:59:A:LEU:H    | 1:59:A:LEU:HG   | 3                   | 0.27     | 0.03                | 0.26       |
| (1,493) | 1:13:A:ALA:HA   | 1:31:A:TYR:H    | 3                   | 0.11     | 0.0                 | 0.11       |
| (1,654) | 1:12:A:ALA:HA   | 1:15:A:GLN:HE21 | 2                   | 0.12     | 0.01                | 0.12       |
| (1,654) | 1:12:A:ALA:HA   | 1:15:A:GLN:HE22 | 2                   | 0.12     | 0.01                | 0.12       |
| (1,732) | 1:37:A:LYS:HA   | 1:37:A:LYS:HD2  | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,732) | 1:37:A:LYS:HA   | 1:37:A:LYS:HD3  | 2                   | 0.11     | 0.0                 | 0.11       |

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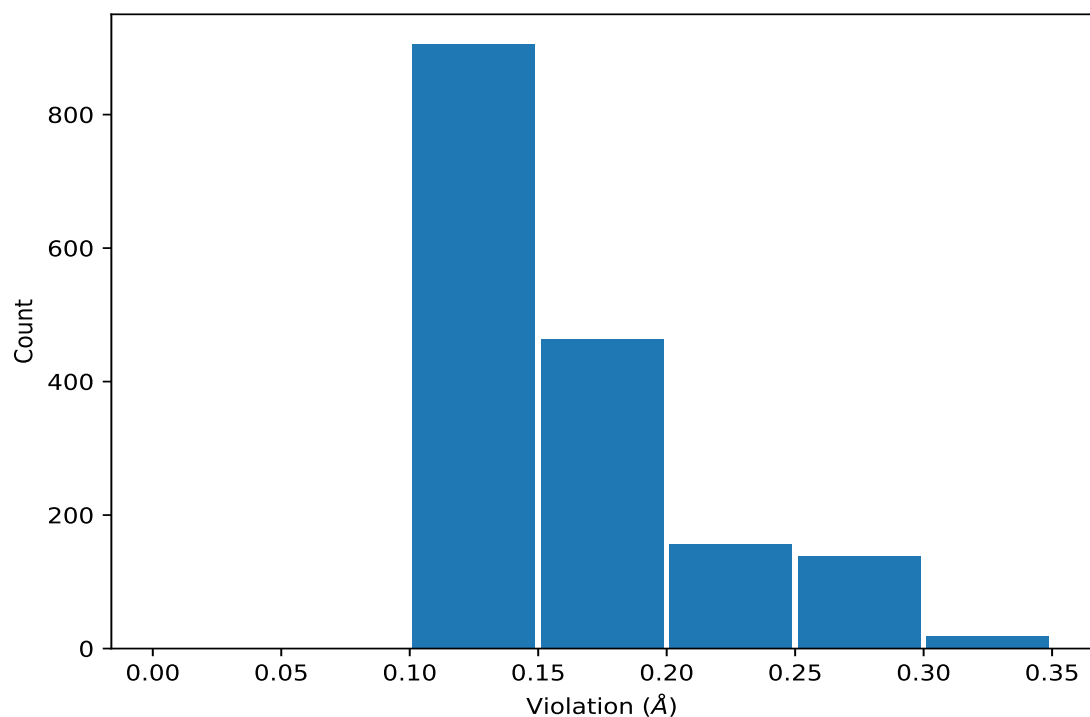
| Key     | Atom-1         | Atom-2         | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|----------------|----------------|---------------------|----------|---------------------|------------|
| (1,565) | 1:31:A:TYR:HD1 | 1:35:A:HIS:HE1 | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,565) | 1:31:A:TYR:HD2 | 1:35:A:HIS:HE1 | 2                   | 0.11     | 0.0                 | 0.11       |

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

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

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

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



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

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

| Key     | Atom-1         | Atom-2       | Model ID | Violation (Å) |
|---------|----------------|--------------|----------|---------------|
| (1,668) | 1:17:A:GLU:HG2 | 1:19:A:ASN:H | 8        | 0.31          |
| (1,668) | 1:17:A:GLU:HG3 | 1:19:A:ASN:H | 8        | 0.31          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,381) | 1:59:A:LEU:H    | 1:59:A:LEU:HG   | 13       | 0.31          |
| (1,6)   | 1:28:A:ILE:HG21 | 1:50:A:ILE:HB   | 14       | 0.31          |
| (1,6)   | 1:28:A:ILE:HG22 | 1:50:A:ILE:HB   | 14       | 0.31          |
| (1,6)   | 1:28:A:ILE:HG23 | 1:50:A:ILE:HB   | 14       | 0.31          |
| (1,644) | 1:10:A:ILE:HG12 | 1:14:A:ILE:HD11 | 12       | 0.3           |
| (1,644) | 1:10:A:ILE:HG12 | 1:14:A:ILE:HD12 | 12       | 0.3           |
| (1,644) | 1:10:A:ILE:HG12 | 1:14:A:ILE:HD13 | 12       | 0.3           |
| (1,644) | 1:10:A:ILE:HG13 | 1:14:A:ILE:HD11 | 12       | 0.3           |
| (1,644) | 1:10:A:ILE:HG13 | 1:14:A:ILE:HD12 | 12       | 0.3           |
| (1,644) | 1:10:A:ILE:HG13 | 1:14:A:ILE:HD13 | 12       | 0.3           |
| (1,6)   | 1:28:A:ILE:HG21 | 1:50:A:ILE:HB   | 6        | 0.3           |
| (1,6)   | 1:28:A:ILE:HG22 | 1:50:A:ILE:HB   | 6        | 0.3           |
| (1,6)   | 1:28:A:ILE:HG23 | 1:50:A:ILE:HB   | 6        | 0.3           |
| (1,6)   | 1:28:A:ILE:HG21 | 1:50:A:ILE:HB   | 13       | 0.3           |
| (1,6)   | 1:28:A:ILE:HG22 | 1:50:A:ILE:HB   | 13       | 0.3           |
| (1,6)   | 1:28:A:ILE:HG23 | 1:50:A:ILE:HB   | 13       | 0.3           |
| (1,820) | 1:63:A:LYS:HG2  | 1:70:A:SER:H    | 3        | 0.29          |
| (1,820) | 1:63:A:LYS:HG3  | 1:70:A:SER:H    | 3        | 0.29          |
| (1,628) | 1:7:A:SER:HB2   | 1:10:A:ILE:HG21 | 4        | 0.29          |
| (1,628) | 1:7:A:SER:HB2   | 1:10:A:ILE:HG22 | 4        | 0.29          |
| (1,628) | 1:7:A:SER:HB2   | 1:10:A:ILE:HG23 | 4        | 0.29          |
| (1,628) | 1:7:A:SER:HB3   | 1:10:A:ILE:HG21 | 4        | 0.29          |
| (1,628) | 1:7:A:SER:HB3   | 1:10:A:ILE:HG22 | 4        | 0.29          |
| (1,628) | 1:7:A:SER:HB3   | 1:10:A:ILE:HG23 | 4        | 0.29          |
| (1,6)   | 1:28:A:ILE:HG21 | 1:50:A:ILE:HB   | 5        | 0.29          |
| (1,6)   | 1:28:A:ILE:HG22 | 1:50:A:ILE:HB   | 5        | 0.29          |
| (1,6)   | 1:28:A:ILE:HG23 | 1:50:A:ILE:HB   | 5        | 0.29          |
| (1,6)   | 1:28:A:ILE:HG21 | 1:50:A:ILE:HB   | 8        | 0.29          |
| (1,6)   | 1:28:A:ILE:HG22 | 1:50:A:ILE:HB   | 8        | 0.29          |
| (1,6)   | 1:28:A:ILE:HG23 | 1:50:A:ILE:HB   | 8        | 0.29          |
| (1,803) | 1:60:A:LYS:HD2  | 1:74:A:ALA:H    | 13       | 0.28          |
| (1,803) | 1:60:A:LYS:HD3  | 1:74:A:ALA:H    | 13       | 0.28          |
| (1,668) | 1:17:A:GLU:HG2  | 1:19:A:ASN:H    | 6        | 0.28          |
| (1,668) | 1:17:A:GLU:HG3  | 1:19:A:ASN:H    | 6        | 0.28          |
| (1,644) | 1:10:A:ILE:HG12 | 1:14:A:ILE:HD11 | 9        | 0.28          |
| (1,644) | 1:10:A:ILE:HG12 | 1:14:A:ILE:HD12 | 9        | 0.28          |
| (1,644) | 1:10:A:ILE:HG12 | 1:14:A:ILE:HD13 | 9        | 0.28          |
| (1,644) | 1:10:A:ILE:HG13 | 1:14:A:ILE:HD11 | 9        | 0.28          |
| (1,644) | 1:10:A:ILE:HG13 | 1:14:A:ILE:HD12 | 9        | 0.28          |
| (1,644) | 1:10:A:ILE:HG13 | 1:14:A:ILE:HD13 | 9        | 0.28          |
| (1,6)   | 1:28:A:ILE:HG21 | 1:50:A:ILE:HB   | 16       | 0.28          |
| (1,6)   | 1:28:A:ILE:HG22 | 1:50:A:ILE:HB   | 16       | 0.28          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,6)   | 1:28:A:ILE:HG23 | 1:50:A:ILE:HB   | 16       | 0.28          |
| (1,820) | 1:63:A:LYS:HG2  | 1:70:A:SER:H    | 11       | 0.27          |
| (1,820) | 1:63:A:LYS:HG3  | 1:70:A:SER:H    | 11       | 0.27          |
| (1,780) | 1:51:A:LYS:HA   | 1:51:A:LYS:HD2  | 6        | 0.27          |
| (1,780) | 1:51:A:LYS:HA   | 1:51:A:LYS:HD3  | 6        | 0.27          |
| (1,688) | 1:25:A:ARG:HB2  | 1:68:A:SER:HB2  | 8        | 0.27          |
| (1,688) | 1:25:A:ARG:HB2  | 1:68:A:SER:HB3  | 8        | 0.27          |
| (1,688) | 1:25:A:ARG:HB3  | 1:68:A:SER:HB2  | 8        | 0.27          |
| (1,688) | 1:25:A:ARG:HB3  | 1:68:A:SER:HB3  | 8        | 0.27          |
| (1,644) | 1:10:A:ILE:HG12 | 1:14:A:ILE:HD11 | 3        | 0.27          |
| (1,644) | 1:10:A:ILE:HG12 | 1:14:A:ILE:HD12 | 3        | 0.27          |
| (1,644) | 1:10:A:ILE:HG12 | 1:14:A:ILE:HD13 | 3        | 0.27          |
| (1,644) | 1:10:A:ILE:HG13 | 1:14:A:ILE:HD11 | 3        | 0.27          |
| (1,644) | 1:10:A:ILE:HG13 | 1:14:A:ILE:HD12 | 3        | 0.27          |
| (1,644) | 1:10:A:ILE:HG13 | 1:14:A:ILE:HD13 | 3        | 0.27          |
| (1,644) | 1:10:A:ILE:HG12 | 1:14:A:ILE:HD11 | 4        | 0.27          |
| (1,644) | 1:10:A:ILE:HG12 | 1:14:A:ILE:HD12 | 4        | 0.27          |
| (1,644) | 1:10:A:ILE:HG12 | 1:14:A:ILE:HD13 | 4        | 0.27          |
| (1,644) | 1:10:A:ILE:HG13 | 1:14:A:ILE:HD11 | 4        | 0.27          |
| (1,644) | 1:10:A:ILE:HG13 | 1:14:A:ILE:HD12 | 4        | 0.27          |
| (1,644) | 1:10:A:ILE:HG13 | 1:14:A:ILE:HD13 | 4        | 0.27          |
| (1,6)   | 1:28:A:ILE:HG21 | 1:50:A:ILE:HB   | 7        | 0.27          |
| (1,6)   | 1:28:A:ILE:HG22 | 1:50:A:ILE:HB   | 7        | 0.27          |
| (1,6)   | 1:28:A:ILE:HG23 | 1:50:A:ILE:HB   | 7        | 0.27          |
| (1,820) | 1:63:A:LYS:HG2  | 1:70:A:SER:H    | 1        | 0.26          |
| (1,820) | 1:63:A:LYS:HG3  | 1:70:A:SER:H    | 1        | 0.26          |
| (1,820) | 1:63:A:LYS:HG2  | 1:70:A:SER:H    | 10       | 0.26          |
| (1,820) | 1:63:A:LYS:HG3  | 1:70:A:SER:H    | 10       | 0.26          |
| (1,820) | 1:63:A:LYS:HG2  | 1:70:A:SER:H    | 12       | 0.26          |
| (1,820) | 1:63:A:LYS:HG3  | 1:70:A:SER:H    | 12       | 0.26          |
| (1,688) | 1:25:A:ARG:HB2  | 1:68:A:SER:HB2  | 13       | 0.26          |
| (1,688) | 1:25:A:ARG:HB2  | 1:68:A:SER:HB3  | 13       | 0.26          |
| (1,688) | 1:25:A:ARG:HB3  | 1:68:A:SER:HB2  | 13       | 0.26          |
| (1,688) | 1:25:A:ARG:HB3  | 1:68:A:SER:HB3  | 13       | 0.26          |
| (1,688) | 1:25:A:ARG:HB2  | 1:68:A:SER:HB2  | 14       | 0.26          |
| (1,688) | 1:25:A:ARG:HB2  | 1:68:A:SER:HB3  | 14       | 0.26          |
| (1,688) | 1:25:A:ARG:HB3  | 1:68:A:SER:HB2  | 14       | 0.26          |
| (1,688) | 1:25:A:ARG:HB3  | 1:68:A:SER:HB3  | 14       | 0.26          |
| (1,688) | 1:25:A:ARG:HB2  | 1:68:A:SER:HB2  | 20       | 0.26          |
| (1,688) | 1:25:A:ARG:HB2  | 1:68:A:SER:HB3  | 20       | 0.26          |
| (1,688) | 1:25:A:ARG:HB3  | 1:68:A:SER:HB2  | 20       | 0.26          |
| (1,688) | 1:25:A:ARG:HB3  | 1:68:A:SER:HB3  | 20       | 0.26          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,661) | 1:15:A:GLN:H    | 1:15:A:GLN:HG2  | 2        | 0.26          |
| (1,661) | 1:15:A:GLN:H    | 1:15:A:GLN:HG3  | 2        | 0.26          |
| (1,661) | 1:15:A:GLN:H    | 1:15:A:GLN:HG2  | 12       | 0.26          |
| (1,661) | 1:15:A:GLN:H    | 1:15:A:GLN:HG3  | 12       | 0.26          |
| (1,661) | 1:15:A:GLN:H    | 1:15:A:GLN:HG2  | 13       | 0.26          |
| (1,661) | 1:15:A:GLN:H    | 1:15:A:GLN:HG3  | 13       | 0.26          |
| (1,661) | 1:15:A:GLN:H    | 1:15:A:GLN:HG2  | 14       | 0.26          |
| (1,661) | 1:15:A:GLN:H    | 1:15:A:GLN:HG3  | 14       | 0.26          |
| (1,661) | 1:15:A:GLN:H    | 1:15:A:GLN:HG2  | 15       | 0.26          |
| (1,661) | 1:15:A:GLN:H    | 1:15:A:GLN:HG3  | 15       | 0.26          |
| (1,661) | 1:15:A:GLN:H    | 1:15:A:GLN:HG2  | 16       | 0.26          |
| (1,661) | 1:15:A:GLN:H    | 1:15:A:GLN:HG3  | 16       | 0.26          |
| (1,661) | 1:15:A:GLN:H    | 1:15:A:GLN:HG2  | 17       | 0.26          |
| (1,661) | 1:15:A:GLN:H    | 1:15:A:GLN:HG3  | 17       | 0.26          |
| (1,661) | 1:15:A:GLN:H    | 1:15:A:GLN:HG2  | 18       | 0.26          |
| (1,661) | 1:15:A:GLN:H    | 1:15:A:GLN:HG3  | 18       | 0.26          |
| (1,661) | 1:15:A:GLN:H    | 1:15:A:GLN:HG2  | 19       | 0.26          |
| (1,661) | 1:15:A:GLN:H    | 1:15:A:GLN:HG3  | 19       | 0.26          |
| (1,644) | 1:10:A:ILE:HG12 | 1:14:A:ILE:HD11 | 11       | 0.26          |
| (1,644) | 1:10:A:ILE:HG12 | 1:14:A:ILE:HD12 | 11       | 0.26          |
| (1,644) | 1:10:A:ILE:HG12 | 1:14:A:ILE:HD13 | 11       | 0.26          |
| (1,644) | 1:10:A:ILE:HG13 | 1:14:A:ILE:HD11 | 11       | 0.26          |
| (1,644) | 1:10:A:ILE:HG13 | 1:14:A:ILE:HD12 | 11       | 0.26          |
| (1,644) | 1:10:A:ILE:HG13 | 1:14:A:ILE:HD13 | 11       | 0.26          |
| (1,381) | 1:59:A:LEU:H    | 1:59:A:LEU:HG   | 1        | 0.26          |
| (1,6)   | 1:28:A:ILE:HG21 | 1:50:A:ILE:HB   | 1        | 0.26          |
| (1,6)   | 1:28:A:ILE:HG22 | 1:50:A:ILE:HB   | 1        | 0.26          |
| (1,6)   | 1:28:A:ILE:HG23 | 1:50:A:ILE:HB   | 1        | 0.26          |
| (1,6)   | 1:28:A:ILE:HG21 | 1:50:A:ILE:HB   | 4        | 0.26          |
| (1,6)   | 1:28:A:ILE:HG22 | 1:50:A:ILE:HB   | 4        | 0.26          |
| (1,6)   | 1:28:A:ILE:HG23 | 1:50:A:ILE:HB   | 4        | 0.26          |
| (1,820) | 1:63:A:LYS:HG2  | 1:70:A:SER:H    | 13       | 0.25          |
| (1,820) | 1:63:A:LYS:HG3  | 1:70:A:SER:H    | 13       | 0.25          |
| (1,820) | 1:63:A:LYS:HG2  | 1:70:A:SER:H    | 18       | 0.25          |
| (1,820) | 1:63:A:LYS:HG3  | 1:70:A:SER:H    | 18       | 0.25          |
| (1,688) | 1:25:A:ARG:HB2  | 1:68:A:SER:HB2  | 3        | 0.25          |
| (1,688) | 1:25:A:ARG:HB2  | 1:68:A:SER:HB3  | 3        | 0.25          |
| (1,688) | 1:25:A:ARG:HB3  | 1:68:A:SER:HB2  | 3        | 0.25          |
| (1,688) | 1:25:A:ARG:HB3  | 1:68:A:SER:HB3  | 3        | 0.25          |
| (1,688) | 1:25:A:ARG:HB2  | 1:68:A:SER:HB2  | 7        | 0.25          |
| (1,688) | 1:25:A:ARG:HB2  | 1:68:A:SER:HB3  | 7        | 0.25          |
| (1,688) | 1:25:A:ARG:HB3  | 1:68:A:SER:HB2  | 7        | 0.25          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,688) | 1:25:A:ARG:HB3  | 1:68:A:SER:HB3 | 7        | 0.25          |
| (1,688) | 1:25:A:ARG:HB2  | 1:68:A:SER:HB2 | 9        | 0.25          |
| (1,688) | 1:25:A:ARG:HB2  | 1:68:A:SER:HB3 | 9        | 0.25          |
| (1,688) | 1:25:A:ARG:HB3  | 1:68:A:SER:HB2 | 9        | 0.25          |
| (1,688) | 1:25:A:ARG:HB3  | 1:68:A:SER:HB3 | 9        | 0.25          |
| (1,688) | 1:25:A:ARG:HB2  | 1:68:A:SER:HB2 | 11       | 0.25          |
| (1,688) | 1:25:A:ARG:HB2  | 1:68:A:SER:HB3 | 11       | 0.25          |
| (1,688) | 1:25:A:ARG:HB3  | 1:68:A:SER:HB2 | 11       | 0.25          |
| (1,688) | 1:25:A:ARG:HB3  | 1:68:A:SER:HB3 | 11       | 0.25          |
| (1,688) | 1:25:A:ARG:HB2  | 1:68:A:SER:HB2 | 17       | 0.25          |
| (1,688) | 1:25:A:ARG:HB2  | 1:68:A:SER:HB3 | 17       | 0.25          |
| (1,688) | 1:25:A:ARG:HB3  | 1:68:A:SER:HB2 | 17       | 0.25          |
| (1,688) | 1:25:A:ARG:HB3  | 1:68:A:SER:HB3 | 17       | 0.25          |
| (1,661) | 1:15:A:GLN:H    | 1:15:A:GLN:HG2 | 7        | 0.25          |
| (1,661) | 1:15:A:GLN:H    | 1:15:A:GLN:HG3 | 7        | 0.25          |
| (1,661) | 1:15:A:GLN:H    | 1:15:A:GLN:HG2 | 20       | 0.25          |
| (1,661) | 1:15:A:GLN:H    | 1:15:A:GLN:HG3 | 20       | 0.25          |
| (1,6)   | 1:28:A:ILE:HG21 | 1:50:A:ILE:HB  | 3        | 0.25          |
| (1,6)   | 1:28:A:ILE:HG22 | 1:50:A:ILE:HB  | 3        | 0.25          |
| (1,6)   | 1:28:A:ILE:HG23 | 1:50:A:ILE:HB  | 3        | 0.25          |
| (1,6)   | 1:28:A:ILE:HG21 | 1:50:A:ILE:HB  | 11       | 0.25          |
| (1,6)   | 1:28:A:ILE:HG22 | 1:50:A:ILE:HB  | 11       | 0.25          |
| (1,6)   | 1:28:A:ILE:HG23 | 1:50:A:ILE:HB  | 11       | 0.25          |
| (1,6)   | 1:28:A:ILE:HG21 | 1:50:A:ILE:HB  | 12       | 0.25          |
| (1,6)   | 1:28:A:ILE:HG22 | 1:50:A:ILE:HB  | 12       | 0.25          |
| (1,6)   | 1:28:A:ILE:HG23 | 1:50:A:ILE:HB  | 12       | 0.25          |
| (1,6)   | 1:28:A:ILE:HG21 | 1:50:A:ILE:HB  | 19       | 0.25          |
| (1,6)   | 1:28:A:ILE:HG22 | 1:50:A:ILE:HB  | 19       | 0.25          |
| (1,6)   | 1:28:A:ILE:HG23 | 1:50:A:ILE:HB  | 19       | 0.25          |
| (1,820) | 1:63:A:LYS:HG2  | 1:70:A:SER:H   | 2        | 0.24          |
| (1,820) | 1:63:A:LYS:HG3  | 1:70:A:SER:H   | 2        | 0.24          |
| (1,820) | 1:63:A:LYS:HG2  | 1:70:A:SER:H   | 4        | 0.24          |
| (1,820) | 1:63:A:LYS:HG3  | 1:70:A:SER:H   | 4        | 0.24          |
| (1,820) | 1:63:A:LYS:HG2  | 1:70:A:SER:H   | 5        | 0.24          |
| (1,820) | 1:63:A:LYS:HG3  | 1:70:A:SER:H   | 5        | 0.24          |
| (1,820) | 1:63:A:LYS:HG2  | 1:70:A:SER:H   | 7        | 0.24          |
| (1,820) | 1:63:A:LYS:HG3  | 1:70:A:SER:H   | 7        | 0.24          |
| (1,820) | 1:63:A:LYS:HG2  | 1:70:A:SER:H   | 14       | 0.24          |
| (1,820) | 1:63:A:LYS:HG3  | 1:70:A:SER:H   | 14       | 0.24          |
| (1,820) | 1:63:A:LYS:HG2  | 1:70:A:SER:H   | 15       | 0.24          |
| (1,820) | 1:63:A:LYS:HG3  | 1:70:A:SER:H   | 15       | 0.24          |
| (1,820) | 1:63:A:LYS:HG2  | 1:70:A:SER:H   | 20       | 0.24          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,820) | 1:63:A:LYS:HG3  | 1:70:A:SER:H   | 20       | 0.24          |
| (1,688) | 1:25:A:ARG:HB2  | 1:68:A:SER:HB2 | 2        | 0.24          |
| (1,688) | 1:25:A:ARG:HB2  | 1:68:A:SER:HB3 | 2        | 0.24          |
| (1,688) | 1:25:A:ARG:HB3  | 1:68:A:SER:HB2 | 2        | 0.24          |
| (1,688) | 1:25:A:ARG:HB3  | 1:68:A:SER:HB3 | 2        | 0.24          |
| (1,688) | 1:25:A:ARG:HB2  | 1:68:A:SER:HB2 | 19       | 0.24          |
| (1,688) | 1:25:A:ARG:HB2  | 1:68:A:SER:HB3 | 19       | 0.24          |
| (1,688) | 1:25:A:ARG:HB3  | 1:68:A:SER:HB2 | 19       | 0.24          |
| (1,688) | 1:25:A:ARG:HB3  | 1:68:A:SER:HB3 | 19       | 0.24          |
| (1,457) | 1:61:A:GLN:H    | 1:72:A:ARG:H   | 4        | 0.24          |
| (1,262) | 1:14:A:ILE:HD11 | 1:71:A:PHE:HA  | 4        | 0.24          |
| (1,262) | 1:14:A:ILE:HD12 | 1:71:A:PHE:HA  | 4        | 0.24          |
| (1,262) | 1:14:A:ILE:HD13 | 1:71:A:PHE:HA  | 4        | 0.24          |
| (1,262) | 1:14:A:ILE:HD11 | 1:71:A:PHE:HA  | 12       | 0.24          |
| (1,262) | 1:14:A:ILE:HD12 | 1:71:A:PHE:HA  | 12       | 0.24          |
| (1,262) | 1:14:A:ILE:HD13 | 1:71:A:PHE:HA  | 12       | 0.24          |
| (1,820) | 1:63:A:LYS:HG2  | 1:70:A:SER:H   | 6        | 0.23          |
| (1,820) | 1:63:A:LYS:HG3  | 1:70:A:SER:H   | 6        | 0.23          |
| (1,820) | 1:63:A:LYS:HG2  | 1:70:A:SER:H   | 9        | 0.23          |
| (1,820) | 1:63:A:LYS:HG3  | 1:70:A:SER:H   | 9        | 0.23          |
| (1,820) | 1:63:A:LYS:HG2  | 1:70:A:SER:H   | 19       | 0.23          |
| (1,820) | 1:63:A:LYS:HG3  | 1:70:A:SER:H   | 19       | 0.23          |
| (1,688) | 1:25:A:ARG:HB2  | 1:68:A:SER:HB2 | 5        | 0.23          |
| (1,688) | 1:25:A:ARG:HB2  | 1:68:A:SER:HB3 | 5        | 0.23          |
| (1,688) | 1:25:A:ARG:HB3  | 1:68:A:SER:HB2 | 5        | 0.23          |
| (1,688) | 1:25:A:ARG:HB3  | 1:68:A:SER:HB3 | 5        | 0.23          |
| (1,688) | 1:25:A:ARG:HB2  | 1:68:A:SER:HB2 | 6        | 0.23          |
| (1,688) | 1:25:A:ARG:HB2  | 1:68:A:SER:HB3 | 6        | 0.23          |
| (1,688) | 1:25:A:ARG:HB3  | 1:68:A:SER:HB2 | 6        | 0.23          |
| (1,688) | 1:25:A:ARG:HB3  | 1:68:A:SER:HB3 | 6        | 0.23          |
| (1,676) | 1:20:A:ARG:HA   | 1:20:A:ARG:HD2 | 3        | 0.23          |
| (1,676) | 1:20:A:ARG:HA   | 1:20:A:ARG:HD3 | 3        | 0.23          |
| (1,668) | 1:17:A:GLU:HG2  | 1:19:A:ASN:H   | 20       | 0.23          |
| (1,668) | 1:17:A:GLU:HG3  | 1:19:A:ASN:H   | 20       | 0.23          |
| (1,531) | 1:61:A:GLN:H    | 1:72:A:ARG:HB2 | 13       | 0.23          |
| (1,531) | 1:61:A:GLN:H    | 1:72:A:ARG:HB3 | 13       | 0.23          |
| (1,381) | 1:59:A:LEU:H    | 1:59:A:LEU:HG  | 12       | 0.23          |
| (1,6)   | 1:28:A:ILE:HG21 | 1:50:A:ILE:HB  | 2        | 0.23          |
| (1,6)   | 1:28:A:ILE:HG22 | 1:50:A:ILE:HB  | 2        | 0.23          |
| (1,6)   | 1:28:A:ILE:HG23 | 1:50:A:ILE:HB  | 2        | 0.23          |
| (1,6)   | 1:28:A:ILE:HG21 | 1:50:A:ILE:HB  | 10       | 0.23          |
| (1,6)   | 1:28:A:ILE:HG22 | 1:50:A:ILE:HB  | 10       | 0.23          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,6)   | 1:28:A:ILE:HG23 | 1:50:A:ILE:HB   | 10       | 0.23          |
| (1,6)   | 1:28:A:ILE:HG21 | 1:50:A:ILE:HB   | 15       | 0.23          |
| (1,6)   | 1:28:A:ILE:HG22 | 1:50:A:ILE:HB   | 15       | 0.23          |
| (1,6)   | 1:28:A:ILE:HG23 | 1:50:A:ILE:HB   | 15       | 0.23          |
| (1,820) | 1:63:A:LYS:HG2  | 1:70:A:SER:H    | 8        | 0.22          |
| (1,820) | 1:63:A:LYS:HG3  | 1:70:A:SER:H    | 8        | 0.22          |
| (1,820) | 1:63:A:LYS:HG2  | 1:70:A:SER:H    | 16       | 0.22          |
| (1,820) | 1:63:A:LYS:HG3  | 1:70:A:SER:H    | 16       | 0.22          |
| (1,819) | 1:63:A:LYS:HB2  | 1:70:A:SER:H    | 7        | 0.22          |
| (1,819) | 1:63:A:LYS:HB3  | 1:70:A:SER:H    | 7        | 0.22          |
| (1,819) | 1:63:A:LYS:HB2  | 1:70:A:SER:H    | 12       | 0.22          |
| (1,819) | 1:63:A:LYS:HB3  | 1:70:A:SER:H    | 12       | 0.22          |
| (1,733) | 1:37:A:LYS:HG2  | 1:38:A:VAL:H    | 9        | 0.22          |
| (1,733) | 1:37:A:LYS:HG3  | 1:38:A:VAL:H    | 9        | 0.22          |
| (1,688) | 1:25:A:ARG:HB2  | 1:68:A:SER:HB2  | 1        | 0.22          |
| (1,688) | 1:25:A:ARG:HB2  | 1:68:A:SER:HB3  | 1        | 0.22          |
| (1,688) | 1:25:A:ARG:HB3  | 1:68:A:SER:HB2  | 1        | 0.22          |
| (1,688) | 1:25:A:ARG:HB3  | 1:68:A:SER:HB3  | 1        | 0.22          |
| (1,688) | 1:25:A:ARG:HB2  | 1:68:A:SER:HB2  | 4        | 0.22          |
| (1,688) | 1:25:A:ARG:HB2  | 1:68:A:SER:HB3  | 4        | 0.22          |
| (1,688) | 1:25:A:ARG:HB3  | 1:68:A:SER:HB2  | 4        | 0.22          |
| (1,688) | 1:25:A:ARG:HB3  | 1:68:A:SER:HB3  | 4        | 0.22          |
| (1,688) | 1:25:A:ARG:HB2  | 1:68:A:SER:HB2  | 15       | 0.22          |
| (1,688) | 1:25:A:ARG:HB2  | 1:68:A:SER:HB3  | 15       | 0.22          |
| (1,688) | 1:25:A:ARG:HB3  | 1:68:A:SER:HB2  | 15       | 0.22          |
| (1,688) | 1:25:A:ARG:HB3  | 1:68:A:SER:HB3  | 15       | 0.22          |
| (1,644) | 1:10:A:ILE:HG12 | 1:14:A:ILE:HD11 | 13       | 0.22          |
| (1,644) | 1:10:A:ILE:HG12 | 1:14:A:ILE:HD12 | 13       | 0.22          |
| (1,644) | 1:10:A:ILE:HG12 | 1:14:A:ILE:HD13 | 13       | 0.22          |
| (1,644) | 1:10:A:ILE:HG13 | 1:14:A:ILE:HD11 | 13       | 0.22          |
| (1,644) | 1:10:A:ILE:HG13 | 1:14:A:ILE:HD12 | 13       | 0.22          |
| (1,644) | 1:10:A:ILE:HG13 | 1:14:A:ILE:HD13 | 13       | 0.22          |
| (1,6)   | 1:28:A:ILE:HG21 | 1:50:A:ILE:HB   | 17       | 0.22          |
| (1,6)   | 1:28:A:ILE:HG22 | 1:50:A:ILE:HB   | 17       | 0.22          |
| (1,6)   | 1:28:A:ILE:HG23 | 1:50:A:ILE:HB   | 17       | 0.22          |
| (1,6)   | 1:28:A:ILE:HG21 | 1:50:A:ILE:HB   | 20       | 0.22          |
| (1,6)   | 1:28:A:ILE:HG22 | 1:50:A:ILE:HB   | 20       | 0.22          |
| (1,6)   | 1:28:A:ILE:HG23 | 1:50:A:ILE:HB   | 20       | 0.22          |
| (1,819) | 1:63:A:LYS:HB2  | 1:70:A:SER:H    | 10       | 0.21          |
| (1,819) | 1:63:A:LYS:HB3  | 1:70:A:SER:H    | 10       | 0.21          |
| (1,819) | 1:63:A:LYS:HB2  | 1:70:A:SER:H    | 15       | 0.21          |
| (1,819) | 1:63:A:LYS:HB3  | 1:70:A:SER:H    | 15       | 0.21          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,819) | 1:63:A:LYS:HB2  | 1:70:A:SER:H    | 19       | 0.21          |
| (1,819) | 1:63:A:LYS:HB3  | 1:70:A:SER:H    | 19       | 0.21          |
| (1,644) | 1:10:A:ILE:HG12 | 1:14:A:ILE:HD11 | 10       | 0.21          |
| (1,644) | 1:10:A:ILE:HG12 | 1:14:A:ILE:HD12 | 10       | 0.21          |
| (1,644) | 1:10:A:ILE:HG12 | 1:14:A:ILE:HD13 | 10       | 0.21          |
| (1,644) | 1:10:A:ILE:HG13 | 1:14:A:ILE:HD11 | 10       | 0.21          |
| (1,644) | 1:10:A:ILE:HG13 | 1:14:A:ILE:HD12 | 10       | 0.21          |
| (1,644) | 1:10:A:ILE:HG13 | 1:14:A:ILE:HD13 | 10       | 0.21          |
| (1,531) | 1:61:A:GLN:H    | 1:72:A:ARG:HB2  | 15       | 0.21          |
| (1,531) | 1:61:A:GLN:H    | 1:72:A:ARG:HB3  | 15       | 0.21          |
| (1,262) | 1:14:A:ILE:HD11 | 1:71:A:PHE:HA   | 10       | 0.21          |
| (1,262) | 1:14:A:ILE:HD12 | 1:71:A:PHE:HA   | 10       | 0.21          |
| (1,262) | 1:14:A:ILE:HD13 | 1:71:A:PHE:HA   | 10       | 0.21          |
| (1,262) | 1:14:A:ILE:HD11 | 1:71:A:PHE:HA   | 11       | 0.21          |
| (1,262) | 1:14:A:ILE:HD12 | 1:71:A:PHE:HA   | 11       | 0.21          |
| (1,262) | 1:14:A:ILE:HD13 | 1:71:A:PHE:HA   | 11       | 0.21          |
| (1,820) | 1:63:A:LYS:HG2  | 1:70:A:SER:H    | 17       | 0.2           |
| (1,820) | 1:63:A:LYS:HG3  | 1:70:A:SER:H    | 17       | 0.2           |
| (1,819) | 1:63:A:LYS:HB2  | 1:70:A:SER:H    | 2        | 0.2           |
| (1,819) | 1:63:A:LYS:HB3  | 1:70:A:SER:H    | 2        | 0.2           |
| (1,819) | 1:63:A:LYS:HB2  | 1:70:A:SER:H    | 3        | 0.2           |
| (1,819) | 1:63:A:LYS:HB3  | 1:70:A:SER:H    | 3        | 0.2           |
| (1,819) | 1:63:A:LYS:HB2  | 1:70:A:SER:H    | 5        | 0.2           |
| (1,819) | 1:63:A:LYS:HB3  | 1:70:A:SER:H    | 5        | 0.2           |
| (1,819) | 1:63:A:LYS:HB2  | 1:70:A:SER:H    | 6        | 0.2           |
| (1,819) | 1:63:A:LYS:HB3  | 1:70:A:SER:H    | 6        | 0.2           |
| (1,819) | 1:63:A:LYS:HB2  | 1:70:A:SER:H    | 8        | 0.2           |
| (1,819) | 1:63:A:LYS:HB3  | 1:70:A:SER:H    | 8        | 0.2           |
| (1,819) | 1:63:A:LYS:HB2  | 1:70:A:SER:H    | 9        | 0.2           |
| (1,819) | 1:63:A:LYS:HB3  | 1:70:A:SER:H    | 9        | 0.2           |
| (1,819) | 1:63:A:LYS:HB2  | 1:70:A:SER:H    | 13       | 0.2           |
| (1,819) | 1:63:A:LYS:HB3  | 1:70:A:SER:H    | 13       | 0.2           |
| (1,819) | 1:63:A:LYS:HB2  | 1:70:A:SER:H    | 14       | 0.2           |
| (1,819) | 1:63:A:LYS:HB3  | 1:70:A:SER:H    | 14       | 0.2           |
| (1,819) | 1:63:A:LYS:HB2  | 1:70:A:SER:H    | 17       | 0.2           |
| (1,819) | 1:63:A:LYS:HB3  | 1:70:A:SER:H    | 17       | 0.2           |
| (1,688) | 1:25:A:ARG:HB2  | 1:68:A:SER:HB2  | 12       | 0.2           |
| (1,688) | 1:25:A:ARG:HB2  | 1:68:A:SER:HB3  | 12       | 0.2           |
| (1,688) | 1:25:A:ARG:HB3  | 1:68:A:SER:HB2  | 12       | 0.2           |
| (1,688) | 1:25:A:ARG:HB3  | 1:68:A:SER:HB3  | 12       | 0.2           |
| (1,688) | 1:25:A:ARG:HB2  | 1:68:A:SER:HB2  | 16       | 0.2           |
| (1,688) | 1:25:A:ARG:HB2  | 1:68:A:SER:HB3  | 16       | 0.2           |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,688) | 1:25:A:ARG:HB3  | 1:68:A:SER:HB2 | 16       | 0.2           |
| (1,688) | 1:25:A:ARG:HB3  | 1:68:A:SER:HB3 | 16       | 0.2           |
| (1,668) | 1:17:A:GLU:HG2  | 1:19:A:ASN:H   | 7        | 0.2           |
| (1,668) | 1:17:A:GLU:HG3  | 1:19:A:ASN:H   | 7        | 0.2           |
| (1,531) | 1:61:A:GLN:H    | 1:72:A:ARG:HB2 | 4        | 0.2           |
| (1,531) | 1:61:A:GLN:H    | 1:72:A:ARG:HB3 | 4        | 0.2           |
| (1,531) | 1:61:A:GLN:H    | 1:72:A:ARG:HB2 | 20       | 0.2           |
| (1,531) | 1:61:A:GLN:H    | 1:72:A:ARG:HB3 | 20       | 0.2           |
| (1,262) | 1:14:A:ILE:HD11 | 1:71:A:PHE:HA  | 8        | 0.2           |
| (1,262) | 1:14:A:ILE:HD12 | 1:71:A:PHE:HA  | 8        | 0.2           |
| (1,262) | 1:14:A:ILE:HD13 | 1:71:A:PHE:HA  | 8        | 0.2           |
| (1,262) | 1:14:A:ILE:HD11 | 1:71:A:PHE:HA  | 9        | 0.2           |
| (1,262) | 1:14:A:ILE:HD12 | 1:71:A:PHE:HA  | 9        | 0.2           |
| (1,262) | 1:14:A:ILE:HD13 | 1:71:A:PHE:HA  | 9        | 0.2           |
| (1,13)  | 1:60:A:LYS:HA   | 1:72:A:ARG:HB2 | 6        | 0.2           |
| (1,13)  | 1:60:A:LYS:HA   | 1:72:A:ARG:HB3 | 6        | 0.2           |
| (1,13)  | 1:60:A:LYS:HA   | 1:72:A:ARG:HB2 | 16       | 0.2           |
| (1,13)  | 1:60:A:LYS:HA   | 1:72:A:ARG:HB3 | 16       | 0.2           |
| (1,819) | 1:63:A:LYS:HB2  | 1:70:A:SER:H   | 16       | 0.19          |
| (1,819) | 1:63:A:LYS:HB3  | 1:70:A:SER:H   | 16       | 0.19          |
| (1,819) | 1:63:A:LYS:HB2  | 1:70:A:SER:H   | 20       | 0.19          |
| (1,819) | 1:63:A:LYS:HB3  | 1:70:A:SER:H   | 20       | 0.19          |
| (1,531) | 1:61:A:GLN:H    | 1:72:A:ARG:HB2 | 9        | 0.19          |
| (1,531) | 1:61:A:GLN:H    | 1:72:A:ARG:HB3 | 9        | 0.19          |
| (1,457) | 1:61:A:GLN:H    | 1:72:A:ARG:H   | 9        | 0.19          |
| (1,457) | 1:61:A:GLN:H    | 1:72:A:ARG:H   | 18       | 0.19          |
| (1,262) | 1:14:A:ILE:HD11 | 1:71:A:PHE:HA  | 20       | 0.19          |
| (1,262) | 1:14:A:ILE:HD12 | 1:71:A:PHE:HA  | 20       | 0.19          |
| (1,262) | 1:14:A:ILE:HD13 | 1:71:A:PHE:HA  | 20       | 0.19          |
| (1,13)  | 1:60:A:LYS:HA   | 1:72:A:ARG:HB2 | 13       | 0.19          |
| (1,13)  | 1:60:A:LYS:HA   | 1:72:A:ARG:HB3 | 13       | 0.19          |
| (1,819) | 1:63:A:LYS:HB2  | 1:70:A:SER:H   | 1        | 0.18          |
| (1,819) | 1:63:A:LYS:HB3  | 1:70:A:SER:H   | 1        | 0.18          |
| (1,819) | 1:63:A:LYS:HB2  | 1:70:A:SER:H   | 11       | 0.18          |
| (1,819) | 1:63:A:LYS:HB3  | 1:70:A:SER:H   | 11       | 0.18          |
| (1,803) | 1:60:A:LYS:HD2  | 1:74:A:ALA:H   | 7        | 0.18          |
| (1,803) | 1:60:A:LYS:HD3  | 1:74:A:ALA:H   | 7        | 0.18          |
| (1,803) | 1:60:A:LYS:HD2  | 1:74:A:ALA:H   | 8        | 0.18          |
| (1,803) | 1:60:A:LYS:HD3  | 1:74:A:ALA:H   | 8        | 0.18          |
| (1,803) | 1:60:A:LYS:HD2  | 1:74:A:ALA:H   | 19       | 0.18          |
| (1,803) | 1:60:A:LYS:HD3  | 1:74:A:ALA:H   | 19       | 0.18          |
| (1,788) | 1:52:A:ARG:HD2  | 1:53:A:LEU:HB2 | 9        | 0.18          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,788) | 1:52:A:ARG:HD2  | 1:53:A:LEU:HB3  | 9        | 0.18          |
| (1,788) | 1:52:A:ARG:HD3  | 1:53:A:LEU:HB2  | 9        | 0.18          |
| (1,788) | 1:52:A:ARG:HD3  | 1:53:A:LEU:HB3  | 9        | 0.18          |
| (1,788) | 1:52:A:ARG:HD2  | 1:53:A:LEU:HB2  | 20       | 0.18          |
| (1,788) | 1:52:A:ARG:HD2  | 1:53:A:LEU:HB3  | 20       | 0.18          |
| (1,788) | 1:52:A:ARG:HD3  | 1:53:A:LEU:HB2  | 20       | 0.18          |
| (1,788) | 1:52:A:ARG:HD3  | 1:53:A:LEU:HB3  | 20       | 0.18          |
| (1,688) | 1:25:A:ARG:HB2  | 1:68:A:SER:HB2  | 10       | 0.18          |
| (1,688) | 1:25:A:ARG:HB2  | 1:68:A:SER:HB3  | 10       | 0.18          |
| (1,688) | 1:25:A:ARG:HB3  | 1:68:A:SER:HB2  | 10       | 0.18          |
| (1,688) | 1:25:A:ARG:HB3  | 1:68:A:SER:HB3  | 10       | 0.18          |
| (1,644) | 1:10:A:ILE:HG12 | 1:14:A:ILE:HD11 | 1        | 0.18          |
| (1,644) | 1:10:A:ILE:HG12 | 1:14:A:ILE:HD12 | 1        | 0.18          |
| (1,644) | 1:10:A:ILE:HG12 | 1:14:A:ILE:HD13 | 1        | 0.18          |
| (1,644) | 1:10:A:ILE:HG13 | 1:14:A:ILE:HD11 | 1        | 0.18          |
| (1,644) | 1:10:A:ILE:HG13 | 1:14:A:ILE:HD12 | 1        | 0.18          |
| (1,644) | 1:10:A:ILE:HG13 | 1:14:A:ILE:HD13 | 1        | 0.18          |
| (1,573) | 1:32:A:ILE:HD11 | 1:36:A:TYR:HD1  | 18       | 0.18          |
| (1,573) | 1:32:A:ILE:HD11 | 1:36:A:TYR:HD2  | 18       | 0.18          |
| (1,573) | 1:32:A:ILE:HD12 | 1:36:A:TYR:HD1  | 18       | 0.18          |
| (1,573) | 1:32:A:ILE:HD12 | 1:36:A:TYR:HD2  | 18       | 0.18          |
| (1,573) | 1:32:A:ILE:HD13 | 1:36:A:TYR:HD1  | 18       | 0.18          |
| (1,573) | 1:32:A:ILE:HD13 | 1:36:A:TYR:HD2  | 18       | 0.18          |
| (1,531) | 1:61:A:GLN:H    | 1:72:A:ARG:HB2  | 1        | 0.18          |
| (1,531) | 1:61:A:GLN:H    | 1:72:A:ARG:HB3  | 1        | 0.18          |
| (1,531) | 1:61:A:GLN:H    | 1:72:A:ARG:HB2  | 3        | 0.18          |
| (1,531) | 1:61:A:GLN:H    | 1:72:A:ARG:HB3  | 3        | 0.18          |
| (1,531) | 1:61:A:GLN:H    | 1:72:A:ARG:HB2  | 6        | 0.18          |
| (1,531) | 1:61:A:GLN:H    | 1:72:A:ARG:HB3  | 6        | 0.18          |
| (1,363) | 1:55:A:THR:HG21 | 1:57:A:GLY:H    | 4        | 0.18          |
| (1,363) | 1:55:A:THR:HG22 | 1:57:A:GLY:H    | 4        | 0.18          |
| (1,363) | 1:55:A:THR:HG23 | 1:57:A:GLY:H    | 4        | 0.18          |
| (1,363) | 1:55:A:THR:HG21 | 1:57:A:GLY:H    | 6        | 0.18          |
| (1,363) | 1:55:A:THR:HG22 | 1:57:A:GLY:H    | 6        | 0.18          |
| (1,363) | 1:55:A:THR:HG23 | 1:57:A:GLY:H    | 6        | 0.18          |
| (1,363) | 1:55:A:THR:HG21 | 1:57:A:GLY:H    | 7        | 0.18          |
| (1,363) | 1:55:A:THR:HG22 | 1:57:A:GLY:H    | 7        | 0.18          |
| (1,363) | 1:55:A:THR:HG23 | 1:57:A:GLY:H    | 7        | 0.18          |
| (1,363) | 1:55:A:THR:HG21 | 1:57:A:GLY:H    | 8        | 0.18          |
| (1,363) | 1:55:A:THR:HG22 | 1:57:A:GLY:H    | 8        | 0.18          |
| (1,363) | 1:55:A:THR:HG23 | 1:57:A:GLY:H    | 8        | 0.18          |
| (1,4)   | 1:14:A:ILE:HD11 | 1:28:A:ILE:HB   | 6        | 0.18          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,4)   | 1:14:A:ILE:HD12 | 1:28:A:ILE:HB   | 6        | 0.18          |
| (1,4)   | 1:14:A:ILE:HD13 | 1:28:A:ILE:HB   | 6        | 0.18          |
| (1,4)   | 1:14:A:ILE:HD11 | 1:28:A:ILE:HB   | 10       | 0.18          |
| (1,4)   | 1:14:A:ILE:HD12 | 1:28:A:ILE:HB   | 10       | 0.18          |
| (1,4)   | 1:14:A:ILE:HD13 | 1:28:A:ILE:HB   | 10       | 0.18          |
| (1,803) | 1:60:A:LYS:HD2  | 1:74:A:ALA:H    | 2        | 0.17          |
| (1,803) | 1:60:A:LYS:HD3  | 1:74:A:ALA:H    | 2        | 0.17          |
| (1,803) | 1:60:A:LYS:HD2  | 1:74:A:ALA:H    | 10       | 0.17          |
| (1,803) | 1:60:A:LYS:HD3  | 1:74:A:ALA:H    | 10       | 0.17          |
| (1,803) | 1:60:A:LYS:HD2  | 1:74:A:ALA:H    | 11       | 0.17          |
| (1,803) | 1:60:A:LYS:HD3  | 1:74:A:ALA:H    | 11       | 0.17          |
| (1,788) | 1:52:A:ARG:HD2  | 1:53:A:LEU:HB2  | 1        | 0.17          |
| (1,788) | 1:52:A:ARG:HD2  | 1:53:A:LEU:HB3  | 1        | 0.17          |
| (1,788) | 1:52:A:ARG:HD3  | 1:53:A:LEU:HB2  | 1        | 0.17          |
| (1,788) | 1:52:A:ARG:HD3  | 1:53:A:LEU:HB3  | 1        | 0.17          |
| (1,788) | 1:52:A:ARG:HD2  | 1:53:A:LEU:HB2  | 3        | 0.17          |
| (1,788) | 1:52:A:ARG:HD2  | 1:53:A:LEU:HB3  | 3        | 0.17          |
| (1,788) | 1:52:A:ARG:HD3  | 1:53:A:LEU:HB2  | 3        | 0.17          |
| (1,788) | 1:52:A:ARG:HD3  | 1:53:A:LEU:HB3  | 3        | 0.17          |
| (1,788) | 1:52:A:ARG:HD2  | 1:53:A:LEU:HB2  | 10       | 0.17          |
| (1,788) | 1:52:A:ARG:HD2  | 1:53:A:LEU:HB3  | 10       | 0.17          |
| (1,788) | 1:52:A:ARG:HD3  | 1:53:A:LEU:HB2  | 10       | 0.17          |
| (1,788) | 1:52:A:ARG:HD3  | 1:53:A:LEU:HB3  | 10       | 0.17          |
| (1,788) | 1:52:A:ARG:HD2  | 1:53:A:LEU:HB2  | 15       | 0.17          |
| (1,788) | 1:52:A:ARG:HD2  | 1:53:A:LEU:HB3  | 15       | 0.17          |
| (1,788) | 1:52:A:ARG:HD3  | 1:53:A:LEU:HB2  | 15       | 0.17          |
| (1,788) | 1:52:A:ARG:HD3  | 1:53:A:LEU:HB3  | 15       | 0.17          |
| (1,788) | 1:52:A:ARG:HD2  | 1:53:A:LEU:HB2  | 17       | 0.17          |
| (1,788) | 1:52:A:ARG:HD2  | 1:53:A:LEU:HB3  | 17       | 0.17          |
| (1,788) | 1:52:A:ARG:HD3  | 1:53:A:LEU:HB2  | 17       | 0.17          |
| (1,788) | 1:52:A:ARG:HD3  | 1:53:A:LEU:HB3  | 17       | 0.17          |
| (1,788) | 1:52:A:ARG:HD2  | 1:53:A:LEU:HB2  | 18       | 0.17          |
| (1,788) | 1:52:A:ARG:HD2  | 1:53:A:LEU:HB3  | 18       | 0.17          |
| (1,788) | 1:52:A:ARG:HD3  | 1:53:A:LEU:HB2  | 18       | 0.17          |
| (1,788) | 1:52:A:ARG:HD3  | 1:53:A:LEU:HB3  | 18       | 0.17          |
| (1,688) | 1:25:A:ARG:HB2  | 1:68:A:SER:HB2  | 18       | 0.17          |
| (1,688) | 1:25:A:ARG:HB2  | 1:68:A:SER:HB3  | 18       | 0.17          |
| (1,688) | 1:25:A:ARG:HB3  | 1:68:A:SER:HB2  | 18       | 0.17          |
| (1,688) | 1:25:A:ARG:HB3  | 1:68:A:SER:HB3  | 18       | 0.17          |
| (1,644) | 1:10:A:ILE:HG12 | 1:14:A:ILE:HD11 | 7        | 0.17          |
| (1,644) | 1:10:A:ILE:HG12 | 1:14:A:ILE:HD12 | 7        | 0.17          |
| (1,644) | 1:10:A:ILE:HG12 | 1:14:A:ILE:HD13 | 7        | 0.17          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,644) | 1:10:A:ILE:HG13 | 1:14:A:ILE:HD11 | 7        | 0.17          |
| (1,644) | 1:10:A:ILE:HG13 | 1:14:A:ILE:HD12 | 7        | 0.17          |
| (1,644) | 1:10:A:ILE:HG13 | 1:14:A:ILE:HD13 | 7        | 0.17          |
| (1,644) | 1:10:A:ILE:HG12 | 1:14:A:ILE:HD11 | 8        | 0.17          |
| (1,644) | 1:10:A:ILE:HG12 | 1:14:A:ILE:HD12 | 8        | 0.17          |
| (1,644) | 1:10:A:ILE:HG12 | 1:14:A:ILE:HD13 | 8        | 0.17          |
| (1,644) | 1:10:A:ILE:HG13 | 1:14:A:ILE:HD11 | 8        | 0.17          |
| (1,644) | 1:10:A:ILE:HG13 | 1:14:A:ILE:HD12 | 8        | 0.17          |
| (1,644) | 1:10:A:ILE:HG13 | 1:14:A:ILE:HD13 | 8        | 0.17          |
| (1,644) | 1:10:A:ILE:HG12 | 1:14:A:ILE:HD11 | 19       | 0.17          |
| (1,644) | 1:10:A:ILE:HG12 | 1:14:A:ILE:HD12 | 19       | 0.17          |
| (1,644) | 1:10:A:ILE:HG12 | 1:14:A:ILE:HD13 | 19       | 0.17          |
| (1,644) | 1:10:A:ILE:HG13 | 1:14:A:ILE:HD11 | 19       | 0.17          |
| (1,644) | 1:10:A:ILE:HG13 | 1:14:A:ILE:HD12 | 19       | 0.17          |
| (1,644) | 1:10:A:ILE:HG13 | 1:14:A:ILE:HD13 | 19       | 0.17          |
| (1,573) | 1:32:A:ILE:HD11 | 1:36:A:TYR:HD1  | 3        | 0.17          |
| (1,573) | 1:32:A:ILE:HD11 | 1:36:A:TYR:HD2  | 3        | 0.17          |
| (1,573) | 1:32:A:ILE:HD12 | 1:36:A:TYR:HD1  | 3        | 0.17          |
| (1,573) | 1:32:A:ILE:HD12 | 1:36:A:TYR:HD2  | 3        | 0.17          |
| (1,573) | 1:32:A:ILE:HD13 | 1:36:A:TYR:HD1  | 3        | 0.17          |
| (1,573) | 1:32:A:ILE:HD13 | 1:36:A:TYR:HD2  | 3        | 0.17          |
| (1,573) | 1:32:A:ILE:HD11 | 1:36:A:TYR:HD1  | 4        | 0.17          |
| (1,573) | 1:32:A:ILE:HD11 | 1:36:A:TYR:HD2  | 4        | 0.17          |
| (1,573) | 1:32:A:ILE:HD12 | 1:36:A:TYR:HD1  | 4        | 0.17          |
| (1,573) | 1:32:A:ILE:HD12 | 1:36:A:TYR:HD2  | 4        | 0.17          |
| (1,573) | 1:32:A:ILE:HD13 | 1:36:A:TYR:HD1  | 4        | 0.17          |
| (1,573) | 1:32:A:ILE:HD13 | 1:36:A:TYR:HD2  | 4        | 0.17          |
| (1,573) | 1:32:A:ILE:HD11 | 1:36:A:TYR:HD1  | 5        | 0.17          |
| (1,573) | 1:32:A:ILE:HD11 | 1:36:A:TYR:HD2  | 5        | 0.17          |
| (1,573) | 1:32:A:ILE:HD12 | 1:36:A:TYR:HD1  | 5        | 0.17          |
| (1,573) | 1:32:A:ILE:HD12 | 1:36:A:TYR:HD2  | 5        | 0.17          |
| (1,573) | 1:32:A:ILE:HD13 | 1:36:A:TYR:HD1  | 5        | 0.17          |
| (1,573) | 1:32:A:ILE:HD13 | 1:36:A:TYR:HD2  | 5        | 0.17          |
| (1,573) | 1:32:A:ILE:HD11 | 1:36:A:TYR:HD1  | 9        | 0.17          |
| (1,573) | 1:32:A:ILE:HD11 | 1:36:A:TYR:HD2  | 9        | 0.17          |
| (1,573) | 1:32:A:ILE:HD12 | 1:36:A:TYR:HD1  | 9        | 0.17          |
| (1,573) | 1:32:A:ILE:HD12 | 1:36:A:TYR:HD2  | 9        | 0.17          |
| (1,573) | 1:32:A:ILE:HD13 | 1:36:A:TYR:HD1  | 9        | 0.17          |
| (1,573) | 1:32:A:ILE:HD13 | 1:36:A:TYR:HD2  | 9        | 0.17          |
| (1,573) | 1:32:A:ILE:HD11 | 1:36:A:TYR:HD1  | 11       | 0.17          |
| (1,573) | 1:32:A:ILE:HD11 | 1:36:A:TYR:HD2  | 11       | 0.17          |
| (1,573) | 1:32:A:ILE:HD12 | 1:36:A:TYR:HD1  | 11       | 0.17          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,573) | 1:32:A:ILE:HD12 | 1:36:A:TYR:HD2 | 11       | 0.17          |
| (1,573) | 1:32:A:ILE:HD13 | 1:36:A:TYR:HD1 | 11       | 0.17          |
| (1,573) | 1:32:A:ILE:HD13 | 1:36:A:TYR:HD2 | 11       | 0.17          |
| (1,573) | 1:32:A:ILE:HD11 | 1:36:A:TYR:HD1 | 12       | 0.17          |
| (1,573) | 1:32:A:ILE:HD11 | 1:36:A:TYR:HD2 | 12       | 0.17          |
| (1,573) | 1:32:A:ILE:HD12 | 1:36:A:TYR:HD1 | 12       | 0.17          |
| (1,573) | 1:32:A:ILE:HD12 | 1:36:A:TYR:HD2 | 12       | 0.17          |
| (1,573) | 1:32:A:ILE:HD13 | 1:36:A:TYR:HD1 | 12       | 0.17          |
| (1,573) | 1:32:A:ILE:HD13 | 1:36:A:TYR:HD2 | 12       | 0.17          |
| (1,573) | 1:32:A:ILE:HD11 | 1:36:A:TYR:HD1 | 19       | 0.17          |
| (1,573) | 1:32:A:ILE:HD11 | 1:36:A:TYR:HD2 | 19       | 0.17          |
| (1,573) | 1:32:A:ILE:HD12 | 1:36:A:TYR:HD1 | 19       | 0.17          |
| (1,573) | 1:32:A:ILE:HD12 | 1:36:A:TYR:HD2 | 19       | 0.17          |
| (1,573) | 1:32:A:ILE:HD13 | 1:36:A:TYR:HD1 | 19       | 0.17          |
| (1,573) | 1:32:A:ILE:HD13 | 1:36:A:TYR:HD2 | 19       | 0.17          |
| (1,531) | 1:61:A:GLN:H    | 1:72:A:ARG:HB2 | 8        | 0.17          |
| (1,531) | 1:61:A:GLN:H    | 1:72:A:ARG:HB3 | 8        | 0.17          |
| (1,531) | 1:61:A:GLN:H    | 1:72:A:ARG:HB2 | 14       | 0.17          |
| (1,531) | 1:61:A:GLN:H    | 1:72:A:ARG:HB3 | 14       | 0.17          |
| (1,531) | 1:61:A:GLN:H    | 1:72:A:ARG:HB2 | 17       | 0.17          |
| (1,531) | 1:61:A:GLN:H    | 1:72:A:ARG:HB3 | 17       | 0.17          |
| (1,457) | 1:61:A:GLN:H    | 1:72:A:ARG:H   | 13       | 0.17          |
| (1,457) | 1:61:A:GLN:H    | 1:72:A:ARG:H   | 14       | 0.17          |
| (1,388) | 1:63:A:LYS:HA   | 1:70:A:SER:H   | 17       | 0.17          |
| (1,388) | 1:63:A:LYS:HA   | 1:70:A:SER:H   | 18       | 0.17          |
| (1,363) | 1:55:A:THR:HG21 | 1:57:A:GLY:H   | 2        | 0.17          |
| (1,363) | 1:55:A:THR:HG22 | 1:57:A:GLY:H   | 2        | 0.17          |
| (1,363) | 1:55:A:THR:HG23 | 1:57:A:GLY:H   | 2        | 0.17          |
| (1,363) | 1:55:A:THR:HG21 | 1:57:A:GLY:H   | 11       | 0.17          |
| (1,363) | 1:55:A:THR:HG22 | 1:57:A:GLY:H   | 11       | 0.17          |
| (1,363) | 1:55:A:THR:HG23 | 1:57:A:GLY:H   | 11       | 0.17          |
| (1,363) | 1:55:A:THR:HG21 | 1:57:A:GLY:H   | 14       | 0.17          |
| (1,363) | 1:55:A:THR:HG22 | 1:57:A:GLY:H   | 14       | 0.17          |
| (1,363) | 1:55:A:THR:HG23 | 1:57:A:GLY:H   | 14       | 0.17          |
| (1,363) | 1:55:A:THR:HG21 | 1:57:A:GLY:H   | 16       | 0.17          |
| (1,363) | 1:55:A:THR:HG22 | 1:57:A:GLY:H   | 16       | 0.17          |
| (1,363) | 1:55:A:THR:HG23 | 1:57:A:GLY:H   | 16       | 0.17          |
| (1,363) | 1:55:A:THR:HG21 | 1:57:A:GLY:H   | 19       | 0.17          |
| (1,363) | 1:55:A:THR:HG22 | 1:57:A:GLY:H   | 19       | 0.17          |
| (1,363) | 1:55:A:THR:HG23 | 1:57:A:GLY:H   | 19       | 0.17          |
| (1,322) | 1:15:A:GLN:HA   | 1:18:A:LYS:H   | 19       | 0.17          |
| (1,262) | 1:14:A:ILE:HD11 | 1:71:A:PHE:HA  | 1        | 0.17          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,262) | 1:14:A:ILE:HD12 | 1:71:A:PHE:HA  | 1        | 0.17          |
| (1,262) | 1:14:A:ILE:HD13 | 1:71:A:PHE:HA  | 1        | 0.17          |
| (1,262) | 1:14:A:ILE:HD11 | 1:71:A:PHE:HA  | 19       | 0.17          |
| (1,262) | 1:14:A:ILE:HD12 | 1:71:A:PHE:HA  | 19       | 0.17          |
| (1,262) | 1:14:A:ILE:HD13 | 1:71:A:PHE:HA  | 19       | 0.17          |
| (1,13)  | 1:60:A:LYS:HA   | 1:72:A:ARG:HB2 | 4        | 0.17          |
| (1,13)  | 1:60:A:LYS:HA   | 1:72:A:ARG:HB3 | 4        | 0.17          |
| (1,8)   | 1:60:A:LYS:HB2  | 1:74:A:ALA:HB1 | 9        | 0.17          |
| (1,8)   | 1:60:A:LYS:HB2  | 1:74:A:ALA:HB2 | 9        | 0.17          |
| (1,8)   | 1:60:A:LYS:HB2  | 1:74:A:ALA:HB3 | 9        | 0.17          |
| (1,8)   | 1:60:A:LYS:HB3  | 1:74:A:ALA:HB1 | 9        | 0.17          |
| (1,8)   | 1:60:A:LYS:HB3  | 1:74:A:ALA:HB2 | 9        | 0.17          |
| (1,8)   | 1:60:A:LYS:HB3  | 1:74:A:ALA:HB3 | 9        | 0.17          |
| (1,8)   | 1:60:A:LYS:HB2  | 1:74:A:ALA:HB1 | 14       | 0.17          |
| (1,8)   | 1:60:A:LYS:HB2  | 1:74:A:ALA:HB2 | 14       | 0.17          |
| (1,8)   | 1:60:A:LYS:HB2  | 1:74:A:ALA:HB3 | 14       | 0.17          |
| (1,8)   | 1:60:A:LYS:HB3  | 1:74:A:ALA:HB1 | 14       | 0.17          |
| (1,8)   | 1:60:A:LYS:HB3  | 1:74:A:ALA:HB2 | 14       | 0.17          |
| (1,8)   | 1:60:A:LYS:HB3  | 1:74:A:ALA:HB3 | 14       | 0.17          |
| (1,4)   | 1:14:A:ILE:HD11 | 1:28:A:ILE:HB  | 1        | 0.17          |
| (1,4)   | 1:14:A:ILE:HD12 | 1:28:A:ILE:HB  | 1        | 0.17          |
| (1,4)   | 1:14:A:ILE:HD13 | 1:28:A:ILE:HB  | 1        | 0.17          |
| (1,4)   | 1:14:A:ILE:HD11 | 1:28:A:ILE:HB  | 5        | 0.17          |
| (1,4)   | 1:14:A:ILE:HD12 | 1:28:A:ILE:HB  | 5        | 0.17          |
| (1,4)   | 1:14:A:ILE:HD13 | 1:28:A:ILE:HB  | 5        | 0.17          |
| (1,4)   | 1:14:A:ILE:HD11 | 1:28:A:ILE:HB  | 8        | 0.17          |
| (1,4)   | 1:14:A:ILE:HD12 | 1:28:A:ILE:HB  | 8        | 0.17          |
| (1,4)   | 1:14:A:ILE:HD13 | 1:28:A:ILE:HB  | 8        | 0.17          |
| (1,4)   | 1:14:A:ILE:HD11 | 1:28:A:ILE:HB  | 18       | 0.17          |
| (1,4)   | 1:14:A:ILE:HD12 | 1:28:A:ILE:HB  | 18       | 0.17          |
| (1,4)   | 1:14:A:ILE:HD13 | 1:28:A:ILE:HB  | 18       | 0.17          |
| (1,819) | 1:63:A:LYS:HB2  | 1:70:A:SER:H   | 4        | 0.16          |
| (1,819) | 1:63:A:LYS:HB3  | 1:70:A:SER:H   | 4        | 0.16          |
| (1,819) | 1:63:A:LYS:HB2  | 1:70:A:SER:H   | 18       | 0.16          |
| (1,819) | 1:63:A:LYS:HB3  | 1:70:A:SER:H   | 18       | 0.16          |
| (1,788) | 1:52:A:ARG:HD2  | 1:53:A:LEU:HB2 | 4        | 0.16          |
| (1,788) | 1:52:A:ARG:HD2  | 1:53:A:LEU:HB3 | 4        | 0.16          |
| (1,788) | 1:52:A:ARG:HD3  | 1:53:A:LEU:HB2 | 4        | 0.16          |
| (1,788) | 1:52:A:ARG:HD3  | 1:53:A:LEU:HB3 | 4        | 0.16          |
| (1,788) | 1:52:A:ARG:HD2  | 1:53:A:LEU:HB2 | 5        | 0.16          |
| (1,788) | 1:52:A:ARG:HD2  | 1:53:A:LEU:HB3 | 5        | 0.16          |
| (1,788) | 1:52:A:ARG:HD3  | 1:53:A:LEU:HB2 | 5        | 0.16          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,788) | 1:52:A:ARG:HD3  | 1:53:A:LEU:HB3  | 5        | 0.16          |
| (1,788) | 1:52:A:ARG:HD2  | 1:53:A:LEU:HB2  | 11       | 0.16          |
| (1,788) | 1:52:A:ARG:HD2  | 1:53:A:LEU:HB3  | 11       | 0.16          |
| (1,788) | 1:52:A:ARG:HD3  | 1:53:A:LEU:HB2  | 11       | 0.16          |
| (1,788) | 1:52:A:ARG:HD3  | 1:53:A:LEU:HB3  | 11       | 0.16          |
| (1,788) | 1:52:A:ARG:HD2  | 1:53:A:LEU:HB2  | 13       | 0.16          |
| (1,788) | 1:52:A:ARG:HD2  | 1:53:A:LEU:HB3  | 13       | 0.16          |
| (1,788) | 1:52:A:ARG:HD3  | 1:53:A:LEU:HB2  | 13       | 0.16          |
| (1,788) | 1:52:A:ARG:HD3  | 1:53:A:LEU:HB3  | 13       | 0.16          |
| (1,788) | 1:52:A:ARG:HD2  | 1:53:A:LEU:HB2  | 14       | 0.16          |
| (1,788) | 1:52:A:ARG:HD2  | 1:53:A:LEU:HB3  | 14       | 0.16          |
| (1,788) | 1:52:A:ARG:HD3  | 1:53:A:LEU:HB2  | 14       | 0.16          |
| (1,788) | 1:52:A:ARG:HD3  | 1:53:A:LEU:HB3  | 14       | 0.16          |
| (1,788) | 1:52:A:ARG:HD2  | 1:53:A:LEU:HB2  | 16       | 0.16          |
| (1,788) | 1:52:A:ARG:HD2  | 1:53:A:LEU:HB3  | 16       | 0.16          |
| (1,788) | 1:52:A:ARG:HD3  | 1:53:A:LEU:HB2  | 16       | 0.16          |
| (1,788) | 1:52:A:ARG:HD3  | 1:53:A:LEU:HB3  | 16       | 0.16          |
| (1,788) | 1:52:A:ARG:HD2  | 1:53:A:LEU:HB2  | 19       | 0.16          |
| (1,788) | 1:52:A:ARG:HD2  | 1:53:A:LEU:HB3  | 19       | 0.16          |
| (1,788) | 1:52:A:ARG:HD3  | 1:53:A:LEU:HB2  | 19       | 0.16          |
| (1,788) | 1:52:A:ARG:HD3  | 1:53:A:LEU:HB3  | 19       | 0.16          |
| (1,644) | 1:10:A:ILE:HG12 | 1:14:A:ILE:HD11 | 6        | 0.16          |
| (1,644) | 1:10:A:ILE:HG12 | 1:14:A:ILE:HD12 | 6        | 0.16          |
| (1,644) | 1:10:A:ILE:HG12 | 1:14:A:ILE:HD13 | 6        | 0.16          |
| (1,644) | 1:10:A:ILE:HG13 | 1:14:A:ILE:HD11 | 6        | 0.16          |
| (1,644) | 1:10:A:ILE:HG13 | 1:14:A:ILE:HD12 | 6        | 0.16          |
| (1,644) | 1:10:A:ILE:HG13 | 1:14:A:ILE:HD13 | 6        | 0.16          |
| (1,644) | 1:10:A:ILE:HG12 | 1:14:A:ILE:HD11 | 20       | 0.16          |
| (1,644) | 1:10:A:ILE:HG12 | 1:14:A:ILE:HD12 | 20       | 0.16          |
| (1,644) | 1:10:A:ILE:HG12 | 1:14:A:ILE:HD13 | 20       | 0.16          |
| (1,644) | 1:10:A:ILE:HG13 | 1:14:A:ILE:HD11 | 20       | 0.16          |
| (1,644) | 1:10:A:ILE:HG13 | 1:14:A:ILE:HD12 | 20       | 0.16          |
| (1,644) | 1:10:A:ILE:HG13 | 1:14:A:ILE:HD13 | 20       | 0.16          |
| (1,636) | 1:9:A:MET:HA    | 1:11:A:VAL:HG11 | 11       | 0.16          |
| (1,636) | 1:9:A:MET:HA    | 1:11:A:VAL:HG12 | 11       | 0.16          |
| (1,636) | 1:9:A:MET:HA    | 1:11:A:VAL:HG13 | 11       | 0.16          |
| (1,636) | 1:9:A:MET:HA    | 1:11:A:VAL:HG21 | 11       | 0.16          |
| (1,636) | 1:9:A:MET:HA    | 1:11:A:VAL:HG22 | 11       | 0.16          |
| (1,636) | 1:9:A:MET:HA    | 1:11:A:VAL:HG23 | 11       | 0.16          |
| (1,628) | 1:7:A:SER:HB2   | 1:10:A:ILE:HG21 | 10       | 0.16          |
| (1,628) | 1:7:A:SER:HB2   | 1:10:A:ILE:HG22 | 10       | 0.16          |
| (1,628) | 1:7:A:SER:HB2   | 1:10:A:ILE:HG23 | 10       | 0.16          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,628) | 1:7:A:SER:HB3   | 1:10:A:ILE:HG21 | 10       | 0.16          |
| (1,628) | 1:7:A:SER:HB3   | 1:10:A:ILE:HG22 | 10       | 0.16          |
| (1,628) | 1:7:A:SER:HB3   | 1:10:A:ILE:HG23 | 10       | 0.16          |
| (1,573) | 1:32:A:ILE:HD11 | 1:36:A:TYR:HD1  | 1        | 0.16          |
| (1,573) | 1:32:A:ILE:HD11 | 1:36:A:TYR:HD2  | 1        | 0.16          |
| (1,573) | 1:32:A:ILE:HD12 | 1:36:A:TYR:HD1  | 1        | 0.16          |
| (1,573) | 1:32:A:ILE:HD12 | 1:36:A:TYR:HD2  | 1        | 0.16          |
| (1,573) | 1:32:A:ILE:HD13 | 1:36:A:TYR:HD1  | 1        | 0.16          |
| (1,573) | 1:32:A:ILE:HD13 | 1:36:A:TYR:HD2  | 1        | 0.16          |
| (1,573) | 1:32:A:ILE:HD11 | 1:36:A:TYR:HD1  | 2        | 0.16          |
| (1,573) | 1:32:A:ILE:HD11 | 1:36:A:TYR:HD2  | 2        | 0.16          |
| (1,573) | 1:32:A:ILE:HD12 | 1:36:A:TYR:HD1  | 2        | 0.16          |
| (1,573) | 1:32:A:ILE:HD12 | 1:36:A:TYR:HD2  | 2        | 0.16          |
| (1,573) | 1:32:A:ILE:HD13 | 1:36:A:TYR:HD1  | 2        | 0.16          |
| (1,573) | 1:32:A:ILE:HD13 | 1:36:A:TYR:HD2  | 2        | 0.16          |
| (1,531) | 1:61:A:GLN:H    | 1:72:A:ARG:HB2  | 7        | 0.16          |
| (1,531) | 1:61:A:GLN:H    | 1:72:A:ARG:HB3  | 7        | 0.16          |
| (1,531) | 1:61:A:GLN:H    | 1:72:A:ARG:HB2  | 12       | 0.16          |
| (1,531) | 1:61:A:GLN:H    | 1:72:A:ARG:HB3  | 12       | 0.16          |
| (1,531) | 1:61:A:GLN:H    | 1:72:A:ARG:HB2  | 19       | 0.16          |
| (1,531) | 1:61:A:GLN:H    | 1:72:A:ARG:HB3  | 19       | 0.16          |
| (1,457) | 1:61:A:GLN:H    | 1:72:A:ARG:H    | 6        | 0.16          |
| (1,457) | 1:61:A:GLN:H    | 1:72:A:ARG:H    | 12       | 0.16          |
| (1,388) | 1:63:A:LYS:HA   | 1:70:A:SER:H    | 4        | 0.16          |
| (1,363) | 1:55:A:THR:HG21 | 1:57:A:GLY:H    | 3        | 0.16          |
| (1,363) | 1:55:A:THR:HG22 | 1:57:A:GLY:H    | 3        | 0.16          |
| (1,363) | 1:55:A:THR:HG23 | 1:57:A:GLY:H    | 3        | 0.16          |
| (1,363) | 1:55:A:THR:HG21 | 1:57:A:GLY:H    | 10       | 0.16          |
| (1,363) | 1:55:A:THR:HG22 | 1:57:A:GLY:H    | 10       | 0.16          |
| (1,363) | 1:55:A:THR:HG23 | 1:57:A:GLY:H    | 10       | 0.16          |
| (1,290) | 1:6:A:TYR:HE1   | 1:10:A:ILE:HD11 | 7        | 0.16          |
| (1,290) | 1:6:A:TYR:HE1   | 1:10:A:ILE:HD12 | 7        | 0.16          |
| (1,290) | 1:6:A:TYR:HE1   | 1:10:A:ILE:HD13 | 7        | 0.16          |
| (1,290) | 1:6:A:TYR:HE2   | 1:10:A:ILE:HD11 | 7        | 0.16          |
| (1,290) | 1:6:A:TYR:HE2   | 1:10:A:ILE:HD12 | 7        | 0.16          |
| (1,290) | 1:6:A:TYR:HE2   | 1:10:A:ILE:HD13 | 7        | 0.16          |
| (1,290) | 1:6:A:TYR:HE1   | 1:10:A:ILE:HD11 | 19       | 0.16          |
| (1,290) | 1:6:A:TYR:HE1   | 1:10:A:ILE:HD12 | 19       | 0.16          |
| (1,290) | 1:6:A:TYR:HE1   | 1:10:A:ILE:HD13 | 19       | 0.16          |
| (1,290) | 1:6:A:TYR:HE2   | 1:10:A:ILE:HD11 | 19       | 0.16          |
| (1,290) | 1:6:A:TYR:HE2   | 1:10:A:ILE:HD12 | 19       | 0.16          |
| (1,290) | 1:6:A:TYR:HE2   | 1:10:A:ILE:HD13 | 19       | 0.16          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,230) | 1:11:A:VAL:HA   | 1:14:A:ILE:HD11 | 12       | 0.16          |
| (1,230) | 1:11:A:VAL:HA   | 1:14:A:ILE:HD12 | 12       | 0.16          |
| (1,230) | 1:11:A:VAL:HA   | 1:14:A:ILE:HD13 | 12       | 0.16          |
| (1,230) | 1:11:A:VAL:HA   | 1:14:A:ILE:HD11 | 13       | 0.16          |
| (1,230) | 1:11:A:VAL:HA   | 1:14:A:ILE:HD12 | 13       | 0.16          |
| (1,230) | 1:11:A:VAL:HA   | 1:14:A:ILE:HD13 | 13       | 0.16          |
| (1,38)  | 1:12:A:ALA:HB1  | 1:32:A:ILE:HG21 | 6        | 0.16          |
| (1,38)  | 1:12:A:ALA:HB1  | 1:32:A:ILE:HG22 | 6        | 0.16          |
| (1,38)  | 1:12:A:ALA:HB1  | 1:32:A:ILE:HG23 | 6        | 0.16          |
| (1,38)  | 1:12:A:ALA:HB2  | 1:32:A:ILE:HG21 | 6        | 0.16          |
| (1,38)  | 1:12:A:ALA:HB2  | 1:32:A:ILE:HG22 | 6        | 0.16          |
| (1,38)  | 1:12:A:ALA:HB2  | 1:32:A:ILE:HG23 | 6        | 0.16          |
| (1,38)  | 1:12:A:ALA:HB3  | 1:32:A:ILE:HG21 | 6        | 0.16          |
| (1,38)  | 1:12:A:ALA:HB3  | 1:32:A:ILE:HG22 | 6        | 0.16          |
| (1,38)  | 1:12:A:ALA:HB3  | 1:32:A:ILE:HG23 | 6        | 0.16          |
| (1,8)   | 1:60:A:LYS:HB2  | 1:74:A:ALA:HB1  | 2        | 0.16          |
| (1,8)   | 1:60:A:LYS:HB2  | 1:74:A:ALA:HB2  | 2        | 0.16          |
| (1,8)   | 1:60:A:LYS:HB2  | 1:74:A:ALA:HB3  | 2        | 0.16          |
| (1,8)   | 1:60:A:LYS:HB3  | 1:74:A:ALA:HB1  | 2        | 0.16          |
| (1,8)   | 1:60:A:LYS:HB3  | 1:74:A:ALA:HB2  | 2        | 0.16          |
| (1,8)   | 1:60:A:LYS:HB3  | 1:74:A:ALA:HB3  | 2        | 0.16          |
| (1,8)   | 1:60:A:LYS:HB2  | 1:74:A:ALA:HB1  | 8        | 0.16          |
| (1,8)   | 1:60:A:LYS:HB2  | 1:74:A:ALA:HB2  | 8        | 0.16          |
| (1,8)   | 1:60:A:LYS:HB2  | 1:74:A:ALA:HB3  | 8        | 0.16          |
| (1,8)   | 1:60:A:LYS:HB3  | 1:74:A:ALA:HB1  | 8        | 0.16          |
| (1,8)   | 1:60:A:LYS:HB3  | 1:74:A:ALA:HB2  | 8        | 0.16          |
| (1,8)   | 1:60:A:LYS:HB3  | 1:74:A:ALA:HB3  | 8        | 0.16          |
| (1,4)   | 1:14:A:ILE:HD11 | 1:28:A:ILE:HB   | 2        | 0.16          |
| (1,4)   | 1:14:A:ILE:HD12 | 1:28:A:ILE:HB   | 2        | 0.16          |
| (1,4)   | 1:14:A:ILE:HD13 | 1:28:A:ILE:HB   | 2        | 0.16          |
| (1,4)   | 1:14:A:ILE:HD11 | 1:28:A:ILE:HB   | 19       | 0.16          |
| (1,4)   | 1:14:A:ILE:HD12 | 1:28:A:ILE:HB   | 19       | 0.16          |
| (1,4)   | 1:14:A:ILE:HD13 | 1:28:A:ILE:HB   | 19       | 0.16          |
| (1,844) | 1:75:A:LYS:H    | 1:75:A:LYS:HB2  | 13       | 0.15          |
| (1,844) | 1:75:A:LYS:H    | 1:75:A:LYS:HB3  | 13       | 0.15          |
| (1,803) | 1:60:A:LYS:HD2  | 1:74:A:ALA:H    | 5        | 0.15          |
| (1,803) | 1:60:A:LYS:HD3  | 1:74:A:ALA:H    | 5        | 0.15          |
| (1,803) | 1:60:A:LYS:HD2  | 1:74:A:ALA:H    | 6        | 0.15          |
| (1,803) | 1:60:A:LYS:HD3  | 1:74:A:ALA:H    | 6        | 0.15          |
| (1,803) | 1:60:A:LYS:HD2  | 1:74:A:ALA:H    | 16       | 0.15          |
| (1,803) | 1:60:A:LYS:HD3  | 1:74:A:ALA:H    | 16       | 0.15          |
| (1,774) | 1:49:A:SER:HB2  | 1:50:A:ILE:HB   | 9        | 0.15          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,774) | 1:49:A:SER:HB3  | 1:50:A:ILE:HB   | 9        | 0.15          |
| (1,764) | 1:47:A:LYS:HB2  | 1:48:A:LEU:H    | 2        | 0.15          |
| (1,764) | 1:47:A:LYS:HB3  | 1:48:A:LEU:H    | 2        | 0.15          |
| (1,709) | 1:29:A:GLN:HE21 | 1:43:A:ASP:HA   | 18       | 0.15          |
| (1,709) | 1:29:A:GLN:HE22 | 1:43:A:ASP:HA   | 18       | 0.15          |
| (1,644) | 1:10:A:ILE:HG12 | 1:14:A:ILE:HD11 | 2        | 0.15          |
| (1,644) | 1:10:A:ILE:HG12 | 1:14:A:ILE:HD12 | 2        | 0.15          |
| (1,644) | 1:10:A:ILE:HG12 | 1:14:A:ILE:HD13 | 2        | 0.15          |
| (1,644) | 1:10:A:ILE:HG13 | 1:14:A:ILE:HD11 | 2        | 0.15          |
| (1,644) | 1:10:A:ILE:HG13 | 1:14:A:ILE:HD12 | 2        | 0.15          |
| (1,644) | 1:10:A:ILE:HG13 | 1:14:A:ILE:HD13 | 2        | 0.15          |
| (1,644) | 1:10:A:ILE:HG12 | 1:14:A:ILE:HD11 | 17       | 0.15          |
| (1,644) | 1:10:A:ILE:HG12 | 1:14:A:ILE:HD12 | 17       | 0.15          |
| (1,644) | 1:10:A:ILE:HG12 | 1:14:A:ILE:HD13 | 17       | 0.15          |
| (1,644) | 1:10:A:ILE:HG13 | 1:14:A:ILE:HD11 | 17       | 0.15          |
| (1,644) | 1:10:A:ILE:HG13 | 1:14:A:ILE:HD12 | 17       | 0.15          |
| (1,644) | 1:10:A:ILE:HG13 | 1:14:A:ILE:HD13 | 17       | 0.15          |
| (1,628) | 1:7:A:SER:HB2   | 1:10:A:ILE:HG21 | 2        | 0.15          |
| (1,628) | 1:7:A:SER:HB2   | 1:10:A:ILE:HG22 | 2        | 0.15          |
| (1,628) | 1:7:A:SER:HB2   | 1:10:A:ILE:HG23 | 2        | 0.15          |
| (1,628) | 1:7:A:SER:HB3   | 1:10:A:ILE:HG21 | 2        | 0.15          |
| (1,628) | 1:7:A:SER:HB3   | 1:10:A:ILE:HG22 | 2        | 0.15          |
| (1,628) | 1:7:A:SER:HB3   | 1:10:A:ILE:HG23 | 2        | 0.15          |
| (1,573) | 1:32:A:ILE:HD11 | 1:36:A:TYR:HD1  | 7        | 0.15          |
| (1,573) | 1:32:A:ILE:HD11 | 1:36:A:TYR:HD2  | 7        | 0.15          |
| (1,573) | 1:32:A:ILE:HD12 | 1:36:A:TYR:HD1  | 7        | 0.15          |
| (1,573) | 1:32:A:ILE:HD12 | 1:36:A:TYR:HD2  | 7        | 0.15          |
| (1,573) | 1:32:A:ILE:HD13 | 1:36:A:TYR:HD1  | 7        | 0.15          |
| (1,573) | 1:32:A:ILE:HD13 | 1:36:A:TYR:HD2  | 7        | 0.15          |
| (1,573) | 1:32:A:ILE:HD11 | 1:36:A:TYR:HD1  | 10       | 0.15          |
| (1,573) | 1:32:A:ILE:HD11 | 1:36:A:TYR:HD2  | 10       | 0.15          |
| (1,573) | 1:32:A:ILE:HD12 | 1:36:A:TYR:HD1  | 10       | 0.15          |
| (1,573) | 1:32:A:ILE:HD12 | 1:36:A:TYR:HD2  | 10       | 0.15          |
| (1,573) | 1:32:A:ILE:HD13 | 1:36:A:TYR:HD1  | 10       | 0.15          |
| (1,573) | 1:32:A:ILE:HD13 | 1:36:A:TYR:HD2  | 10       | 0.15          |
| (1,573) | 1:32:A:ILE:HD11 | 1:36:A:TYR:HD1  | 13       | 0.15          |
| (1,573) | 1:32:A:ILE:HD11 | 1:36:A:TYR:HD2  | 13       | 0.15          |
| (1,573) | 1:32:A:ILE:HD12 | 1:36:A:TYR:HD1  | 13       | 0.15          |
| (1,573) | 1:32:A:ILE:HD12 | 1:36:A:TYR:HD2  | 13       | 0.15          |
| (1,573) | 1:32:A:ILE:HD13 | 1:36:A:TYR:HD1  | 13       | 0.15          |
| (1,573) | 1:32:A:ILE:HD13 | 1:36:A:TYR:HD2  | 13       | 0.15          |
| (1,573) | 1:32:A:ILE:HD11 | 1:36:A:TYR:HD1  | 15       | 0.15          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,573) | 1:32:A:ILE:HD11 | 1:36:A:TYR:HD2  | 15       | 0.15          |
| (1,573) | 1:32:A:ILE:HD12 | 1:36:A:TYR:HD1  | 15       | 0.15          |
| (1,573) | 1:32:A:ILE:HD12 | 1:36:A:TYR:HD2  | 15       | 0.15          |
| (1,573) | 1:32:A:ILE:HD13 | 1:36:A:TYR:HD1  | 15       | 0.15          |
| (1,573) | 1:32:A:ILE:HD13 | 1:36:A:TYR:HD2  | 15       | 0.15          |
| (1,573) | 1:32:A:ILE:HD11 | 1:36:A:TYR:HD1  | 16       | 0.15          |
| (1,573) | 1:32:A:ILE:HD11 | 1:36:A:TYR:HD2  | 16       | 0.15          |
| (1,573) | 1:32:A:ILE:HD12 | 1:36:A:TYR:HD1  | 16       | 0.15          |
| (1,573) | 1:32:A:ILE:HD12 | 1:36:A:TYR:HD2  | 16       | 0.15          |
| (1,573) | 1:32:A:ILE:HD13 | 1:36:A:TYR:HD1  | 16       | 0.15          |
| (1,573) | 1:32:A:ILE:HD13 | 1:36:A:TYR:HD2  | 16       | 0.15          |
| (1,573) | 1:32:A:ILE:HD11 | 1:36:A:TYR:HD1  | 17       | 0.15          |
| (1,573) | 1:32:A:ILE:HD11 | 1:36:A:TYR:HD2  | 17       | 0.15          |
| (1,573) | 1:32:A:ILE:HD12 | 1:36:A:TYR:HD1  | 17       | 0.15          |
| (1,573) | 1:32:A:ILE:HD12 | 1:36:A:TYR:HD2  | 17       | 0.15          |
| (1,573) | 1:32:A:ILE:HD13 | 1:36:A:TYR:HD1  | 17       | 0.15          |
| (1,573) | 1:32:A:ILE:HD13 | 1:36:A:TYR:HD2  | 17       | 0.15          |
| (1,457) | 1:61:A:GLN:H    | 1:72:A:ARG:H    | 1        | 0.15          |
| (1,457) | 1:61:A:GLN:H    | 1:72:A:ARG:H    | 8        | 0.15          |
| (1,457) | 1:61:A:GLN:H    | 1:72:A:ARG:H    | 17       | 0.15          |
| (1,398) | 1:46:A:ILE:HG21 | 1:51:A:LYS:H    | 2        | 0.15          |
| (1,398) | 1:46:A:ILE:HG22 | 1:51:A:LYS:H    | 2        | 0.15          |
| (1,398) | 1:46:A:ILE:HG23 | 1:51:A:LYS:H    | 2        | 0.15          |
| (1,388) | 1:63:A:LYS:HA   | 1:70:A:SER:H    | 1        | 0.15          |
| (1,388) | 1:63:A:LYS:HA   | 1:70:A:SER:H    | 6        | 0.15          |
| (1,388) | 1:63:A:LYS:HA   | 1:70:A:SER:H    | 19       | 0.15          |
| (1,290) | 1:6:A:TYR:HE1   | 1:10:A:ILE:HD11 | 8        | 0.15          |
| (1,290) | 1:6:A:TYR:HE1   | 1:10:A:ILE:HD12 | 8        | 0.15          |
| (1,290) | 1:6:A:TYR:HE1   | 1:10:A:ILE:HD13 | 8        | 0.15          |
| (1,290) | 1:6:A:TYR:HE2   | 1:10:A:ILE:HD11 | 8        | 0.15          |
| (1,290) | 1:6:A:TYR:HE2   | 1:10:A:ILE:HD12 | 8        | 0.15          |
| (1,290) | 1:6:A:TYR:HE2   | 1:10:A:ILE:HD13 | 8        | 0.15          |
| (1,290) | 1:6:A:TYR:HE1   | 1:10:A:ILE:HD11 | 15       | 0.15          |
| (1,290) | 1:6:A:TYR:HE1   | 1:10:A:ILE:HD12 | 15       | 0.15          |
| (1,290) | 1:6:A:TYR:HE1   | 1:10:A:ILE:HD13 | 15       | 0.15          |
| (1,290) | 1:6:A:TYR:HE2   | 1:10:A:ILE:HD11 | 15       | 0.15          |
| (1,290) | 1:6:A:TYR:HE2   | 1:10:A:ILE:HD12 | 15       | 0.15          |
| (1,290) | 1:6:A:TYR:HE2   | 1:10:A:ILE:HD13 | 15       | 0.15          |
| (1,274) | 1:52:A:ARG:HA   | 1:55:A:THR:HG21 | 4        | 0.15          |
| (1,274) | 1:52:A:ARG:HA   | 1:55:A:THR:HG22 | 4        | 0.15          |
| (1,274) | 1:52:A:ARG:HA   | 1:55:A:THR:HG23 | 4        | 0.15          |
| (1,274) | 1:52:A:ARG:HA   | 1:55:A:THR:HG21 | 7        | 0.15          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,274) | 1:52:A:ARG:HA   | 1:55:A:THR:HG22 | 7        | 0.15          |
| (1,274) | 1:52:A:ARG:HA   | 1:55:A:THR:HG23 | 7        | 0.15          |
| (1,262) | 1:14:A:ILE:HD11 | 1:71:A:PHE:HA   | 2        | 0.15          |
| (1,262) | 1:14:A:ILE:HD12 | 1:71:A:PHE:HA   | 2        | 0.15          |
| (1,262) | 1:14:A:ILE:HD13 | 1:71:A:PHE:HA   | 2        | 0.15          |
| (1,262) | 1:14:A:ILE:HD11 | 1:71:A:PHE:HA   | 7        | 0.15          |
| (1,262) | 1:14:A:ILE:HD12 | 1:71:A:PHE:HA   | 7        | 0.15          |
| (1,262) | 1:14:A:ILE:HD13 | 1:71:A:PHE:HA   | 7        | 0.15          |
| (1,262) | 1:14:A:ILE:HD11 | 1:71:A:PHE:HA   | 14       | 0.15          |
| (1,262) | 1:14:A:ILE:HD12 | 1:71:A:PHE:HA   | 14       | 0.15          |
| (1,262) | 1:14:A:ILE:HD13 | 1:71:A:PHE:HA   | 14       | 0.15          |
| (1,230) | 1:11:A:VAL:HA   | 1:14:A:ILE:HD11 | 4        | 0.15          |
| (1,230) | 1:11:A:VAL:HA   | 1:14:A:ILE:HD12 | 4        | 0.15          |
| (1,230) | 1:11:A:VAL:HA   | 1:14:A:ILE:HD13 | 4        | 0.15          |
| (1,8)   | 1:60:A:LYS:HB2  | 1:74:A:ALA:HB1  | 12       | 0.15          |
| (1,8)   | 1:60:A:LYS:HB2  | 1:74:A:ALA:HB2  | 12       | 0.15          |
| (1,8)   | 1:60:A:LYS:HB2  | 1:74:A:ALA:HB3  | 12       | 0.15          |
| (1,8)   | 1:60:A:LYS:HB3  | 1:74:A:ALA:HB1  | 12       | 0.15          |
| (1,8)   | 1:60:A:LYS:HB3  | 1:74:A:ALA:HB2  | 12       | 0.15          |
| (1,8)   | 1:60:A:LYS:HB3  | 1:74:A:ALA:HB3  | 12       | 0.15          |
| (1,803) | 1:60:A:LYS:HD2  | 1:74:A:ALA:H    | 4        | 0.14          |
| (1,803) | 1:60:A:LYS:HD3  | 1:74:A:ALA:H    | 4        | 0.14          |
| (1,694) | 1:26:A:GLN:HG2  | 1:27:A:SER:H    | 11       | 0.14          |
| (1,694) | 1:26:A:GLN:HG3  | 1:27:A:SER:H    | 11       | 0.14          |
| (1,668) | 1:17:A:GLU:HG2  | 1:19:A:ASN:H    | 12       | 0.14          |
| (1,668) | 1:17:A:GLU:HG3  | 1:19:A:ASN:H    | 12       | 0.14          |
| (1,668) | 1:17:A:GLU:HG2  | 1:19:A:ASN:H    | 19       | 0.14          |
| (1,668) | 1:17:A:GLU:HG3  | 1:19:A:ASN:H    | 19       | 0.14          |
| (1,644) | 1:10:A:ILE:HG12 | 1:14:A:ILE:HD11 | 14       | 0.14          |
| (1,644) | 1:10:A:ILE:HG12 | 1:14:A:ILE:HD12 | 14       | 0.14          |
| (1,644) | 1:10:A:ILE:HG12 | 1:14:A:ILE:HD13 | 14       | 0.14          |
| (1,644) | 1:10:A:ILE:HG13 | 1:14:A:ILE:HD11 | 14       | 0.14          |
| (1,644) | 1:10:A:ILE:HG13 | 1:14:A:ILE:HD12 | 14       | 0.14          |
| (1,644) | 1:10:A:ILE:HG13 | 1:14:A:ILE:HD13 | 14       | 0.14          |
| (1,636) | 1:9:A:MET:HA    | 1:11:A:VAL:HG11 | 6        | 0.14          |
| (1,636) | 1:9:A:MET:HA    | 1:11:A:VAL:HG12 | 6        | 0.14          |
| (1,636) | 1:9:A:MET:HA    | 1:11:A:VAL:HG13 | 6        | 0.14          |
| (1,636) | 1:9:A:MET:HA    | 1:11:A:VAL:HG21 | 6        | 0.14          |
| (1,636) | 1:9:A:MET:HA    | 1:11:A:VAL:HG22 | 6        | 0.14          |
| (1,636) | 1:9:A:MET:HA    | 1:11:A:VAL:HG23 | 6        | 0.14          |
| (1,575) | 1:12:A:ALA:HB1  | 1:36:A:TYR:HD1  | 8        | 0.14          |
| (1,575) | 1:12:A:ALA:HB1  | 1:36:A:TYR:HD2  | 8        | 0.14          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,575) | 1:12:A:ALA:HB2  | 1:36:A:TYR:HD1  | 8        | 0.14          |
| (1,575) | 1:12:A:ALA:HB2  | 1:36:A:TYR:HD2  | 8        | 0.14          |
| (1,575) | 1:12:A:ALA:HB3  | 1:36:A:TYR:HD1  | 8        | 0.14          |
| (1,575) | 1:12:A:ALA:HB3  | 1:36:A:TYR:HD2  | 8        | 0.14          |
| (1,573) | 1:32:A:ILE:HD11 | 1:36:A:TYR:HD1  | 8        | 0.14          |
| (1,573) | 1:32:A:ILE:HD11 | 1:36:A:TYR:HD2  | 8        | 0.14          |
| (1,573) | 1:32:A:ILE:HD12 | 1:36:A:TYR:HD1  | 8        | 0.14          |
| (1,573) | 1:32:A:ILE:HD12 | 1:36:A:TYR:HD2  | 8        | 0.14          |
| (1,573) | 1:32:A:ILE:HD13 | 1:36:A:TYR:HD1  | 8        | 0.14          |
| (1,573) | 1:32:A:ILE:HD13 | 1:36:A:TYR:HD2  | 8        | 0.14          |
| (1,531) | 1:61:A:GLN:H    | 1:72:A:ARG:HB2  | 2        | 0.14          |
| (1,531) | 1:61:A:GLN:H    | 1:72:A:ARG:HB3  | 2        | 0.14          |
| (1,531) | 1:61:A:GLN:H    | 1:72:A:ARG:HB2  | 10       | 0.14          |
| (1,531) | 1:61:A:GLN:H    | 1:72:A:ARG:HB3  | 10       | 0.14          |
| (1,531) | 1:61:A:GLN:H    | 1:72:A:ARG:HB2  | 16       | 0.14          |
| (1,531) | 1:61:A:GLN:H    | 1:72:A:ARG:HB3  | 16       | 0.14          |
| (1,531) | 1:61:A:GLN:H    | 1:72:A:ARG:HB2  | 18       | 0.14          |
| (1,531) | 1:61:A:GLN:H    | 1:72:A:ARG:HB3  | 18       | 0.14          |
| (1,457) | 1:61:A:GLN:H    | 1:72:A:ARG:H    | 10       | 0.14          |
| (1,457) | 1:61:A:GLN:H    | 1:72:A:ARG:H    | 20       | 0.14          |
| (1,388) | 1:63:A:LYS:HA   | 1:70:A:SER:H    | 9        | 0.14          |
| (1,388) | 1:63:A:LYS:HA   | 1:70:A:SER:H    | 16       | 0.14          |
| (1,322) | 1:15:A:GLN:HA   | 1:18:A:LYS:H    | 12       | 0.14          |
| (1,290) | 1:6:A:TYR:HE1   | 1:10:A:ILE:HD11 | 1        | 0.14          |
| (1,290) | 1:6:A:TYR:HE1   | 1:10:A:ILE:HD12 | 1        | 0.14          |
| (1,290) | 1:6:A:TYR:HE1   | 1:10:A:ILE:HD13 | 1        | 0.14          |
| (1,290) | 1:6:A:TYR:HE2   | 1:10:A:ILE:HD11 | 1        | 0.14          |
| (1,290) | 1:6:A:TYR:HE2   | 1:10:A:ILE:HD12 | 1        | 0.14          |
| (1,290) | 1:6:A:TYR:HE2   | 1:10:A:ILE:HD13 | 1        | 0.14          |
| (1,290) | 1:6:A:TYR:HE1   | 1:10:A:ILE:HD11 | 3        | 0.14          |
| (1,290) | 1:6:A:TYR:HE1   | 1:10:A:ILE:HD12 | 3        | 0.14          |
| (1,290) | 1:6:A:TYR:HE1   | 1:10:A:ILE:HD13 | 3        | 0.14          |
| (1,290) | 1:6:A:TYR:HE2   | 1:10:A:ILE:HD11 | 3        | 0.14          |
| (1,290) | 1:6:A:TYR:HE2   | 1:10:A:ILE:HD12 | 3        | 0.14          |
| (1,290) | 1:6:A:TYR:HE2   | 1:10:A:ILE:HD13 | 3        | 0.14          |
| (1,290) | 1:6:A:TYR:HE1   | 1:10:A:ILE:HD11 | 12       | 0.14          |
| (1,290) | 1:6:A:TYR:HE1   | 1:10:A:ILE:HD12 | 12       | 0.14          |
| (1,290) | 1:6:A:TYR:HE1   | 1:10:A:ILE:HD13 | 12       | 0.14          |
| (1,290) | 1:6:A:TYR:HE2   | 1:10:A:ILE:HD11 | 12       | 0.14          |
| (1,290) | 1:6:A:TYR:HE2   | 1:10:A:ILE:HD12 | 12       | 0.14          |
| (1,290) | 1:6:A:TYR:HE2   | 1:10:A:ILE:HD13 | 12       | 0.14          |
| (1,290) | 1:6:A:TYR:HE1   | 1:10:A:ILE:HD11 | 17       | 0.14          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,290) | 1:6:A:TYR:HE1   | 1:10:A:ILE:HD12 | 17       | 0.14          |
| (1,290) | 1:6:A:TYR:HE1   | 1:10:A:ILE:HD13 | 17       | 0.14          |
| (1,290) | 1:6:A:TYR:HE2   | 1:10:A:ILE:HD11 | 17       | 0.14          |
| (1,290) | 1:6:A:TYR:HE2   | 1:10:A:ILE:HD12 | 17       | 0.14          |
| (1,290) | 1:6:A:TYR:HE2   | 1:10:A:ILE:HD13 | 17       | 0.14          |
| (1,274) | 1:52:A:ARG:HA   | 1:55:A:THR:HG21 | 6        | 0.14          |
| (1,274) | 1:52:A:ARG:HA   | 1:55:A:THR:HG22 | 6        | 0.14          |
| (1,274) | 1:52:A:ARG:HA   | 1:55:A:THR:HG23 | 6        | 0.14          |
| (1,262) | 1:14:A:ILE:HD11 | 1:71:A:PHE:HA   | 6        | 0.14          |
| (1,262) | 1:14:A:ILE:HD12 | 1:71:A:PHE:HA   | 6        | 0.14          |
| (1,262) | 1:14:A:ILE:HD13 | 1:71:A:PHE:HA   | 6        | 0.14          |
| (1,262) | 1:14:A:ILE:HD11 | 1:71:A:PHE:HA   | 15       | 0.14          |
| (1,262) | 1:14:A:ILE:HD12 | 1:71:A:PHE:HA   | 15       | 0.14          |
| (1,262) | 1:14:A:ILE:HD13 | 1:71:A:PHE:HA   | 15       | 0.14          |
| (1,262) | 1:14:A:ILE:HD11 | 1:71:A:PHE:HA   | 17       | 0.14          |
| (1,262) | 1:14:A:ILE:HD12 | 1:71:A:PHE:HA   | 17       | 0.14          |
| (1,262) | 1:14:A:ILE:HD13 | 1:71:A:PHE:HA   | 17       | 0.14          |
| (1,262) | 1:14:A:ILE:HD11 | 1:71:A:PHE:HA   | 18       | 0.14          |
| (1,262) | 1:14:A:ILE:HD12 | 1:71:A:PHE:HA   | 18       | 0.14          |
| (1,262) | 1:14:A:ILE:HD13 | 1:71:A:PHE:HA   | 18       | 0.14          |
| (1,38)  | 1:12:A:ALA:HB1  | 1:32:A:ILE:HG21 | 14       | 0.14          |
| (1,38)  | 1:12:A:ALA:HB1  | 1:32:A:ILE:HG22 | 14       | 0.14          |
| (1,38)  | 1:12:A:ALA:HB1  | 1:32:A:ILE:HG23 | 14       | 0.14          |
| (1,38)  | 1:12:A:ALA:HB2  | 1:32:A:ILE:HG21 | 14       | 0.14          |
| (1,38)  | 1:12:A:ALA:HB2  | 1:32:A:ILE:HG22 | 14       | 0.14          |
| (1,38)  | 1:12:A:ALA:HB2  | 1:32:A:ILE:HG23 | 14       | 0.14          |
| (1,38)  | 1:12:A:ALA:HB3  | 1:32:A:ILE:HG21 | 14       | 0.14          |
| (1,38)  | 1:12:A:ALA:HB3  | 1:32:A:ILE:HG22 | 14       | 0.14          |
| (1,38)  | 1:12:A:ALA:HB3  | 1:32:A:ILE:HG23 | 14       | 0.14          |
| (1,35)  | 1:10:A:ILE:HA   | 1:10:A:ILE:HD11 | 6        | 0.14          |
| (1,35)  | 1:10:A:ILE:HA   | 1:10:A:ILE:HD12 | 6        | 0.14          |
| (1,35)  | 1:10:A:ILE:HA   | 1:10:A:ILE:HD13 | 6        | 0.14          |
| (1,35)  | 1:10:A:ILE:HA   | 1:10:A:ILE:HD11 | 7        | 0.14          |
| (1,35)  | 1:10:A:ILE:HA   | 1:10:A:ILE:HD12 | 7        | 0.14          |
| (1,35)  | 1:10:A:ILE:HA   | 1:10:A:ILE:HD13 | 7        | 0.14          |
| (1,35)  | 1:10:A:ILE:HA   | 1:10:A:ILE:HD11 | 14       | 0.14          |
| (1,35)  | 1:10:A:ILE:HA   | 1:10:A:ILE:HD12 | 14       | 0.14          |
| (1,35)  | 1:10:A:ILE:HA   | 1:10:A:ILE:HD13 | 14       | 0.14          |
| (1,35)  | 1:10:A:ILE:HA   | 1:10:A:ILE:HD11 | 18       | 0.14          |
| (1,35)  | 1:10:A:ILE:HA   | 1:10:A:ILE:HD12 | 18       | 0.14          |
| (1,35)  | 1:10:A:ILE:HA   | 1:10:A:ILE:HD13 | 18       | 0.14          |
| (1,35)  | 1:10:A:ILE:HA   | 1:10:A:ILE:HD11 | 19       | 0.14          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,35)  | 1:10:A:ILE:HA   | 1:10:A:ILE:HD12 | 19       | 0.14          |
| (1,35)  | 1:10:A:ILE:HA   | 1:10:A:ILE:HD13 | 19       | 0.14          |
| (1,13)  | 1:60:A:LYS:HA   | 1:72:A:ARG:HB2  | 3        | 0.14          |
| (1,13)  | 1:60:A:LYS:HA   | 1:72:A:ARG:HB3  | 3        | 0.14          |
| (1,8)   | 1:60:A:LYS:HB2  | 1:74:A:ALA:HB1  | 1        | 0.14          |
| (1,8)   | 1:60:A:LYS:HB2  | 1:74:A:ALA:HB2  | 1        | 0.14          |
| (1,8)   | 1:60:A:LYS:HB2  | 1:74:A:ALA:HB3  | 1        | 0.14          |
| (1,8)   | 1:60:A:LYS:HB3  | 1:74:A:ALA:HB1  | 1        | 0.14          |
| (1,8)   | 1:60:A:LYS:HB3  | 1:74:A:ALA:HB2  | 1        | 0.14          |
| (1,8)   | 1:60:A:LYS:HB3  | 1:74:A:ALA:HB3  | 1        | 0.14          |
| (1,8)   | 1:60:A:LYS:HB2  | 1:74:A:ALA:HB1  | 3        | 0.14          |
| (1,8)   | 1:60:A:LYS:HB2  | 1:74:A:ALA:HB2  | 3        | 0.14          |
| (1,8)   | 1:60:A:LYS:HB2  | 1:74:A:ALA:HB3  | 3        | 0.14          |
| (1,8)   | 1:60:A:LYS:HB3  | 1:74:A:ALA:HB1  | 3        | 0.14          |
| (1,8)   | 1:60:A:LYS:HB3  | 1:74:A:ALA:HB2  | 3        | 0.14          |
| (1,8)   | 1:60:A:LYS:HB3  | 1:74:A:ALA:HB3  | 3        | 0.14          |
| (1,8)   | 1:60:A:LYS:HB2  | 1:74:A:ALA:HB1  | 7        | 0.14          |
| (1,8)   | 1:60:A:LYS:HB2  | 1:74:A:ALA:HB2  | 7        | 0.14          |
| (1,8)   | 1:60:A:LYS:HB2  | 1:74:A:ALA:HB3  | 7        | 0.14          |
| (1,8)   | 1:60:A:LYS:HB3  | 1:74:A:ALA:HB1  | 7        | 0.14          |
| (1,8)   | 1:60:A:LYS:HB3  | 1:74:A:ALA:HB2  | 7        | 0.14          |
| (1,8)   | 1:60:A:LYS:HB3  | 1:74:A:ALA:HB3  | 7        | 0.14          |
| (1,8)   | 1:60:A:LYS:HB2  | 1:74:A:ALA:HB1  | 10       | 0.14          |
| (1,8)   | 1:60:A:LYS:HB2  | 1:74:A:ALA:HB2  | 10       | 0.14          |
| (1,8)   | 1:60:A:LYS:HB2  | 1:74:A:ALA:HB3  | 10       | 0.14          |
| (1,8)   | 1:60:A:LYS:HB3  | 1:74:A:ALA:HB1  | 10       | 0.14          |
| (1,8)   | 1:60:A:LYS:HB3  | 1:74:A:ALA:HB2  | 10       | 0.14          |
| (1,8)   | 1:60:A:LYS:HB3  | 1:74:A:ALA:HB3  | 10       | 0.14          |
| (1,4)   | 1:14:A:ILE:HD11 | 1:28:A:ILE:HB   | 20       | 0.14          |
| (1,4)   | 1:14:A:ILE:HD12 | 1:28:A:ILE:HB   | 20       | 0.14          |
| (1,4)   | 1:14:A:ILE:HD13 | 1:28:A:ILE:HB   | 20       | 0.14          |
| (1,821) | 1:64:A:GLY:HA2  | 1:65:A:VAL:HG11 | 13       | 0.13          |
| (1,821) | 1:64:A:GLY:HA2  | 1:65:A:VAL:HG12 | 13       | 0.13          |
| (1,821) | 1:64:A:GLY:HA2  | 1:65:A:VAL:HG13 | 13       | 0.13          |
| (1,821) | 1:64:A:GLY:HA2  | 1:65:A:VAL:HG21 | 13       | 0.13          |
| (1,821) | 1:64:A:GLY:HA2  | 1:65:A:VAL:HG22 | 13       | 0.13          |
| (1,821) | 1:64:A:GLY:HA2  | 1:65:A:VAL:HG23 | 13       | 0.13          |
| (1,821) | 1:64:A:GLY:HA3  | 1:65:A:VAL:HG11 | 13       | 0.13          |
| (1,821) | 1:64:A:GLY:HA3  | 1:65:A:VAL:HG12 | 13       | 0.13          |
| (1,821) | 1:64:A:GLY:HA3  | 1:65:A:VAL:HG13 | 13       | 0.13          |
| (1,821) | 1:64:A:GLY:HA3  | 1:65:A:VAL:HG21 | 13       | 0.13          |
| (1,821) | 1:64:A:GLY:HA3  | 1:65:A:VAL:HG22 | 13       | 0.13          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,821) | 1:64:A:GLY:HA3  | 1:65:A:VAL:HG23 | 13       | 0.13          |
| (1,803) | 1:60:A:LYS:HD2  | 1:74:A:ALA:H    | 12       | 0.13          |
| (1,803) | 1:60:A:LYS:HD3  | 1:74:A:ALA:H    | 12       | 0.13          |
| (1,654) | 1:12:A:ALA:HA   | 1:15:A:GLN:HE21 | 20       | 0.13          |
| (1,654) | 1:12:A:ALA:HA   | 1:15:A:GLN:HE22 | 20       | 0.13          |
| (1,644) | 1:10:A:ILE:HG12 | 1:14:A:ILE:HD11 | 15       | 0.13          |
| (1,644) | 1:10:A:ILE:HG12 | 1:14:A:ILE:HD12 | 15       | 0.13          |
| (1,644) | 1:10:A:ILE:HG12 | 1:14:A:ILE:HD13 | 15       | 0.13          |
| (1,644) | 1:10:A:ILE:HG13 | 1:14:A:ILE:HD11 | 15       | 0.13          |
| (1,644) | 1:10:A:ILE:HG13 | 1:14:A:ILE:HD12 | 15       | 0.13          |
| (1,644) | 1:10:A:ILE:HG13 | 1:14:A:ILE:HD13 | 15       | 0.13          |
| (1,644) | 1:10:A:ILE:HG12 | 1:14:A:ILE:HD11 | 16       | 0.13          |
| (1,644) | 1:10:A:ILE:HG12 | 1:14:A:ILE:HD12 | 16       | 0.13          |
| (1,644) | 1:10:A:ILE:HG12 | 1:14:A:ILE:HD13 | 16       | 0.13          |
| (1,644) | 1:10:A:ILE:HG13 | 1:14:A:ILE:HD11 | 16       | 0.13          |
| (1,644) | 1:10:A:ILE:HG13 | 1:14:A:ILE:HD12 | 16       | 0.13          |
| (1,644) | 1:10:A:ILE:HG13 | 1:14:A:ILE:HD13 | 16       | 0.13          |
| (1,636) | 1:9:A:MET:HA    | 1:11:A:VAL:HG11 | 2        | 0.13          |
| (1,636) | 1:9:A:MET:HA    | 1:11:A:VAL:HG12 | 2        | 0.13          |
| (1,636) | 1:9:A:MET:HA    | 1:11:A:VAL:HG13 | 2        | 0.13          |
| (1,636) | 1:9:A:MET:HA    | 1:11:A:VAL:HG21 | 2        | 0.13          |
| (1,636) | 1:9:A:MET:HA    | 1:11:A:VAL:HG22 | 2        | 0.13          |
| (1,636) | 1:9:A:MET:HA    | 1:11:A:VAL:HG23 | 2        | 0.13          |
| (1,636) | 1:9:A:MET:HA    | 1:11:A:VAL:HG11 | 8        | 0.13          |
| (1,636) | 1:9:A:MET:HA    | 1:11:A:VAL:HG12 | 8        | 0.13          |
| (1,636) | 1:9:A:MET:HA    | 1:11:A:VAL:HG13 | 8        | 0.13          |
| (1,636) | 1:9:A:MET:HA    | 1:11:A:VAL:HG21 | 8        | 0.13          |
| (1,636) | 1:9:A:MET:HA    | 1:11:A:VAL:HG22 | 8        | 0.13          |
| (1,636) | 1:9:A:MET:HA    | 1:11:A:VAL:HG23 | 8        | 0.13          |
| (1,628) | 1:7:A:SER:HB2   | 1:10:A:ILE:HG21 | 13       | 0.13          |
| (1,628) | 1:7:A:SER:HB2   | 1:10:A:ILE:HG22 | 13       | 0.13          |
| (1,628) | 1:7:A:SER:HB2   | 1:10:A:ILE:HG23 | 13       | 0.13          |
| (1,628) | 1:7:A:SER:HB3   | 1:10:A:ILE:HG21 | 13       | 0.13          |
| (1,628) | 1:7:A:SER:HB3   | 1:10:A:ILE:HG22 | 13       | 0.13          |
| (1,628) | 1:7:A:SER:HB3   | 1:10:A:ILE:HG23 | 13       | 0.13          |
| (1,573) | 1:32:A:ILE:HD11 | 1:36:A:TYR:HD1  | 6        | 0.13          |
| (1,573) | 1:32:A:ILE:HD11 | 1:36:A:TYR:HD2  | 6        | 0.13          |
| (1,573) | 1:32:A:ILE:HD12 | 1:36:A:TYR:HD1  | 6        | 0.13          |
| (1,573) | 1:32:A:ILE:HD12 | 1:36:A:TYR:HD2  | 6        | 0.13          |
| (1,573) | 1:32:A:ILE:HD13 | 1:36:A:TYR:HD1  | 6        | 0.13          |
| (1,573) | 1:32:A:ILE:HD13 | 1:36:A:TYR:HD2  | 6        | 0.13          |
| (1,457) | 1:61:A:GLN:H    | 1:72:A:ARG:H    | 5        | 0.13          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,457) | 1:61:A:GLN:H    | 1:72:A:ARG:H    | 15       | 0.13          |
| (1,388) | 1:63:A:LYS:HA   | 1:70:A:SER:H    | 5        | 0.13          |
| (1,388) | 1:63:A:LYS:HA   | 1:70:A:SER:H    | 8        | 0.13          |
| (1,388) | 1:63:A:LYS:HA   | 1:70:A:SER:H    | 11       | 0.13          |
| (1,388) | 1:63:A:LYS:HA   | 1:70:A:SER:H    | 13       | 0.13          |
| (1,388) | 1:63:A:LYS:HA   | 1:70:A:SER:H    | 20       | 0.13          |
| (1,344) | 1:52:A:ARG:HD2  | 1:55:A:THR:HG21 | 19       | 0.13          |
| (1,344) | 1:52:A:ARG:HD2  | 1:55:A:THR:HG22 | 19       | 0.13          |
| (1,344) | 1:52:A:ARG:HD2  | 1:55:A:THR:HG23 | 19       | 0.13          |
| (1,344) | 1:52:A:ARG:HD3  | 1:55:A:THR:HG21 | 19       | 0.13          |
| (1,344) | 1:52:A:ARG:HD3  | 1:55:A:THR:HG22 | 19       | 0.13          |
| (1,344) | 1:52:A:ARG:HD3  | 1:55:A:THR:HG23 | 19       | 0.13          |
| (1,343) | 1:52:A:ARG:HD2  | 1:55:A:THR:HG21 | 19       | 0.13          |
| (1,343) | 1:52:A:ARG:HD2  | 1:55:A:THR:HG22 | 19       | 0.13          |
| (1,343) | 1:52:A:ARG:HD2  | 1:55:A:THR:HG23 | 19       | 0.13          |
| (1,343) | 1:52:A:ARG:HD3  | 1:55:A:THR:HG21 | 19       | 0.13          |
| (1,343) | 1:52:A:ARG:HD3  | 1:55:A:THR:HG22 | 19       | 0.13          |
| (1,343) | 1:52:A:ARG:HD3  | 1:55:A:THR:HG23 | 19       | 0.13          |
| (1,322) | 1:15:A:GLN:HA   | 1:18:A:LYS:H    | 2        | 0.13          |
| (1,322) | 1:15:A:GLN:HA   | 1:18:A:LYS:H    | 20       | 0.13          |
| (1,290) | 1:6:A:TYR:HE1   | 1:10:A:ILE:HD11 | 2        | 0.13          |
| (1,290) | 1:6:A:TYR:HE1   | 1:10:A:ILE:HD12 | 2        | 0.13          |
| (1,290) | 1:6:A:TYR:HE1   | 1:10:A:ILE:HD13 | 2        | 0.13          |
| (1,290) | 1:6:A:TYR:HE2   | 1:10:A:ILE:HD11 | 2        | 0.13          |
| (1,290) | 1:6:A:TYR:HE2   | 1:10:A:ILE:HD12 | 2        | 0.13          |
| (1,290) | 1:6:A:TYR:HE2   | 1:10:A:ILE:HD13 | 2        | 0.13          |
| (1,290) | 1:6:A:TYR:HE1   | 1:10:A:ILE:HD11 | 9        | 0.13          |
| (1,290) | 1:6:A:TYR:HE1   | 1:10:A:ILE:HD12 | 9        | 0.13          |
| (1,290) | 1:6:A:TYR:HE1   | 1:10:A:ILE:HD13 | 9        | 0.13          |
| (1,290) | 1:6:A:TYR:HE2   | 1:10:A:ILE:HD11 | 9        | 0.13          |
| (1,290) | 1:6:A:TYR:HE2   | 1:10:A:ILE:HD12 | 9        | 0.13          |
| (1,290) | 1:6:A:TYR:HE2   | 1:10:A:ILE:HD13 | 9        | 0.13          |
| (1,274) | 1:52:A:ARG:HA   | 1:55:A:THR:HG21 | 8        | 0.13          |
| (1,274) | 1:52:A:ARG:HA   | 1:55:A:THR:HG22 | 8        | 0.13          |
| (1,274) | 1:52:A:ARG:HA   | 1:55:A:THR:HG23 | 8        | 0.13          |
| (1,274) | 1:52:A:ARG:HA   | 1:55:A:THR:HG21 | 12       | 0.13          |
| (1,274) | 1:52:A:ARG:HA   | 1:55:A:THR:HG22 | 12       | 0.13          |
| (1,274) | 1:52:A:ARG:HA   | 1:55:A:THR:HG23 | 12       | 0.13          |
| (1,262) | 1:14:A:ILE:HD11 | 1:71:A:PHE:HA   | 3        | 0.13          |
| (1,262) | 1:14:A:ILE:HD12 | 1:71:A:PHE:HA   | 3        | 0.13          |
| (1,262) | 1:14:A:ILE:HD13 | 1:71:A:PHE:HA   | 3        | 0.13          |
| (1,262) | 1:14:A:ILE:HD11 | 1:71:A:PHE:HA   | 5        | 0.13          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,262) | 1:14:A:ILE:HD12 | 1:71:A:PHE:HA   | 5        | 0.13          |
| (1,262) | 1:14:A:ILE:HD13 | 1:71:A:PHE:HA   | 5        | 0.13          |
| (1,262) | 1:14:A:ILE:HD11 | 1:71:A:PHE:HA   | 16       | 0.13          |
| (1,262) | 1:14:A:ILE:HD12 | 1:71:A:PHE:HA   | 16       | 0.13          |
| (1,262) | 1:14:A:ILE:HD13 | 1:71:A:PHE:HA   | 16       | 0.13          |
| (1,230) | 1:11:A:VAL:HA   | 1:14:A:ILE:HD11 | 11       | 0.13          |
| (1,230) | 1:11:A:VAL:HA   | 1:14:A:ILE:HD12 | 11       | 0.13          |
| (1,230) | 1:11:A:VAL:HA   | 1:14:A:ILE:HD13 | 11       | 0.13          |
| (1,35)  | 1:10:A:ILE:HA   | 1:10:A:ILE:HD11 | 1        | 0.13          |
| (1,35)  | 1:10:A:ILE:HA   | 1:10:A:ILE:HD12 | 1        | 0.13          |
| (1,35)  | 1:10:A:ILE:HA   | 1:10:A:ILE:HD13 | 1        | 0.13          |
| (1,35)  | 1:10:A:ILE:HA   | 1:10:A:ILE:HD11 | 2        | 0.13          |
| (1,35)  | 1:10:A:ILE:HA   | 1:10:A:ILE:HD12 | 2        | 0.13          |
| (1,35)  | 1:10:A:ILE:HA   | 1:10:A:ILE:HD13 | 2        | 0.13          |
| (1,35)  | 1:10:A:ILE:HA   | 1:10:A:ILE:HD11 | 3        | 0.13          |
| (1,35)  | 1:10:A:ILE:HA   | 1:10:A:ILE:HD12 | 3        | 0.13          |
| (1,35)  | 1:10:A:ILE:HA   | 1:10:A:ILE:HD13 | 3        | 0.13          |
| (1,35)  | 1:10:A:ILE:HA   | 1:10:A:ILE:HD11 | 5        | 0.13          |
| (1,35)  | 1:10:A:ILE:HA   | 1:10:A:ILE:HD12 | 5        | 0.13          |
| (1,35)  | 1:10:A:ILE:HA   | 1:10:A:ILE:HD13 | 5        | 0.13          |
| (1,35)  | 1:10:A:ILE:HA   | 1:10:A:ILE:HD11 | 8        | 0.13          |
| (1,35)  | 1:10:A:ILE:HA   | 1:10:A:ILE:HD12 | 8        | 0.13          |
| (1,35)  | 1:10:A:ILE:HA   | 1:10:A:ILE:HD13 | 8        | 0.13          |
| (1,35)  | 1:10:A:ILE:HA   | 1:10:A:ILE:HD11 | 9        | 0.13          |
| (1,35)  | 1:10:A:ILE:HA   | 1:10:A:ILE:HD12 | 9        | 0.13          |
| (1,35)  | 1:10:A:ILE:HA   | 1:10:A:ILE:HD13 | 9        | 0.13          |
| (1,35)  | 1:10:A:ILE:HA   | 1:10:A:ILE:HD11 | 10       | 0.13          |
| (1,35)  | 1:10:A:ILE:HA   | 1:10:A:ILE:HD12 | 10       | 0.13          |
| (1,35)  | 1:10:A:ILE:HA   | 1:10:A:ILE:HD13 | 10       | 0.13          |
| (1,35)  | 1:10:A:ILE:HA   | 1:10:A:ILE:HD11 | 11       | 0.13          |
| (1,35)  | 1:10:A:ILE:HA   | 1:10:A:ILE:HD12 | 11       | 0.13          |
| (1,35)  | 1:10:A:ILE:HA   | 1:10:A:ILE:HD13 | 11       | 0.13          |
| (1,35)  | 1:10:A:ILE:HA   | 1:10:A:ILE:HD11 | 12       | 0.13          |
| (1,35)  | 1:10:A:ILE:HA   | 1:10:A:ILE:HD12 | 12       | 0.13          |
| (1,35)  | 1:10:A:ILE:HA   | 1:10:A:ILE:HD13 | 12       | 0.13          |
| (1,35)  | 1:10:A:ILE:HA   | 1:10:A:ILE:HD11 | 13       | 0.13          |
| (1,35)  | 1:10:A:ILE:HA   | 1:10:A:ILE:HD12 | 13       | 0.13          |
| (1,35)  | 1:10:A:ILE:HA   | 1:10:A:ILE:HD13 | 13       | 0.13          |
| (1,35)  | 1:10:A:ILE:HA   | 1:10:A:ILE:HD11 | 15       | 0.13          |
| (1,35)  | 1:10:A:ILE:HA   | 1:10:A:ILE:HD12 | 15       | 0.13          |
| (1,35)  | 1:10:A:ILE:HA   | 1:10:A:ILE:HD13 | 15       | 0.13          |
| (1,35)  | 1:10:A:ILE:HA   | 1:10:A:ILE:HD11 | 16       | 0.13          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,35)  | 1:10:A:ILE:HA   | 1:10:A:ILE:HD12 | 16       | 0.13          |
| (1,35)  | 1:10:A:ILE:HA   | 1:10:A:ILE:HD13 | 16       | 0.13          |
| (1,35)  | 1:10:A:ILE:HA   | 1:10:A:ILE:HD11 | 17       | 0.13          |
| (1,35)  | 1:10:A:ILE:HA   | 1:10:A:ILE:HD12 | 17       | 0.13          |
| (1,35)  | 1:10:A:ILE:HA   | 1:10:A:ILE:HD13 | 17       | 0.13          |
| (1,35)  | 1:10:A:ILE:HA   | 1:10:A:ILE:HD11 | 20       | 0.13          |
| (1,35)  | 1:10:A:ILE:HA   | 1:10:A:ILE:HD12 | 20       | 0.13          |
| (1,35)  | 1:10:A:ILE:HA   | 1:10:A:ILE:HD13 | 20       | 0.13          |
| (1,4)   | 1:14:A:ILE:HD11 | 1:28:A:ILE:HB   | 7        | 0.13          |
| (1,4)   | 1:14:A:ILE:HD12 | 1:28:A:ILE:HB   | 7        | 0.13          |
| (1,4)   | 1:14:A:ILE:HD13 | 1:28:A:ILE:HB   | 7        | 0.13          |
| (1,4)   | 1:14:A:ILE:HD11 | 1:28:A:ILE:HB   | 14       | 0.13          |
| (1,4)   | 1:14:A:ILE:HD12 | 1:28:A:ILE:HB   | 14       | 0.13          |
| (1,4)   | 1:14:A:ILE:HD13 | 1:28:A:ILE:HB   | 14       | 0.13          |
| (1,4)   | 1:14:A:ILE:HD11 | 1:28:A:ILE:HB   | 15       | 0.13          |
| (1,4)   | 1:14:A:ILE:HD12 | 1:28:A:ILE:HB   | 15       | 0.13          |
| (1,4)   | 1:14:A:ILE:HD13 | 1:28:A:ILE:HB   | 15       | 0.13          |
| (1,821) | 1:64:A:GLY:HA2  | 1:65:A:VAL:HG11 | 9        | 0.12          |
| (1,821) | 1:64:A:GLY:HA2  | 1:65:A:VAL:HG12 | 9        | 0.12          |
| (1,821) | 1:64:A:GLY:HA2  | 1:65:A:VAL:HG13 | 9        | 0.12          |
| (1,821) | 1:64:A:GLY:HA2  | 1:65:A:VAL:HG21 | 9        | 0.12          |
| (1,821) | 1:64:A:GLY:HA2  | 1:65:A:VAL:HG22 | 9        | 0.12          |
| (1,821) | 1:64:A:GLY:HA2  | 1:65:A:VAL:HG23 | 9        | 0.12          |
| (1,821) | 1:64:A:GLY:HA3  | 1:65:A:VAL:HG11 | 9        | 0.12          |
| (1,821) | 1:64:A:GLY:HA3  | 1:65:A:VAL:HG12 | 9        | 0.12          |
| (1,821) | 1:64:A:GLY:HA3  | 1:65:A:VAL:HG13 | 9        | 0.12          |
| (1,821) | 1:64:A:GLY:HA3  | 1:65:A:VAL:HG21 | 9        | 0.12          |
| (1,821) | 1:64:A:GLY:HA3  | 1:65:A:VAL:HG22 | 9        | 0.12          |
| (1,821) | 1:64:A:GLY:HA3  | 1:65:A:VAL:HG23 | 9        | 0.12          |
| (1,803) | 1:60:A:LYS:HD2  | 1:74:A:ALA:H    | 3        | 0.12          |
| (1,803) | 1:60:A:LYS:HD3  | 1:74:A:ALA:H    | 3        | 0.12          |
| (1,754) | 1:45:A:GLN:HE21 | 1:48:A:LEU:HD11 | 16       | 0.12          |
| (1,754) | 1:45:A:GLN:HE21 | 1:48:A:LEU:HD12 | 16       | 0.12          |
| (1,754) | 1:45:A:GLN:HE21 | 1:48:A:LEU:HD13 | 16       | 0.12          |
| (1,754) | 1:45:A:GLN:HE21 | 1:48:A:LEU:HD21 | 16       | 0.12          |
| (1,754) | 1:45:A:GLN:HE21 | 1:48:A:LEU:HD22 | 16       | 0.12          |
| (1,754) | 1:45:A:GLN:HE21 | 1:48:A:LEU:HD23 | 16       | 0.12          |
| (1,754) | 1:45:A:GLN:HE22 | 1:48:A:LEU:HD11 | 16       | 0.12          |
| (1,754) | 1:45:A:GLN:HE22 | 1:48:A:LEU:HD12 | 16       | 0.12          |
| (1,754) | 1:45:A:GLN:HE22 | 1:48:A:LEU:HD13 | 16       | 0.12          |
| (1,754) | 1:45:A:GLN:HE22 | 1:48:A:LEU:HD21 | 16       | 0.12          |
| (1,754) | 1:45:A:GLN:HE22 | 1:48:A:LEU:HD22 | 16       | 0.12          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,754) | 1:45:A:GLN:HE22 | 1:48:A:LEU:HD23 | 16       | 0.12          |
| (1,754) | 1:45:A:GLN:HE21 | 1:48:A:LEU:HD11 | 18       | 0.12          |
| (1,754) | 1:45:A:GLN:HE21 | 1:48:A:LEU:HD12 | 18       | 0.12          |
| (1,754) | 1:45:A:GLN:HE21 | 1:48:A:LEU:HD13 | 18       | 0.12          |
| (1,754) | 1:45:A:GLN:HE21 | 1:48:A:LEU:HD21 | 18       | 0.12          |
| (1,754) | 1:45:A:GLN:HE21 | 1:48:A:LEU:HD22 | 18       | 0.12          |
| (1,754) | 1:45:A:GLN:HE21 | 1:48:A:LEU:HD23 | 18       | 0.12          |
| (1,754) | 1:45:A:GLN:HE22 | 1:48:A:LEU:HD11 | 18       | 0.12          |
| (1,754) | 1:45:A:GLN:HE22 | 1:48:A:LEU:HD12 | 18       | 0.12          |
| (1,754) | 1:45:A:GLN:HE22 | 1:48:A:LEU:HD13 | 18       | 0.12          |
| (1,754) | 1:45:A:GLN:HE22 | 1:48:A:LEU:HD21 | 18       | 0.12          |
| (1,754) | 1:45:A:GLN:HE22 | 1:48:A:LEU:HD22 | 18       | 0.12          |
| (1,754) | 1:45:A:GLN:HE22 | 1:48:A:LEU:HD23 | 18       | 0.12          |
| (1,654) | 1:12:A:ALA:HA   | 1:15:A:GLN:HE21 | 7        | 0.12          |
| (1,654) | 1:12:A:ALA:HA   | 1:15:A:GLN:HE22 | 7        | 0.12          |
| (1,644) | 1:10:A:ILE:HG12 | 1:14:A:ILE:HD11 | 5        | 0.12          |
| (1,644) | 1:10:A:ILE:HG12 | 1:14:A:ILE:HD12 | 5        | 0.12          |
| (1,644) | 1:10:A:ILE:HG12 | 1:14:A:ILE:HD13 | 5        | 0.12          |
| (1,644) | 1:10:A:ILE:HG13 | 1:14:A:ILE:HD11 | 5        | 0.12          |
| (1,644) | 1:10:A:ILE:HG13 | 1:14:A:ILE:HD12 | 5        | 0.12          |
| (1,644) | 1:10:A:ILE:HG13 | 1:14:A:ILE:HD13 | 5        | 0.12          |
| (1,636) | 1:9:A:MET:HA    | 1:11:A:VAL:HG11 | 5        | 0.12          |
| (1,636) | 1:9:A:MET:HA    | 1:11:A:VAL:HG12 | 5        | 0.12          |
| (1,636) | 1:9:A:MET:HA    | 1:11:A:VAL:HG13 | 5        | 0.12          |
| (1,636) | 1:9:A:MET:HA    | 1:11:A:VAL:HG21 | 5        | 0.12          |
| (1,636) | 1:9:A:MET:HA    | 1:11:A:VAL:HG22 | 5        | 0.12          |
| (1,636) | 1:9:A:MET:HA    | 1:11:A:VAL:HG23 | 5        | 0.12          |
| (1,636) | 1:9:A:MET:HA    | 1:11:A:VAL:HG11 | 9        | 0.12          |
| (1,636) | 1:9:A:MET:HA    | 1:11:A:VAL:HG12 | 9        | 0.12          |
| (1,636) | 1:9:A:MET:HA    | 1:11:A:VAL:HG13 | 9        | 0.12          |
| (1,636) | 1:9:A:MET:HA    | 1:11:A:VAL:HG21 | 9        | 0.12          |
| (1,636) | 1:9:A:MET:HA    | 1:11:A:VAL:HG22 | 9        | 0.12          |
| (1,636) | 1:9:A:MET:HA    | 1:11:A:VAL:HG23 | 9        | 0.12          |
| (1,636) | 1:9:A:MET:HA    | 1:11:A:VAL:HG11 | 10       | 0.12          |
| (1,636) | 1:9:A:MET:HA    | 1:11:A:VAL:HG12 | 10       | 0.12          |
| (1,636) | 1:9:A:MET:HA    | 1:11:A:VAL:HG13 | 10       | 0.12          |
| (1,636) | 1:9:A:MET:HA    | 1:11:A:VAL:HG21 | 10       | 0.12          |
| (1,636) | 1:9:A:MET:HA    | 1:11:A:VAL:HG22 | 10       | 0.12          |
| (1,636) | 1:9:A:MET:HA    | 1:11:A:VAL:HG23 | 10       | 0.12          |
| (1,636) | 1:9:A:MET:HA    | 1:11:A:VAL:HG11 | 19       | 0.12          |
| (1,636) | 1:9:A:MET:HA    | 1:11:A:VAL:HG12 | 19       | 0.12          |
| (1,636) | 1:9:A:MET:HA    | 1:11:A:VAL:HG13 | 19       | 0.12          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,636) | 1:9:A:MET:HA    | 1:11:A:VAL:HG21 | 19       | 0.12          |
| (1,636) | 1:9:A:MET:HA    | 1:11:A:VAL:HG22 | 19       | 0.12          |
| (1,636) | 1:9:A:MET:HA    | 1:11:A:VAL:HG23 | 19       | 0.12          |
| (1,636) | 1:9:A:MET:HA    | 1:11:A:VAL:HG11 | 20       | 0.12          |
| (1,636) | 1:9:A:MET:HA    | 1:11:A:VAL:HG12 | 20       | 0.12          |
| (1,636) | 1:9:A:MET:HA    | 1:11:A:VAL:HG13 | 20       | 0.12          |
| (1,636) | 1:9:A:MET:HA    | 1:11:A:VAL:HG21 | 20       | 0.12          |
| (1,636) | 1:9:A:MET:HA    | 1:11:A:VAL:HG22 | 20       | 0.12          |
| (1,636) | 1:9:A:MET:HA    | 1:11:A:VAL:HG23 | 20       | 0.12          |
| (1,628) | 1:7:A:SER:HB2   | 1:10:A:ILE:HG21 | 1        | 0.12          |
| (1,628) | 1:7:A:SER:HB2   | 1:10:A:ILE:HG22 | 1        | 0.12          |
| (1,628) | 1:7:A:SER:HB2   | 1:10:A:ILE:HG23 | 1        | 0.12          |
| (1,628) | 1:7:A:SER:HB3   | 1:10:A:ILE:HG21 | 1        | 0.12          |
| (1,628) | 1:7:A:SER:HB3   | 1:10:A:ILE:HG22 | 1        | 0.12          |
| (1,628) | 1:7:A:SER:HB3   | 1:10:A:ILE:HG23 | 1        | 0.12          |
| (1,573) | 1:32:A:ILE:HD11 | 1:36:A:TYR:HD1  | 20       | 0.12          |
| (1,573) | 1:32:A:ILE:HD11 | 1:36:A:TYR:HD2  | 20       | 0.12          |
| (1,573) | 1:32:A:ILE:HD12 | 1:36:A:TYR:HD1  | 20       | 0.12          |
| (1,573) | 1:32:A:ILE:HD12 | 1:36:A:TYR:HD2  | 20       | 0.12          |
| (1,573) | 1:32:A:ILE:HD13 | 1:36:A:TYR:HD1  | 20       | 0.12          |
| (1,573) | 1:32:A:ILE:HD13 | 1:36:A:TYR:HD2  | 20       | 0.12          |
| (1,531) | 1:61:A:GLN:H    | 1:72:A:ARG:HB2  | 11       | 0.12          |
| (1,531) | 1:61:A:GLN:H    | 1:72:A:ARG:HB3  | 11       | 0.12          |
| (1,457) | 1:61:A:GLN:H    | 1:72:A:ARG:H    | 2        | 0.12          |
| (1,457) | 1:61:A:GLN:H    | 1:72:A:ARG:H    | 11       | 0.12          |
| (1,457) | 1:61:A:GLN:H    | 1:72:A:ARG:H    | 16       | 0.12          |
| (1,457) | 1:61:A:GLN:H    | 1:72:A:ARG:H    | 19       | 0.12          |
| (1,398) | 1:46:A:ILE:HG21 | 1:51:A:LYS:H    | 7        | 0.12          |
| (1,398) | 1:46:A:ILE:HG22 | 1:51:A:LYS:H    | 7        | 0.12          |
| (1,398) | 1:46:A:ILE:HG23 | 1:51:A:LYS:H    | 7        | 0.12          |
| (1,398) | 1:46:A:ILE:HG21 | 1:51:A:LYS:H    | 20       | 0.12          |
| (1,398) | 1:46:A:ILE:HG22 | 1:51:A:LYS:H    | 20       | 0.12          |
| (1,398) | 1:46:A:ILE:HG23 | 1:51:A:LYS:H    | 20       | 0.12          |
| (1,388) | 1:63:A:LYS:HA   | 1:70:A:SER:H    | 2        | 0.12          |
| (1,388) | 1:63:A:LYS:HA   | 1:70:A:SER:H    | 12       | 0.12          |
| (1,388) | 1:63:A:LYS:HA   | 1:70:A:SER:H    | 14       | 0.12          |
| (1,388) | 1:63:A:LYS:HA   | 1:70:A:SER:H    | 15       | 0.12          |
| (1,344) | 1:52:A:ARG:HD2  | 1:55:A:THR:HG21 | 3        | 0.12          |
| (1,344) | 1:52:A:ARG:HD2  | 1:55:A:THR:HG22 | 3        | 0.12          |
| (1,344) | 1:52:A:ARG:HD2  | 1:55:A:THR:HG23 | 3        | 0.12          |
| (1,344) | 1:52:A:ARG:HD3  | 1:55:A:THR:HG21 | 3        | 0.12          |
| (1,344) | 1:52:A:ARG:HD3  | 1:55:A:THR:HG22 | 3        | 0.12          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,344) | 1:52:A:ARG:HD3 | 1:55:A:THR:HG23 | 3        | 0.12          |
| (1,344) | 1:52:A:ARG:HD2 | 1:55:A:THR:HG21 | 5        | 0.12          |
| (1,344) | 1:52:A:ARG:HD2 | 1:55:A:THR:HG22 | 5        | 0.12          |
| (1,344) | 1:52:A:ARG:HD2 | 1:55:A:THR:HG23 | 5        | 0.12          |
| (1,344) | 1:52:A:ARG:HD3 | 1:55:A:THR:HG21 | 5        | 0.12          |
| (1,344) | 1:52:A:ARG:HD3 | 1:55:A:THR:HG22 | 5        | 0.12          |
| (1,344) | 1:52:A:ARG:HD3 | 1:55:A:THR:HG23 | 5        | 0.12          |
| (1,344) | 1:52:A:ARG:HD2 | 1:55:A:THR:HG21 | 11       | 0.12          |
| (1,344) | 1:52:A:ARG:HD2 | 1:55:A:THR:HG22 | 11       | 0.12          |
| (1,344) | 1:52:A:ARG:HD2 | 1:55:A:THR:HG23 | 11       | 0.12          |
| (1,344) | 1:52:A:ARG:HD3 | 1:55:A:THR:HG21 | 11       | 0.12          |
| (1,344) | 1:52:A:ARG:HD3 | 1:55:A:THR:HG22 | 11       | 0.12          |
| (1,344) | 1:52:A:ARG:HD3 | 1:55:A:THR:HG23 | 11       | 0.12          |
| (1,344) | 1:52:A:ARG:HD2 | 1:55:A:THR:HG21 | 13       | 0.12          |
| (1,344) | 1:52:A:ARG:HD2 | 1:55:A:THR:HG22 | 13       | 0.12          |
| (1,344) | 1:52:A:ARG:HD2 | 1:55:A:THR:HG23 | 13       | 0.12          |
| (1,344) | 1:52:A:ARG:HD3 | 1:55:A:THR:HG21 | 13       | 0.12          |
| (1,344) | 1:52:A:ARG:HD3 | 1:55:A:THR:HG22 | 13       | 0.12          |
| (1,344) | 1:52:A:ARG:HD3 | 1:55:A:THR:HG23 | 13       | 0.12          |
| (1,344) | 1:52:A:ARG:HD2 | 1:55:A:THR:HG21 | 14       | 0.12          |
| (1,344) | 1:52:A:ARG:HD2 | 1:55:A:THR:HG22 | 14       | 0.12          |
| (1,344) | 1:52:A:ARG:HD2 | 1:55:A:THR:HG23 | 14       | 0.12          |
| (1,344) | 1:52:A:ARG:HD3 | 1:55:A:THR:HG21 | 14       | 0.12          |
| (1,344) | 1:52:A:ARG:HD3 | 1:55:A:THR:HG22 | 14       | 0.12          |
| (1,344) | 1:52:A:ARG:HD3 | 1:55:A:THR:HG23 | 14       | 0.12          |
| (1,344) | 1:52:A:ARG:HD2 | 1:55:A:THR:HG21 | 15       | 0.12          |
| (1,344) | 1:52:A:ARG:HD2 | 1:55:A:THR:HG22 | 15       | 0.12          |
| (1,344) | 1:52:A:ARG:HD2 | 1:55:A:THR:HG23 | 15       | 0.12          |
| (1,344) | 1:52:A:ARG:HD3 | 1:55:A:THR:HG21 | 15       | 0.12          |
| (1,344) | 1:52:A:ARG:HD3 | 1:55:A:THR:HG22 | 15       | 0.12          |
| (1,344) | 1:52:A:ARG:HD3 | 1:55:A:THR:HG23 | 15       | 0.12          |
| (1,344) | 1:52:A:ARG:HD2 | 1:55:A:THR:HG21 | 16       | 0.12          |
| (1,344) | 1:52:A:ARG:HD2 | 1:55:A:THR:HG22 | 16       | 0.12          |
| (1,344) | 1:52:A:ARG:HD2 | 1:55:A:THR:HG23 | 16       | 0.12          |
| (1,344) | 1:52:A:ARG:HD3 | 1:55:A:THR:HG21 | 16       | 0.12          |
| (1,344) | 1:52:A:ARG:HD3 | 1:55:A:THR:HG22 | 16       | 0.12          |
| (1,344) | 1:52:A:ARG:HD3 | 1:55:A:THR:HG23 | 16       | 0.12          |
| (1,343) | 1:52:A:ARG:HD2 | 1:55:A:THR:HG21 | 3        | 0.12          |
| (1,343) | 1:52:A:ARG:HD2 | 1:55:A:THR:HG22 | 3        | 0.12          |
| (1,343) | 1:52:A:ARG:HD2 | 1:55:A:THR:HG23 | 3        | 0.12          |
| (1,343) | 1:52:A:ARG:HD3 | 1:55:A:THR:HG21 | 3        | 0.12          |
| (1,343) | 1:52:A:ARG:HD3 | 1:55:A:THR:HG22 | 3        | 0.12          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,343) | 1:52:A:ARG:HD3 | 1:55:A:THR:HG23 | 3        | 0.12          |
| (1,343) | 1:52:A:ARG:HD2 | 1:55:A:THR:HG21 | 5        | 0.12          |
| (1,343) | 1:52:A:ARG:HD2 | 1:55:A:THR:HG22 | 5        | 0.12          |
| (1,343) | 1:52:A:ARG:HD2 | 1:55:A:THR:HG23 | 5        | 0.12          |
| (1,343) | 1:52:A:ARG:HD3 | 1:55:A:THR:HG21 | 5        | 0.12          |
| (1,343) | 1:52:A:ARG:HD3 | 1:55:A:THR:HG22 | 5        | 0.12          |
| (1,343) | 1:52:A:ARG:HD3 | 1:55:A:THR:HG23 | 5        | 0.12          |
| (1,343) | 1:52:A:ARG:HD2 | 1:55:A:THR:HG21 | 11       | 0.12          |
| (1,343) | 1:52:A:ARG:HD2 | 1:55:A:THR:HG22 | 11       | 0.12          |
| (1,343) | 1:52:A:ARG:HD2 | 1:55:A:THR:HG23 | 11       | 0.12          |
| (1,343) | 1:52:A:ARG:HD3 | 1:55:A:THR:HG21 | 11       | 0.12          |
| (1,343) | 1:52:A:ARG:HD3 | 1:55:A:THR:HG22 | 11       | 0.12          |
| (1,343) | 1:52:A:ARG:HD3 | 1:55:A:THR:HG23 | 11       | 0.12          |
| (1,343) | 1:52:A:ARG:HD2 | 1:55:A:THR:HG21 | 13       | 0.12          |
| (1,343) | 1:52:A:ARG:HD2 | 1:55:A:THR:HG22 | 13       | 0.12          |
| (1,343) | 1:52:A:ARG:HD2 | 1:55:A:THR:HG23 | 13       | 0.12          |
| (1,343) | 1:52:A:ARG:HD3 | 1:55:A:THR:HG21 | 13       | 0.12          |
| (1,343) | 1:52:A:ARG:HD3 | 1:55:A:THR:HG22 | 13       | 0.12          |
| (1,343) | 1:52:A:ARG:HD3 | 1:55:A:THR:HG23 | 13       | 0.12          |
| (1,343) | 1:52:A:ARG:HD2 | 1:55:A:THR:HG21 | 14       | 0.12          |
| (1,343) | 1:52:A:ARG:HD2 | 1:55:A:THR:HG22 | 14       | 0.12          |
| (1,343) | 1:52:A:ARG:HD2 | 1:55:A:THR:HG23 | 14       | 0.12          |
| (1,343) | 1:52:A:ARG:HD3 | 1:55:A:THR:HG21 | 14       | 0.12          |
| (1,343) | 1:52:A:ARG:HD3 | 1:55:A:THR:HG22 | 14       | 0.12          |
| (1,343) | 1:52:A:ARG:HD3 | 1:55:A:THR:HG23 | 14       | 0.12          |
| (1,343) | 1:52:A:ARG:HD2 | 1:55:A:THR:HG21 | 15       | 0.12          |
| (1,343) | 1:52:A:ARG:HD2 | 1:55:A:THR:HG22 | 15       | 0.12          |
| (1,343) | 1:52:A:ARG:HD2 | 1:55:A:THR:HG23 | 15       | 0.12          |
| (1,343) | 1:52:A:ARG:HD3 | 1:55:A:THR:HG21 | 15       | 0.12          |
| (1,343) | 1:52:A:ARG:HD3 | 1:55:A:THR:HG22 | 15       | 0.12          |
| (1,343) | 1:52:A:ARG:HD3 | 1:55:A:THR:HG23 | 15       | 0.12          |
| (1,343) | 1:52:A:ARG:HD2 | 1:55:A:THR:HG21 | 16       | 0.12          |
| (1,343) | 1:52:A:ARG:HD2 | 1:55:A:THR:HG22 | 16       | 0.12          |
| (1,343) | 1:52:A:ARG:HD2 | 1:55:A:THR:HG23 | 16       | 0.12          |
| (1,343) | 1:52:A:ARG:HD3 | 1:55:A:THR:HG21 | 16       | 0.12          |
| (1,343) | 1:52:A:ARG:HD3 | 1:55:A:THR:HG22 | 16       | 0.12          |
| (1,343) | 1:52:A:ARG:HD3 | 1:55:A:THR:HG23 | 16       | 0.12          |
| (1,322) | 1:15:A:GLN:HA  | 1:18:A:LYS:H    | 6        | 0.12          |
| (1,322) | 1:15:A:GLN:HA  | 1:18:A:LYS:H    | 8        | 0.12          |
| (1,290) | 1:6:A:TYR:HE1  | 1:10:A:ILE:HD11 | 5        | 0.12          |
| (1,290) | 1:6:A:TYR:HE1  | 1:10:A:ILE:HD12 | 5        | 0.12          |
| (1,290) | 1:6:A:TYR:HE1  | 1:10:A:ILE:HD13 | 5        | 0.12          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,290) | 1:6:A:TYR:HE2  | 1:10:A:ILE:HD11 | 5        | 0.12          |
| (1,290) | 1:6:A:TYR:HE2  | 1:10:A:ILE:HD12 | 5        | 0.12          |
| (1,290) | 1:6:A:TYR:HE2  | 1:10:A:ILE:HD13 | 5        | 0.12          |
| (1,290) | 1:6:A:TYR:HE1  | 1:10:A:ILE:HD11 | 6        | 0.12          |
| (1,290) | 1:6:A:TYR:HE1  | 1:10:A:ILE:HD12 | 6        | 0.12          |
| (1,290) | 1:6:A:TYR:HE1  | 1:10:A:ILE:HD13 | 6        | 0.12          |
| (1,290) | 1:6:A:TYR:HE2  | 1:10:A:ILE:HD11 | 6        | 0.12          |
| (1,290) | 1:6:A:TYR:HE2  | 1:10:A:ILE:HD12 | 6        | 0.12          |
| (1,290) | 1:6:A:TYR:HE2  | 1:10:A:ILE:HD13 | 6        | 0.12          |
| (1,290) | 1:6:A:TYR:HE1  | 1:10:A:ILE:HD11 | 10       | 0.12          |
| (1,290) | 1:6:A:TYR:HE1  | 1:10:A:ILE:HD12 | 10       | 0.12          |
| (1,290) | 1:6:A:TYR:HE1  | 1:10:A:ILE:HD13 | 10       | 0.12          |
| (1,290) | 1:6:A:TYR:HE2  | 1:10:A:ILE:HD11 | 10       | 0.12          |
| (1,290) | 1:6:A:TYR:HE2  | 1:10:A:ILE:HD12 | 10       | 0.12          |
| (1,290) | 1:6:A:TYR:HE2  | 1:10:A:ILE:HD13 | 10       | 0.12          |
| (1,290) | 1:6:A:TYR:HE1  | 1:10:A:ILE:HD11 | 11       | 0.12          |
| (1,290) | 1:6:A:TYR:HE1  | 1:10:A:ILE:HD12 | 11       | 0.12          |
| (1,290) | 1:6:A:TYR:HE1  | 1:10:A:ILE:HD13 | 11       | 0.12          |
| (1,290) | 1:6:A:TYR:HE2  | 1:10:A:ILE:HD11 | 11       | 0.12          |
| (1,290) | 1:6:A:TYR:HE2  | 1:10:A:ILE:HD12 | 11       | 0.12          |
| (1,290) | 1:6:A:TYR:HE2  | 1:10:A:ILE:HD13 | 11       | 0.12          |
| (1,274) | 1:52:A:ARG:HA  | 1:55:A:THR:HG21 | 10       | 0.12          |
| (1,274) | 1:52:A:ARG:HA  | 1:55:A:THR:HG22 | 10       | 0.12          |
| (1,274) | 1:52:A:ARG:HA  | 1:55:A:THR:HG23 | 10       | 0.12          |
| (1,230) | 1:11:A:VAL:HA  | 1:14:A:ILE:HD11 | 9        | 0.12          |
| (1,230) | 1:11:A:VAL:HA  | 1:14:A:ILE:HD12 | 9        | 0.12          |
| (1,230) | 1:11:A:VAL:HA  | 1:14:A:ILE:HD13 | 9        | 0.12          |
| (1,35)  | 1:10:A:ILE:HA  | 1:10:A:ILE:HD11 | 4        | 0.12          |
| (1,35)  | 1:10:A:ILE:HA  | 1:10:A:ILE:HD12 | 4        | 0.12          |
| (1,35)  | 1:10:A:ILE:HA  | 1:10:A:ILE:HD13 | 4        | 0.12          |
| (1,13)  | 1:60:A:LYS:HA  | 1:72:A:ARG:HB2  | 7        | 0.12          |
| (1,13)  | 1:60:A:LYS:HA  | 1:72:A:ARG:HB3  | 7        | 0.12          |
| (1,13)  | 1:60:A:LYS:HA  | 1:72:A:ARG:HB2  | 8        | 0.12          |
| (1,13)  | 1:60:A:LYS:HA  | 1:72:A:ARG:HB3  | 8        | 0.12          |
| (1,13)  | 1:60:A:LYS:HA  | 1:72:A:ARG:HB2  | 19       | 0.12          |
| (1,13)  | 1:60:A:LYS:HA  | 1:72:A:ARG:HB3  | 19       | 0.12          |
| (1,8)   | 1:60:A:LYS:HB2 | 1:74:A:ALA:HB1  | 5        | 0.12          |
| (1,8)   | 1:60:A:LYS:HB2 | 1:74:A:ALA:HB2  | 5        | 0.12          |
| (1,8)   | 1:60:A:LYS:HB2 | 1:74:A:ALA:HB3  | 5        | 0.12          |
| (1,8)   | 1:60:A:LYS:HB3 | 1:74:A:ALA:HB1  | 5        | 0.12          |
| (1,8)   | 1:60:A:LYS:HB3 | 1:74:A:ALA:HB2  | 5        | 0.12          |
| (1,8)   | 1:60:A:LYS:HB3 | 1:74:A:ALA:HB3  | 5        | 0.12          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,8)   | 1:60:A:LYS:HB2  | 1:74:A:ALA:HB1  | 11       | 0.12          |
| (1,8)   | 1:60:A:LYS:HB2  | 1:74:A:ALA:HB2  | 11       | 0.12          |
| (1,8)   | 1:60:A:LYS:HB2  | 1:74:A:ALA:HB3  | 11       | 0.12          |
| (1,8)   | 1:60:A:LYS:HB3  | 1:74:A:ALA:HB1  | 11       | 0.12          |
| (1,8)   | 1:60:A:LYS:HB3  | 1:74:A:ALA:HB2  | 11       | 0.12          |
| (1,8)   | 1:60:A:LYS:HB3  | 1:74:A:ALA:HB3  | 11       | 0.12          |
| (1,8)   | 1:60:A:LYS:HB2  | 1:74:A:ALA:HB1  | 18       | 0.12          |
| (1,8)   | 1:60:A:LYS:HB2  | 1:74:A:ALA:HB2  | 18       | 0.12          |
| (1,8)   | 1:60:A:LYS:HB2  | 1:74:A:ALA:HB3  | 18       | 0.12          |
| (1,8)   | 1:60:A:LYS:HB3  | 1:74:A:ALA:HB1  | 18       | 0.12          |
| (1,8)   | 1:60:A:LYS:HB3  | 1:74:A:ALA:HB2  | 18       | 0.12          |
| (1,8)   | 1:60:A:LYS:HB3  | 1:74:A:ALA:HB3  | 18       | 0.12          |
| (1,6)   | 1:28:A:ILE:HG21 | 1:50:A:ILE:HB   | 18       | 0.12          |
| (1,6)   | 1:28:A:ILE:HG22 | 1:50:A:ILE:HB   | 18       | 0.12          |
| (1,6)   | 1:28:A:ILE:HG23 | 1:50:A:ILE:HB   | 18       | 0.12          |
| (1,4)   | 1:14:A:ILE:HD11 | 1:28:A:ILE:HB   | 16       | 0.12          |
| (1,4)   | 1:14:A:ILE:HD12 | 1:28:A:ILE:HB   | 16       | 0.12          |
| (1,4)   | 1:14:A:ILE:HD13 | 1:28:A:ILE:HB   | 16       | 0.12          |
| (1,4)   | 1:14:A:ILE:HD11 | 1:28:A:ILE:HB   | 17       | 0.12          |
| (1,4)   | 1:14:A:ILE:HD12 | 1:28:A:ILE:HB   | 17       | 0.12          |
| (1,4)   | 1:14:A:ILE:HD13 | 1:28:A:ILE:HB   | 17       | 0.12          |
| (1,821) | 1:64:A:GLY:HA2  | 1:65:A:VAL:HG11 | 1        | 0.11          |
| (1,821) | 1:64:A:GLY:HA2  | 1:65:A:VAL:HG12 | 1        | 0.11          |
| (1,821) | 1:64:A:GLY:HA2  | 1:65:A:VAL:HG13 | 1        | 0.11          |
| (1,821) | 1:64:A:GLY:HA2  | 1:65:A:VAL:HG21 | 1        | 0.11          |
| (1,821) | 1:64:A:GLY:HA2  | 1:65:A:VAL:HG22 | 1        | 0.11          |
| (1,821) | 1:64:A:GLY:HA2  | 1:65:A:VAL:HG23 | 1        | 0.11          |
| (1,821) | 1:64:A:GLY:HA3  | 1:65:A:VAL:HG11 | 1        | 0.11          |
| (1,821) | 1:64:A:GLY:HA3  | 1:65:A:VAL:HG12 | 1        | 0.11          |
| (1,821) | 1:64:A:GLY:HA3  | 1:65:A:VAL:HG13 | 1        | 0.11          |
| (1,821) | 1:64:A:GLY:HA3  | 1:65:A:VAL:HG21 | 1        | 0.11          |
| (1,821) | 1:64:A:GLY:HA3  | 1:65:A:VAL:HG22 | 1        | 0.11          |
| (1,821) | 1:64:A:GLY:HA3  | 1:65:A:VAL:HG23 | 1        | 0.11          |
| (1,821) | 1:64:A:GLY:HA2  | 1:65:A:VAL:HG11 | 4        | 0.11          |
| (1,821) | 1:64:A:GLY:HA2  | 1:65:A:VAL:HG12 | 4        | 0.11          |
| (1,821) | 1:64:A:GLY:HA2  | 1:65:A:VAL:HG13 | 4        | 0.11          |
| (1,821) | 1:64:A:GLY:HA2  | 1:65:A:VAL:HG21 | 4        | 0.11          |
| (1,821) | 1:64:A:GLY:HA2  | 1:65:A:VAL:HG22 | 4        | 0.11          |
| (1,821) | 1:64:A:GLY:HA2  | 1:65:A:VAL:HG23 | 4        | 0.11          |
| (1,821) | 1:64:A:GLY:HA3  | 1:65:A:VAL:HG11 | 4        | 0.11          |
| (1,821) | 1:64:A:GLY:HA3  | 1:65:A:VAL:HG12 | 4        | 0.11          |
| (1,821) | 1:64:A:GLY:HA3  | 1:65:A:VAL:HG13 | 4        | 0.11          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,821) | 1:64:A:GLY:HA3 | 1:65:A:VAL:HG21 | 4        | 0.11          |
| (1,821) | 1:64:A:GLY:HA3 | 1:65:A:VAL:HG22 | 4        | 0.11          |
| (1,821) | 1:64:A:GLY:HA3 | 1:65:A:VAL:HG23 | 4        | 0.11          |
| (1,821) | 1:64:A:GLY:HA2 | 1:65:A:VAL:HG11 | 6        | 0.11          |
| (1,821) | 1:64:A:GLY:HA2 | 1:65:A:VAL:HG12 | 6        | 0.11          |
| (1,821) | 1:64:A:GLY:HA2 | 1:65:A:VAL:HG13 | 6        | 0.11          |
| (1,821) | 1:64:A:GLY:HA2 | 1:65:A:VAL:HG21 | 6        | 0.11          |
| (1,821) | 1:64:A:GLY:HA2 | 1:65:A:VAL:HG22 | 6        | 0.11          |
| (1,821) | 1:64:A:GLY:HA2 | 1:65:A:VAL:HG23 | 6        | 0.11          |
| (1,821) | 1:64:A:GLY:HA3 | 1:65:A:VAL:HG11 | 6        | 0.11          |
| (1,821) | 1:64:A:GLY:HA3 | 1:65:A:VAL:HG12 | 6        | 0.11          |
| (1,821) | 1:64:A:GLY:HA3 | 1:65:A:VAL:HG13 | 6        | 0.11          |
| (1,821) | 1:64:A:GLY:HA3 | 1:65:A:VAL:HG21 | 6        | 0.11          |
| (1,821) | 1:64:A:GLY:HA3 | 1:65:A:VAL:HG22 | 6        | 0.11          |
| (1,821) | 1:64:A:GLY:HA3 | 1:65:A:VAL:HG23 | 6        | 0.11          |
| (1,821) | 1:64:A:GLY:HA2 | 1:65:A:VAL:HG11 | 12       | 0.11          |
| (1,821) | 1:64:A:GLY:HA2 | 1:65:A:VAL:HG12 | 12       | 0.11          |
| (1,821) | 1:64:A:GLY:HA2 | 1:65:A:VAL:HG13 | 12       | 0.11          |
| (1,821) | 1:64:A:GLY:HA2 | 1:65:A:VAL:HG21 | 12       | 0.11          |
| (1,821) | 1:64:A:GLY:HA2 | 1:65:A:VAL:HG22 | 12       | 0.11          |
| (1,821) | 1:64:A:GLY:HA2 | 1:65:A:VAL:HG23 | 12       | 0.11          |
| (1,821) | 1:64:A:GLY:HA3 | 1:65:A:VAL:HG11 | 12       | 0.11          |
| (1,821) | 1:64:A:GLY:HA3 | 1:65:A:VAL:HG12 | 12       | 0.11          |
| (1,821) | 1:64:A:GLY:HA3 | 1:65:A:VAL:HG13 | 12       | 0.11          |
| (1,821) | 1:64:A:GLY:HA3 | 1:65:A:VAL:HG21 | 12       | 0.11          |
| (1,821) | 1:64:A:GLY:HA3 | 1:65:A:VAL:HG22 | 12       | 0.11          |
| (1,821) | 1:64:A:GLY:HA3 | 1:65:A:VAL:HG23 | 12       | 0.11          |
| (1,821) | 1:64:A:GLY:HA2 | 1:65:A:VAL:HG11 | 16       | 0.11          |
| (1,821) | 1:64:A:GLY:HA2 | 1:65:A:VAL:HG12 | 16       | 0.11          |
| (1,821) | 1:64:A:GLY:HA2 | 1:65:A:VAL:HG13 | 16       | 0.11          |
| (1,821) | 1:64:A:GLY:HA2 | 1:65:A:VAL:HG21 | 16       | 0.11          |
| (1,821) | 1:64:A:GLY:HA2 | 1:65:A:VAL:HG22 | 16       | 0.11          |
| (1,821) | 1:64:A:GLY:HA2 | 1:65:A:VAL:HG23 | 16       | 0.11          |
| (1,821) | 1:64:A:GLY:HA3 | 1:65:A:VAL:HG11 | 16       | 0.11          |
| (1,821) | 1:64:A:GLY:HA3 | 1:65:A:VAL:HG12 | 16       | 0.11          |
| (1,821) | 1:64:A:GLY:HA3 | 1:65:A:VAL:HG13 | 16       | 0.11          |
| (1,821) | 1:64:A:GLY:HA3 | 1:65:A:VAL:HG21 | 16       | 0.11          |
| (1,821) | 1:64:A:GLY:HA3 | 1:65:A:VAL:HG22 | 16       | 0.11          |
| (1,821) | 1:64:A:GLY:HA3 | 1:65:A:VAL:HG23 | 16       | 0.11          |
| (1,821) | 1:64:A:GLY:HA2 | 1:65:A:VAL:HG11 | 20       | 0.11          |
| (1,821) | 1:64:A:GLY:HA2 | 1:65:A:VAL:HG12 | 20       | 0.11          |
| (1,821) | 1:64:A:GLY:HA2 | 1:65:A:VAL:HG13 | 20       | 0.11          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,821) | 1:64:A:GLY:HA2  | 1:65:A:VAL:HG21 | 20       | 0.11          |
| (1,821) | 1:64:A:GLY:HA2  | 1:65:A:VAL:HG22 | 20       | 0.11          |
| (1,821) | 1:64:A:GLY:HA2  | 1:65:A:VAL:HG23 | 20       | 0.11          |
| (1,821) | 1:64:A:GLY:HA3  | 1:65:A:VAL:HG11 | 20       | 0.11          |
| (1,821) | 1:64:A:GLY:HA3  | 1:65:A:VAL:HG12 | 20       | 0.11          |
| (1,821) | 1:64:A:GLY:HA3  | 1:65:A:VAL:HG13 | 20       | 0.11          |
| (1,821) | 1:64:A:GLY:HA3  | 1:65:A:VAL:HG21 | 20       | 0.11          |
| (1,821) | 1:64:A:GLY:HA3  | 1:65:A:VAL:HG22 | 20       | 0.11          |
| (1,821) | 1:64:A:GLY:HA3  | 1:65:A:VAL:HG23 | 20       | 0.11          |
| (1,754) | 1:45:A:GLN:HE21 | 1:48:A:LEU:HD11 | 14       | 0.11          |
| (1,754) | 1:45:A:GLN:HE21 | 1:48:A:LEU:HD12 | 14       | 0.11          |
| (1,754) | 1:45:A:GLN:HE21 | 1:48:A:LEU:HD13 | 14       | 0.11          |
| (1,754) | 1:45:A:GLN:HE21 | 1:48:A:LEU:HD21 | 14       | 0.11          |
| (1,754) | 1:45:A:GLN:HE21 | 1:48:A:LEU:HD22 | 14       | 0.11          |
| (1,754) | 1:45:A:GLN:HE21 | 1:48:A:LEU:HD23 | 14       | 0.11          |
| (1,754) | 1:45:A:GLN:HE22 | 1:48:A:LEU:HD11 | 14       | 0.11          |
| (1,754) | 1:45:A:GLN:HE22 | 1:48:A:LEU:HD12 | 14       | 0.11          |
| (1,754) | 1:45:A:GLN:HE22 | 1:48:A:LEU:HD13 | 14       | 0.11          |
| (1,754) | 1:45:A:GLN:HE22 | 1:48:A:LEU:HD21 | 14       | 0.11          |
| (1,754) | 1:45:A:GLN:HE22 | 1:48:A:LEU:HD22 | 14       | 0.11          |
| (1,754) | 1:45:A:GLN:HE22 | 1:48:A:LEU:HD23 | 14       | 0.11          |
| (1,732) | 1:37:A:LYS:HA   | 1:37:A:LYS:HD2  | 1        | 0.11          |
| (1,732) | 1:37:A:LYS:HA   | 1:37:A:LYS:HD3  | 1        | 0.11          |
| (1,732) | 1:37:A:LYS:HA   | 1:37:A:LYS:HD2  | 19       | 0.11          |
| (1,732) | 1:37:A:LYS:HA   | 1:37:A:LYS:HD3  | 19       | 0.11          |
| (1,644) | 1:10:A:ILE:HG12 | 1:14:A:ILE:HD11 | 18       | 0.11          |
| (1,644) | 1:10:A:ILE:HG12 | 1:14:A:ILE:HD12 | 18       | 0.11          |
| (1,644) | 1:10:A:ILE:HG12 | 1:14:A:ILE:HD13 | 18       | 0.11          |
| (1,644) | 1:10:A:ILE:HG13 | 1:14:A:ILE:HD11 | 18       | 0.11          |
| (1,644) | 1:10:A:ILE:HG13 | 1:14:A:ILE:HD12 | 18       | 0.11          |
| (1,644) | 1:10:A:ILE:HG13 | 1:14:A:ILE:HD13 | 18       | 0.11          |
| (1,636) | 1:9:A:MET:HA    | 1:11:A:VAL:HG11 | 1        | 0.11          |
| (1,636) | 1:9:A:MET:HA    | 1:11:A:VAL:HG12 | 1        | 0.11          |
| (1,636) | 1:9:A:MET:HA    | 1:11:A:VAL:HG13 | 1        | 0.11          |
| (1,636) | 1:9:A:MET:HA    | 1:11:A:VAL:HG21 | 1        | 0.11          |
| (1,636) | 1:9:A:MET:HA    | 1:11:A:VAL:HG22 | 1        | 0.11          |
| (1,636) | 1:9:A:MET:HA    | 1:11:A:VAL:HG23 | 1        | 0.11          |
| (1,636) | 1:9:A:MET:HA    | 1:11:A:VAL:HG11 | 7        | 0.11          |
| (1,636) | 1:9:A:MET:HA    | 1:11:A:VAL:HG12 | 7        | 0.11          |
| (1,636) | 1:9:A:MET:HA    | 1:11:A:VAL:HG13 | 7        | 0.11          |
| (1,636) | 1:9:A:MET:HA    | 1:11:A:VAL:HG21 | 7        | 0.11          |
| (1,636) | 1:9:A:MET:HA    | 1:11:A:VAL:HG22 | 7        | 0.11          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,636) | 1:9:A:MET:HA   | 1:11:A:VAL:HG23 | 7        | 0.11          |
| (1,636) | 1:9:A:MET:HA   | 1:11:A:VAL:HG11 | 12       | 0.11          |
| (1,636) | 1:9:A:MET:HA   | 1:11:A:VAL:HG12 | 12       | 0.11          |
| (1,636) | 1:9:A:MET:HA   | 1:11:A:VAL:HG13 | 12       | 0.11          |
| (1,636) | 1:9:A:MET:HA   | 1:11:A:VAL:HG21 | 12       | 0.11          |
| (1,636) | 1:9:A:MET:HA   | 1:11:A:VAL:HG22 | 12       | 0.11          |
| (1,636) | 1:9:A:MET:HA   | 1:11:A:VAL:HG23 | 12       | 0.11          |
| (1,636) | 1:9:A:MET:HA   | 1:11:A:VAL:HG11 | 13       | 0.11          |
| (1,636) | 1:9:A:MET:HA   | 1:11:A:VAL:HG12 | 13       | 0.11          |
| (1,636) | 1:9:A:MET:HA   | 1:11:A:VAL:HG13 | 13       | 0.11          |
| (1,636) | 1:9:A:MET:HA   | 1:11:A:VAL:HG21 | 13       | 0.11          |
| (1,636) | 1:9:A:MET:HA   | 1:11:A:VAL:HG22 | 13       | 0.11          |
| (1,636) | 1:9:A:MET:HA   | 1:11:A:VAL:HG23 | 13       | 0.11          |
| (1,636) | 1:9:A:MET:HA   | 1:11:A:VAL:HG11 | 15       | 0.11          |
| (1,636) | 1:9:A:MET:HA   | 1:11:A:VAL:HG12 | 15       | 0.11          |
| (1,636) | 1:9:A:MET:HA   | 1:11:A:VAL:HG13 | 15       | 0.11          |
| (1,636) | 1:9:A:MET:HA   | 1:11:A:VAL:HG21 | 15       | 0.11          |
| (1,636) | 1:9:A:MET:HA   | 1:11:A:VAL:HG22 | 15       | 0.11          |
| (1,636) | 1:9:A:MET:HA   | 1:11:A:VAL:HG23 | 15       | 0.11          |
| (1,636) | 1:9:A:MET:HA   | 1:11:A:VAL:HG11 | 18       | 0.11          |
| (1,636) | 1:9:A:MET:HA   | 1:11:A:VAL:HG12 | 18       | 0.11          |
| (1,636) | 1:9:A:MET:HA   | 1:11:A:VAL:HG13 | 18       | 0.11          |
| (1,636) | 1:9:A:MET:HA   | 1:11:A:VAL:HG21 | 18       | 0.11          |
| (1,636) | 1:9:A:MET:HA   | 1:11:A:VAL:HG22 | 18       | 0.11          |
| (1,636) | 1:9:A:MET:HA   | 1:11:A:VAL:HG23 | 18       | 0.11          |
| (1,628) | 1:7:A:SER:HB2  | 1:10:A:ILE:HG21 | 15       | 0.11          |
| (1,628) | 1:7:A:SER:HB2  | 1:10:A:ILE:HG22 | 15       | 0.11          |
| (1,628) | 1:7:A:SER:HB2  | 1:10:A:ILE:HG23 | 15       | 0.11          |
| (1,628) | 1:7:A:SER:HB3  | 1:10:A:ILE:HG21 | 15       | 0.11          |
| (1,628) | 1:7:A:SER:HB3  | 1:10:A:ILE:HG22 | 15       | 0.11          |
| (1,628) | 1:7:A:SER:HB3  | 1:10:A:ILE:HG23 | 15       | 0.11          |
| (1,628) | 1:7:A:SER:HB2  | 1:10:A:ILE:HG21 | 18       | 0.11          |
| (1,628) | 1:7:A:SER:HB2  | 1:10:A:ILE:HG22 | 18       | 0.11          |
| (1,628) | 1:7:A:SER:HB2  | 1:10:A:ILE:HG23 | 18       | 0.11          |
| (1,628) | 1:7:A:SER:HB3  | 1:10:A:ILE:HG21 | 18       | 0.11          |
| (1,628) | 1:7:A:SER:HB3  | 1:10:A:ILE:HG22 | 18       | 0.11          |
| (1,628) | 1:7:A:SER:HB3  | 1:10:A:ILE:HG23 | 18       | 0.11          |
| (1,575) | 1:12:A:ALA:HB1 | 1:36:A:TYR:HD1  | 3        | 0.11          |
| (1,575) | 1:12:A:ALA:HB1 | 1:36:A:TYR:HD2  | 3        | 0.11          |
| (1,575) | 1:12:A:ALA:HB2 | 1:36:A:TYR:HD1  | 3        | 0.11          |
| (1,575) | 1:12:A:ALA:HB2 | 1:36:A:TYR:HD2  | 3        | 0.11          |
| (1,575) | 1:12:A:ALA:HB3 | 1:36:A:TYR:HD1  | 3        | 0.11          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,575) | 1:12:A:ALA:HB3  | 1:36:A:TYR:HD2  | 3        | 0.11          |
| (1,575) | 1:12:A:ALA:HB1  | 1:36:A:TYR:HD1  | 17       | 0.11          |
| (1,575) | 1:12:A:ALA:HB1  | 1:36:A:TYR:HD2  | 17       | 0.11          |
| (1,575) | 1:12:A:ALA:HB2  | 1:36:A:TYR:HD1  | 17       | 0.11          |
| (1,575) | 1:12:A:ALA:HB2  | 1:36:A:TYR:HD2  | 17       | 0.11          |
| (1,575) | 1:12:A:ALA:HB3  | 1:36:A:TYR:HD1  | 17       | 0.11          |
| (1,575) | 1:12:A:ALA:HB3  | 1:36:A:TYR:HD2  | 17       | 0.11          |
| (1,575) | 1:12:A:ALA:HB1  | 1:36:A:TYR:HD1  | 18       | 0.11          |
| (1,575) | 1:12:A:ALA:HB1  | 1:36:A:TYR:HD2  | 18       | 0.11          |
| (1,575) | 1:12:A:ALA:HB2  | 1:36:A:TYR:HD1  | 18       | 0.11          |
| (1,575) | 1:12:A:ALA:HB2  | 1:36:A:TYR:HD2  | 18       | 0.11          |
| (1,575) | 1:12:A:ALA:HB3  | 1:36:A:TYR:HD1  | 18       | 0.11          |
| (1,575) | 1:12:A:ALA:HB3  | 1:36:A:TYR:HD2  | 18       | 0.11          |
| (1,573) | 1:32:A:ILE:HD11 | 1:36:A:TYR:HD1  | 14       | 0.11          |
| (1,573) | 1:32:A:ILE:HD11 | 1:36:A:TYR:HD2  | 14       | 0.11          |
| (1,573) | 1:32:A:ILE:HD12 | 1:36:A:TYR:HD1  | 14       | 0.11          |
| (1,573) | 1:32:A:ILE:HD12 | 1:36:A:TYR:HD2  | 14       | 0.11          |
| (1,573) | 1:32:A:ILE:HD13 | 1:36:A:TYR:HD1  | 14       | 0.11          |
| (1,573) | 1:32:A:ILE:HD13 | 1:36:A:TYR:HD2  | 14       | 0.11          |
| (1,565) | 1:31:A:TYR:HD1  | 1:35:A:HIS:HE1  | 6        | 0.11          |
| (1,565) | 1:31:A:TYR:HD2  | 1:35:A:HIS:HE1  | 6        | 0.11          |
| (1,526) | 1:59:A:LEU:HD11 | 1:74:A:ALA:H    | 13       | 0.11          |
| (1,526) | 1:59:A:LEU:HD12 | 1:74:A:ALA:H    | 13       | 0.11          |
| (1,526) | 1:59:A:LEU:HD13 | 1:74:A:ALA:H    | 13       | 0.11          |
| (1,526) | 1:59:A:LEU:HD21 | 1:74:A:ALA:H    | 13       | 0.11          |
| (1,526) | 1:59:A:LEU:HD22 | 1:74:A:ALA:H    | 13       | 0.11          |
| (1,526) | 1:59:A:LEU:HD23 | 1:74:A:ALA:H    | 13       | 0.11          |
| (1,493) | 1:13:A:ALA:HA   | 1:31:A:TYR:H    | 10       | 0.11          |
| (1,493) | 1:13:A:ALA:HA   | 1:31:A:TYR:H    | 19       | 0.11          |
| (1,398) | 1:46:A:ILE:HG21 | 1:51:A:LYS:H    | 11       | 0.11          |
| (1,398) | 1:46:A:ILE:HG22 | 1:51:A:LYS:H    | 11       | 0.11          |
| (1,398) | 1:46:A:ILE:HG23 | 1:51:A:LYS:H    | 11       | 0.11          |
| (1,388) | 1:63:A:LYS:HA   | 1:70:A:SER:H    | 3        | 0.11          |
| (1,344) | 1:52:A:ARG:HD2  | 1:55:A:THR:HG21 | 1        | 0.11          |
| (1,344) | 1:52:A:ARG:HD2  | 1:55:A:THR:HG22 | 1        | 0.11          |
| (1,344) | 1:52:A:ARG:HD2  | 1:55:A:THR:HG23 | 1        | 0.11          |
| (1,344) | 1:52:A:ARG:HD3  | 1:55:A:THR:HG21 | 1        | 0.11          |
| (1,344) | 1:52:A:ARG:HD3  | 1:55:A:THR:HG22 | 1        | 0.11          |
| (1,344) | 1:52:A:ARG:HD3  | 1:55:A:THR:HG23 | 1        | 0.11          |
| (1,344) | 1:52:A:ARG:HD2  | 1:55:A:THR:HG21 | 17       | 0.11          |
| (1,344) | 1:52:A:ARG:HD2  | 1:55:A:THR:HG22 | 17       | 0.11          |
| (1,344) | 1:52:A:ARG:HD2  | 1:55:A:THR:HG23 | 17       | 0.11          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,344) | 1:52:A:ARG:HD3  | 1:55:A:THR:HG21 | 17       | 0.11          |
| (1,344) | 1:52:A:ARG:HD3  | 1:55:A:THR:HG22 | 17       | 0.11          |
| (1,344) | 1:52:A:ARG:HD3  | 1:55:A:THR:HG23 | 17       | 0.11          |
| (1,344) | 1:52:A:ARG:HD2  | 1:55:A:THR:HG21 | 20       | 0.11          |
| (1,344) | 1:52:A:ARG:HD2  | 1:55:A:THR:HG22 | 20       | 0.11          |
| (1,344) | 1:52:A:ARG:HD2  | 1:55:A:THR:HG23 | 20       | 0.11          |
| (1,344) | 1:52:A:ARG:HD3  | 1:55:A:THR:HG21 | 20       | 0.11          |
| (1,344) | 1:52:A:ARG:HD3  | 1:55:A:THR:HG22 | 20       | 0.11          |
| (1,344) | 1:52:A:ARG:HD3  | 1:55:A:THR:HG23 | 20       | 0.11          |
| (1,343) | 1:52:A:ARG:HD2  | 1:55:A:THR:HG21 | 1        | 0.11          |
| (1,343) | 1:52:A:ARG:HD2  | 1:55:A:THR:HG22 | 1        | 0.11          |
| (1,343) | 1:52:A:ARG:HD2  | 1:55:A:THR:HG23 | 1        | 0.11          |
| (1,343) | 1:52:A:ARG:HD3  | 1:55:A:THR:HG21 | 1        | 0.11          |
| (1,343) | 1:52:A:ARG:HD3  | 1:55:A:THR:HG22 | 1        | 0.11          |
| (1,343) | 1:52:A:ARG:HD3  | 1:55:A:THR:HG23 | 1        | 0.11          |
| (1,343) | 1:52:A:ARG:HD2  | 1:55:A:THR:HG21 | 17       | 0.11          |
| (1,343) | 1:52:A:ARG:HD2  | 1:55:A:THR:HG22 | 17       | 0.11          |
| (1,343) | 1:52:A:ARG:HD2  | 1:55:A:THR:HG23 | 17       | 0.11          |
| (1,343) | 1:52:A:ARG:HD3  | 1:55:A:THR:HG21 | 17       | 0.11          |
| (1,343) | 1:52:A:ARG:HD3  | 1:55:A:THR:HG22 | 17       | 0.11          |
| (1,343) | 1:52:A:ARG:HD3  | 1:55:A:THR:HG23 | 17       | 0.11          |
| (1,343) | 1:52:A:ARG:HD2  | 1:55:A:THR:HG21 | 20       | 0.11          |
| (1,343) | 1:52:A:ARG:HD2  | 1:55:A:THR:HG22 | 20       | 0.11          |
| (1,343) | 1:52:A:ARG:HD2  | 1:55:A:THR:HG23 | 20       | 0.11          |
| (1,343) | 1:52:A:ARG:HD3  | 1:55:A:THR:HG21 | 20       | 0.11          |
| (1,343) | 1:52:A:ARG:HD3  | 1:55:A:THR:HG22 | 20       | 0.11          |
| (1,343) | 1:52:A:ARG:HD3  | 1:55:A:THR:HG23 | 20       | 0.11          |
| (1,322) | 1:15:A:GLN:HA   | 1:18:A:LYS:H    | 5        | 0.11          |
| (1,322) | 1:15:A:GLN:HA   | 1:18:A:LYS:H    | 16       | 0.11          |
| (1,230) | 1:11:A:VAL:HA   | 1:14:A:ILE:HD11 | 3        | 0.11          |
| (1,230) | 1:11:A:VAL:HA   | 1:14:A:ILE:HD12 | 3        | 0.11          |
| (1,230) | 1:11:A:VAL:HA   | 1:14:A:ILE:HD13 | 3        | 0.11          |
| (1,43)  | 1:46:A:ILE:HG21 | 1:50:A:ILE:HB   | 9        | 0.11          |
| (1,43)  | 1:46:A:ILE:HG22 | 1:50:A:ILE:HB   | 9        | 0.11          |
| (1,43)  | 1:46:A:ILE:HG23 | 1:50:A:ILE:HB   | 9        | 0.11          |
| (1,38)  | 1:12:A:ALA:HB1  | 1:32:A:ILE:HG21 | 20       | 0.11          |
| (1,38)  | 1:12:A:ALA:HB1  | 1:32:A:ILE:HG22 | 20       | 0.11          |
| (1,38)  | 1:12:A:ALA:HB1  | 1:32:A:ILE:HG23 | 20       | 0.11          |
| (1,38)  | 1:12:A:ALA:HB2  | 1:32:A:ILE:HG21 | 20       | 0.11          |
| (1,38)  | 1:12:A:ALA:HB2  | 1:32:A:ILE:HG22 | 20       | 0.11          |
| (1,38)  | 1:12:A:ALA:HB2  | 1:32:A:ILE:HG23 | 20       | 0.11          |
| (1,38)  | 1:12:A:ALA:HB3  | 1:32:A:ILE:HG21 | 20       | 0.11          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,38)  | 1:12:A:ALA:HB3  | 1:32:A:ILE:HG22 | 20       | 0.11          |
| (1,38)  | 1:12:A:ALA:HB3  | 1:32:A:ILE:HG23 | 20       | 0.11          |
| (1,13)  | 1:60:A:LYS:HA   | 1:72:A:ARG:HB2  | 1        | 0.11          |
| (1,13)  | 1:60:A:LYS:HA   | 1:72:A:ARG:HB3  | 1        | 0.11          |
| (1,13)  | 1:60:A:LYS:HA   | 1:72:A:ARG:HB2  | 12       | 0.11          |
| (1,13)  | 1:60:A:LYS:HA   | 1:72:A:ARG:HB3  | 12       | 0.11          |
| (1,13)  | 1:60:A:LYS:HA   | 1:72:A:ARG:HB2  | 14       | 0.11          |
| (1,13)  | 1:60:A:LYS:HA   | 1:72:A:ARG:HB3  | 14       | 0.11          |
| (1,13)  | 1:60:A:LYS:HA   | 1:72:A:ARG:HB2  | 18       | 0.11          |
| (1,13)  | 1:60:A:LYS:HA   | 1:72:A:ARG:HB3  | 18       | 0.11          |
| (1,821) | 1:64:A:GLY:HA2  | 1:65:A:VAL:HG11 | 7        | 0.1           |
| (1,821) | 1:64:A:GLY:HA2  | 1:65:A:VAL:HG12 | 7        | 0.1           |
| (1,821) | 1:64:A:GLY:HA2  | 1:65:A:VAL:HG13 | 7        | 0.1           |
| (1,821) | 1:64:A:GLY:HA2  | 1:65:A:VAL:HG21 | 7        | 0.1           |
| (1,821) | 1:64:A:GLY:HA2  | 1:65:A:VAL:HG22 | 7        | 0.1           |
| (1,821) | 1:64:A:GLY:HA2  | 1:65:A:VAL:HG23 | 7        | 0.1           |
| (1,821) | 1:64:A:GLY:HA3  | 1:65:A:VAL:HG11 | 7        | 0.1           |
| (1,821) | 1:64:A:GLY:HA3  | 1:65:A:VAL:HG12 | 7        | 0.1           |
| (1,821) | 1:64:A:GLY:HA3  | 1:65:A:VAL:HG13 | 7        | 0.1           |
| (1,821) | 1:64:A:GLY:HA3  | 1:65:A:VAL:HG21 | 7        | 0.1           |
| (1,821) | 1:64:A:GLY:HA3  | 1:65:A:VAL:HG22 | 7        | 0.1           |
| (1,821) | 1:64:A:GLY:HA3  | 1:65:A:VAL:HG23 | 7        | 0.1           |
| (1,821) | 1:64:A:GLY:HA2  | 1:65:A:VAL:HG11 | 15       | 0.1           |
| (1,821) | 1:64:A:GLY:HA2  | 1:65:A:VAL:HG12 | 15       | 0.1           |
| (1,821) | 1:64:A:GLY:HA2  | 1:65:A:VAL:HG13 | 15       | 0.1           |
| (1,821) | 1:64:A:GLY:HA2  | 1:65:A:VAL:HG21 | 15       | 0.1           |
| (1,821) | 1:64:A:GLY:HA2  | 1:65:A:VAL:HG22 | 15       | 0.1           |
| (1,821) | 1:64:A:GLY:HA2  | 1:65:A:VAL:HG23 | 15       | 0.1           |
| (1,821) | 1:64:A:GLY:HA3  | 1:65:A:VAL:HG11 | 15       | 0.1           |
| (1,821) | 1:64:A:GLY:HA3  | 1:65:A:VAL:HG12 | 15       | 0.1           |
| (1,821) | 1:64:A:GLY:HA3  | 1:65:A:VAL:HG13 | 15       | 0.1           |
| (1,821) | 1:64:A:GLY:HA3  | 1:65:A:VAL:HG21 | 15       | 0.1           |
| (1,821) | 1:64:A:GLY:HA3  | 1:65:A:VAL:HG22 | 15       | 0.1           |
| (1,821) | 1:64:A:GLY:HA3  | 1:65:A:VAL:HG23 | 15       | 0.1           |
| (1,754) | 1:45:A:GLN:HE21 | 1:48:A:LEU:HD11 | 3        | 0.1           |
| (1,754) | 1:45:A:GLN:HE21 | 1:48:A:LEU:HD12 | 3        | 0.1           |
| (1,754) | 1:45:A:GLN:HE21 | 1:48:A:LEU:HD13 | 3        | 0.1           |
| (1,754) | 1:45:A:GLN:HE21 | 1:48:A:LEU:HD21 | 3        | 0.1           |
| (1,754) | 1:45:A:GLN:HE21 | 1:48:A:LEU:HD22 | 3        | 0.1           |
| (1,754) | 1:45:A:GLN:HE21 | 1:48:A:LEU:HD23 | 3        | 0.1           |
| (1,754) | 1:45:A:GLN:HE22 | 1:48:A:LEU:HD11 | 3        | 0.1           |
| (1,754) | 1:45:A:GLN:HE22 | 1:48:A:LEU:HD12 | 3        | 0.1           |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,754) | 1:45:A:GLN:HE22 | 1:48:A:LEU:HD13 | 3        | 0.1           |
| (1,754) | 1:45:A:GLN:HE22 | 1:48:A:LEU:HD21 | 3        | 0.1           |
| (1,754) | 1:45:A:GLN:HE22 | 1:48:A:LEU:HD22 | 3        | 0.1           |
| (1,754) | 1:45:A:GLN:HE22 | 1:48:A:LEU:HD23 | 3        | 0.1           |
| (1,754) | 1:45:A:GLN:HE21 | 1:48:A:LEU:HD11 | 15       | 0.1           |
| (1,754) | 1:45:A:GLN:HE21 | 1:48:A:LEU:HD12 | 15       | 0.1           |
| (1,754) | 1:45:A:GLN:HE21 | 1:48:A:LEU:HD13 | 15       | 0.1           |
| (1,754) | 1:45:A:GLN:HE21 | 1:48:A:LEU:HD21 | 15       | 0.1           |
| (1,754) | 1:45:A:GLN:HE21 | 1:48:A:LEU:HD22 | 15       | 0.1           |
| (1,754) | 1:45:A:GLN:HE21 | 1:48:A:LEU:HD23 | 15       | 0.1           |
| (1,754) | 1:45:A:GLN:HE22 | 1:48:A:LEU:HD11 | 15       | 0.1           |
| (1,754) | 1:45:A:GLN:HE22 | 1:48:A:LEU:HD12 | 15       | 0.1           |
| (1,754) | 1:45:A:GLN:HE22 | 1:48:A:LEU:HD13 | 15       | 0.1           |
| (1,754) | 1:45:A:GLN:HE22 | 1:48:A:LEU:HD21 | 15       | 0.1           |
| (1,754) | 1:45:A:GLN:HE22 | 1:48:A:LEU:HD22 | 15       | 0.1           |
| (1,754) | 1:45:A:GLN:HE22 | 1:48:A:LEU:HD23 | 15       | 0.1           |
| (1,748) | 1:45:A:GLN:H    | 1:46:A:ILE:HG12 | 11       | 0.1           |
| (1,748) | 1:45:A:GLN:H    | 1:46:A:ILE:HG13 | 11       | 0.1           |
| (1,668) | 1:17:A:GLU:HG2  | 1:19:A:ASN:H    | 14       | 0.1           |
| (1,668) | 1:17:A:GLU:HG3  | 1:19:A:ASN:H    | 14       | 0.1           |
| (1,636) | 1:9:A:MET:HA    | 1:11:A:VAL:HG11 | 4        | 0.1           |
| (1,636) | 1:9:A:MET:HA    | 1:11:A:VAL:HG12 | 4        | 0.1           |
| (1,636) | 1:9:A:MET:HA    | 1:11:A:VAL:HG13 | 4        | 0.1           |
| (1,636) | 1:9:A:MET:HA    | 1:11:A:VAL:HG21 | 4        | 0.1           |
| (1,636) | 1:9:A:MET:HA    | 1:11:A:VAL:HG22 | 4        | 0.1           |
| (1,636) | 1:9:A:MET:HA    | 1:11:A:VAL:HG23 | 4        | 0.1           |
| (1,628) | 1:7:A:SER:HB2   | 1:10:A:ILE:HG21 | 3        | 0.1           |
| (1,628) | 1:7:A:SER:HB2   | 1:10:A:ILE:HG22 | 3        | 0.1           |
| (1,628) | 1:7:A:SER:HB2   | 1:10:A:ILE:HG23 | 3        | 0.1           |
| (1,628) | 1:7:A:SER:HB3   | 1:10:A:ILE:HG21 | 3        | 0.1           |
| (1,628) | 1:7:A:SER:HB3   | 1:10:A:ILE:HG22 | 3        | 0.1           |
| (1,628) | 1:7:A:SER:HB3   | 1:10:A:ILE:HG23 | 3        | 0.1           |
| (1,628) | 1:7:A:SER:HB2   | 1:10:A:ILE:HG21 | 12       | 0.1           |
| (1,628) | 1:7:A:SER:HB2   | 1:10:A:ILE:HG22 | 12       | 0.1           |
| (1,628) | 1:7:A:SER:HB2   | 1:10:A:ILE:HG23 | 12       | 0.1           |
| (1,628) | 1:7:A:SER:HB3   | 1:10:A:ILE:HG21 | 12       | 0.1           |
| (1,628) | 1:7:A:SER:HB3   | 1:10:A:ILE:HG22 | 12       | 0.1           |
| (1,628) | 1:7:A:SER:HB3   | 1:10:A:ILE:HG23 | 12       | 0.1           |
| (1,565) | 1:31:A:TYR:HD1  | 1:35:A:HIS:HE1  | 8        | 0.1           |
| (1,565) | 1:31:A:TYR:HD2  | 1:35:A:HIS:HE1  | 8        | 0.1           |
| (1,493) | 1:13:A:ALA:HA   | 1:31:A:TYR:H    | 9        | 0.1           |
| (1,398) | 1:46:A:ILE:HG21 | 1:51:A:LYS:H    | 3        | 0.1           |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,398) | 1:46:A:ILE:HG22 | 1:51:A:LYS:H    | 3        | 0.1           |
| (1,398) | 1:46:A:ILE:HG23 | 1:51:A:LYS:H    | 3        | 0.1           |
| (1,398) | 1:46:A:ILE:HG21 | 1:51:A:LYS:H    | 10       | 0.1           |
| (1,398) | 1:46:A:ILE:HG22 | 1:51:A:LYS:H    | 10       | 0.1           |
| (1,398) | 1:46:A:ILE:HG23 | 1:51:A:LYS:H    | 10       | 0.1           |
| (1,398) | 1:46:A:ILE:HG21 | 1:51:A:LYS:H    | 17       | 0.1           |
| (1,398) | 1:46:A:ILE:HG22 | 1:51:A:LYS:H    | 17       | 0.1           |
| (1,398) | 1:46:A:ILE:HG23 | 1:51:A:LYS:H    | 17       | 0.1           |
| (1,388) | 1:63:A:LYS:HA   | 1:70:A:SER:H    | 7        | 0.1           |
| (1,290) | 1:6:A:TYR:HE1   | 1:10:A:ILE:HD11 | 14       | 0.1           |
| (1,290) | 1:6:A:TYR:HE1   | 1:10:A:ILE:HD12 | 14       | 0.1           |
| (1,290) | 1:6:A:TYR:HE1   | 1:10:A:ILE:HD13 | 14       | 0.1           |
| (1,290) | 1:6:A:TYR:HE2   | 1:10:A:ILE:HD11 | 14       | 0.1           |
| (1,290) | 1:6:A:TYR:HE2   | 1:10:A:ILE:HD12 | 14       | 0.1           |
| (1,290) | 1:6:A:TYR:HE2   | 1:10:A:ILE:HD13 | 14       | 0.1           |
| (1,290) | 1:6:A:TYR:HE1   | 1:10:A:ILE:HD11 | 20       | 0.1           |
| (1,290) | 1:6:A:TYR:HE1   | 1:10:A:ILE:HD12 | 20       | 0.1           |
| (1,290) | 1:6:A:TYR:HE1   | 1:10:A:ILE:HD13 | 20       | 0.1           |
| (1,290) | 1:6:A:TYR:HE2   | 1:10:A:ILE:HD11 | 20       | 0.1           |
| (1,290) | 1:6:A:TYR:HE2   | 1:10:A:ILE:HD12 | 20       | 0.1           |
| (1,290) | 1:6:A:TYR:HE2   | 1:10:A:ILE:HD13 | 20       | 0.1           |
| (1,38)  | 1:12:A:ALA:HB1  | 1:32:A:ILE:HG21 | 7        | 0.1           |
| (1,38)  | 1:12:A:ALA:HB1  | 1:32:A:ILE:HG22 | 7        | 0.1           |
| (1,38)  | 1:12:A:ALA:HB1  | 1:32:A:ILE:HG23 | 7        | 0.1           |
| (1,38)  | 1:12:A:ALA:HB2  | 1:32:A:ILE:HG21 | 7        | 0.1           |
| (1,38)  | 1:12:A:ALA:HB2  | 1:32:A:ILE:HG22 | 7        | 0.1           |
| (1,38)  | 1:12:A:ALA:HB2  | 1:32:A:ILE:HG23 | 7        | 0.1           |
| (1,38)  | 1:12:A:ALA:HB3  | 1:32:A:ILE:HG21 | 7        | 0.1           |
| (1,38)  | 1:12:A:ALA:HB3  | 1:32:A:ILE:HG22 | 7        | 0.1           |
| (1,38)  | 1:12:A:ALA:HB3  | 1:32:A:ILE:HG23 | 7        | 0.1           |
| (1,38)  | 1:12:A:ALA:HB1  | 1:32:A:ILE:HG21 | 18       | 0.1           |
| (1,38)  | 1:12:A:ALA:HB1  | 1:32:A:ILE:HG22 | 18       | 0.1           |
| (1,38)  | 1:12:A:ALA:HB1  | 1:32:A:ILE:HG23 | 18       | 0.1           |
| (1,38)  | 1:12:A:ALA:HB2  | 1:32:A:ILE:HG21 | 18       | 0.1           |
| (1,38)  | 1:12:A:ALA:HB2  | 1:32:A:ILE:HG22 | 18       | 0.1           |
| (1,38)  | 1:12:A:ALA:HB2  | 1:32:A:ILE:HG23 | 18       | 0.1           |
| (1,38)  | 1:12:A:ALA:HB3  | 1:32:A:ILE:HG21 | 18       | 0.1           |
| (1,38)  | 1:12:A:ALA:HB3  | 1:32:A:ILE:HG22 | 18       | 0.1           |
| (1,38)  | 1:12:A:ALA:HB3  | 1:32:A:ILE:HG23 | 18       | 0.1           |
| (1,13)  | 1:60:A:LYS:HA   | 1:72:A:ARG:HB2  | 2        | 0.1           |
| (1,13)  | 1:60:A:LYS:HA   | 1:72:A:ARG:HB3  | 2        | 0.1           |
| (1,13)  | 1:60:A:LYS:HA   | 1:72:A:ARG:HB2  | 9        | 0.1           |

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| Key    | Atom-1        | Atom-2         | Model ID | Violation (Å) |
|--------|---------------|----------------|----------|---------------|
| (1,13) | 1:60:A:LYS:HA | 1:72:A:ARG:HB3 | 9        | 0.1           |

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

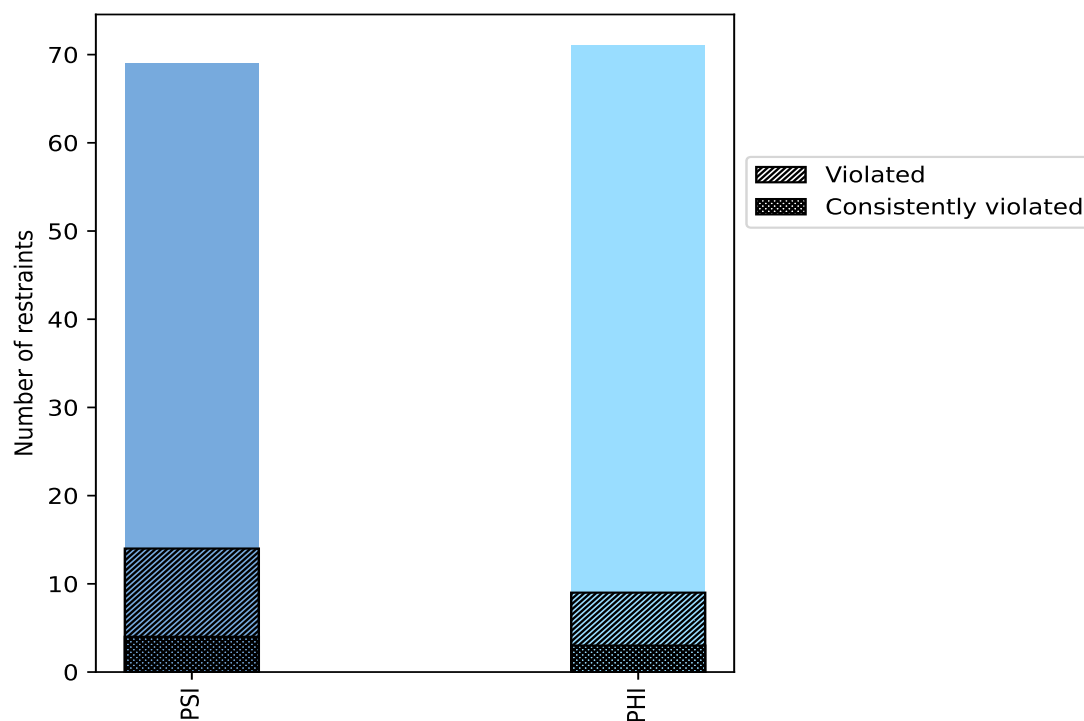
### 10.1 Summary of dihedral-angle violations [i](#)

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

| Angle type | Count | % <sup>1</sup> | Violated <sup>3</sup> |                |                | Consistently Violated <sup>4</sup> |                |                |
|------------|-------|----------------|-----------------------|----------------|----------------|------------------------------------|----------------|----------------|
|            |       |                | Count                 | % <sup>2</sup> | % <sup>1</sup> | Count                              | % <sup>2</sup> | % <sup>1</sup> |
| PSI        | 69    | 49.3           | 14                    | 20.3           | 10.0           | 4                                  | 5.8            | 2.9            |
| PHI        | 71    | 50.7           | 9                     | 12.7           | 6.4            | 3                                  | 4.2            | 2.1            |
| Total      | 140   | 100.0          | 23                    | 16.4           | 16.4           | 7                                  | 5.0            | 5.0            |

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

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



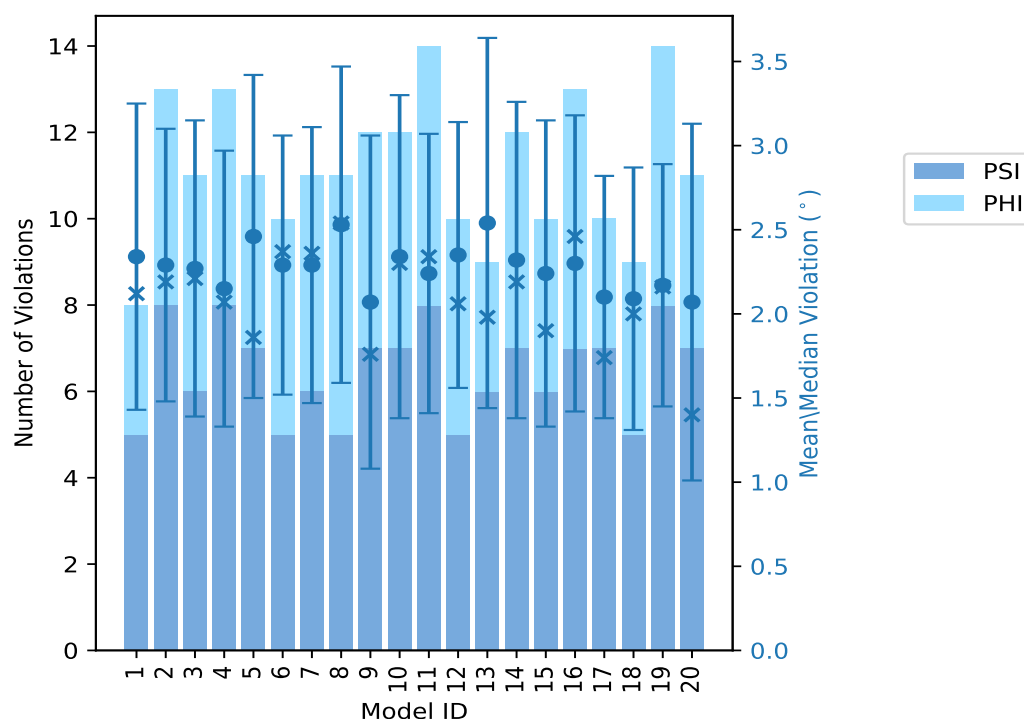
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

## 10.2 Dihedral-angle violation statistics for each model

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

| Model ID | Number of violations |     |       | Mean (°) | Max (°) | SD (°) | Median (°) |
|----------|----------------------|-----|-------|----------|---------|--------|------------|
|          | PSI                  | PHI | Total |          |         |        |            |
| 1        | 5                    | 3   | 8     | 2.34     | 4.11    | 0.91   | 2.12       |
| 2        | 8                    | 5   | 13    | 2.29     | 4.09    | 0.81   | 2.19       |
| 3        | 6                    | 5   | 11    | 2.27     | 4.51    | 0.88   | 2.21       |
| 4        | 8                    | 5   | 13    | 2.15     | 3.77    | 0.82   | 2.07       |
| 5        | 7                    | 4   | 11    | 2.46     | 4.26    | 0.96   | 1.86       |
| 6        | 5                    | 5   | 10    | 2.29     | 3.87    | 0.77   | 2.37       |
| 7        | 6                    | 5   | 11    | 2.29     | 4.04    | 0.82   | 2.36       |
| 8        | 5                    | 6   | 11    | 2.53     | 4.17    | 0.94   | 2.54       |
| 9        | 7                    | 5   | 12    | 2.07     | 4.15    | 0.99   | 1.76       |
| 10       | 7                    | 5   | 12    | 2.34     | 4.66    | 0.96   | 2.3        |
| 11       | 8                    | 6   | 14    | 2.24     | 4.21    | 0.83   | 2.34       |
| 12       | 5                    | 5   | 10    | 2.35     | 4.27    | 0.79   | 2.06       |
| 13       | 6                    | 3   | 9     | 2.54     | 4.36    | 1.1    | 1.98       |
| 14       | 7                    | 5   | 12    | 2.32     | 3.98    | 0.94   | 2.19       |
| 15       | 6                    | 4   | 10    | 2.24     | 3.87    | 0.91   | 1.9        |
| 16       | 7                    | 6   | 13    | 2.3      | 3.87    | 0.88   | 2.46       |
| 17       | 7                    | 3   | 10    | 2.1      | 3.86    | 0.72   | 1.74       |
| 18       | 5                    | 4   | 9     | 2.09     | 3.86    | 0.78   | 2.0        |
| 19       | 8                    | 6   | 14    | 2.17     | 4.09    | 0.72   | 2.16       |
| 20       | 7                    | 4   | 11    | 2.07     | 4.09    | 1.06   | 1.4        |

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



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

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

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

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

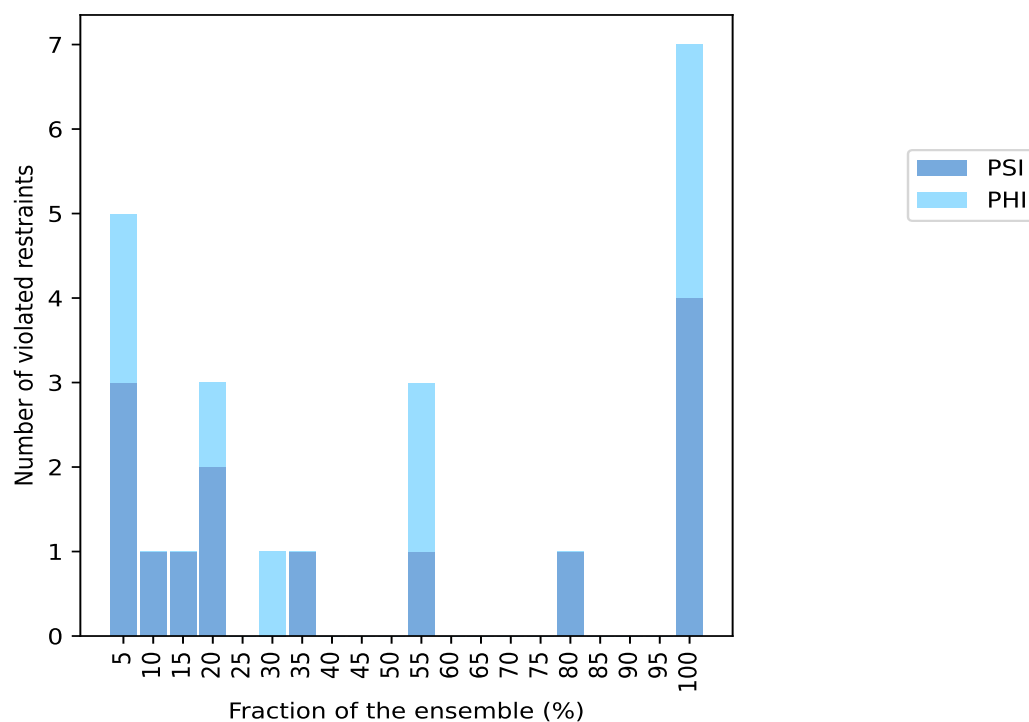
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| Number of violated restraints |     |       | Fraction of the ensemble |       |
|-------------------------------|-----|-------|--------------------------|-------|
| PSI                           | PHI | Total | Count <sup>1</sup>       | %     |
| 0                             | 0   | 0     | 12                       | 60.0  |
| 0                             | 0   | 0     | 13                       | 65.0  |
| 0                             | 0   | 0     | 14                       | 70.0  |
| 0                             | 0   | 0     | 15                       | 75.0  |
| 1                             | 0   | 1     | 16                       | 80.0  |
| 0                             | 0   | 0     | 17                       | 85.0  |
| 0                             | 0   | 0     | 18                       | 90.0  |
| 0                             | 0   | 0     | 19                       | 95.0  |
| 4                             | 3   | 7     | 20                       | 100.0 |

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

### 10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble ⓘ

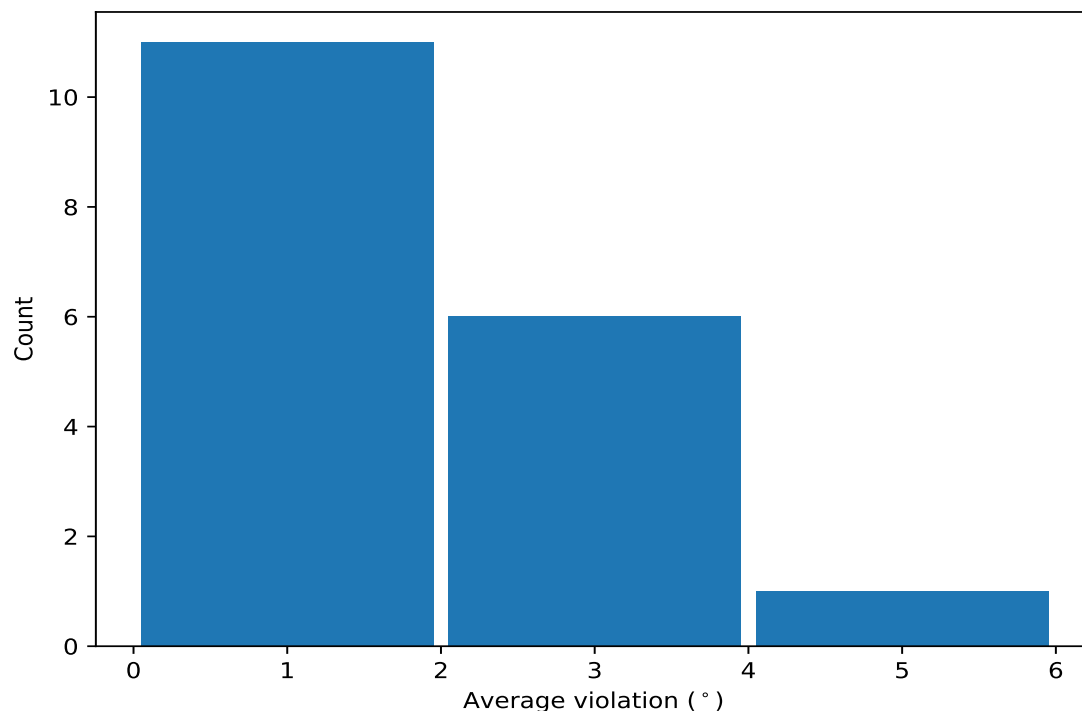


## 10.4 Most violated dihedral-angle restraints in the ensemble ⓘ

### 10.4.1 Histogram : Distribution of mean dihedral-angle 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



#### 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.

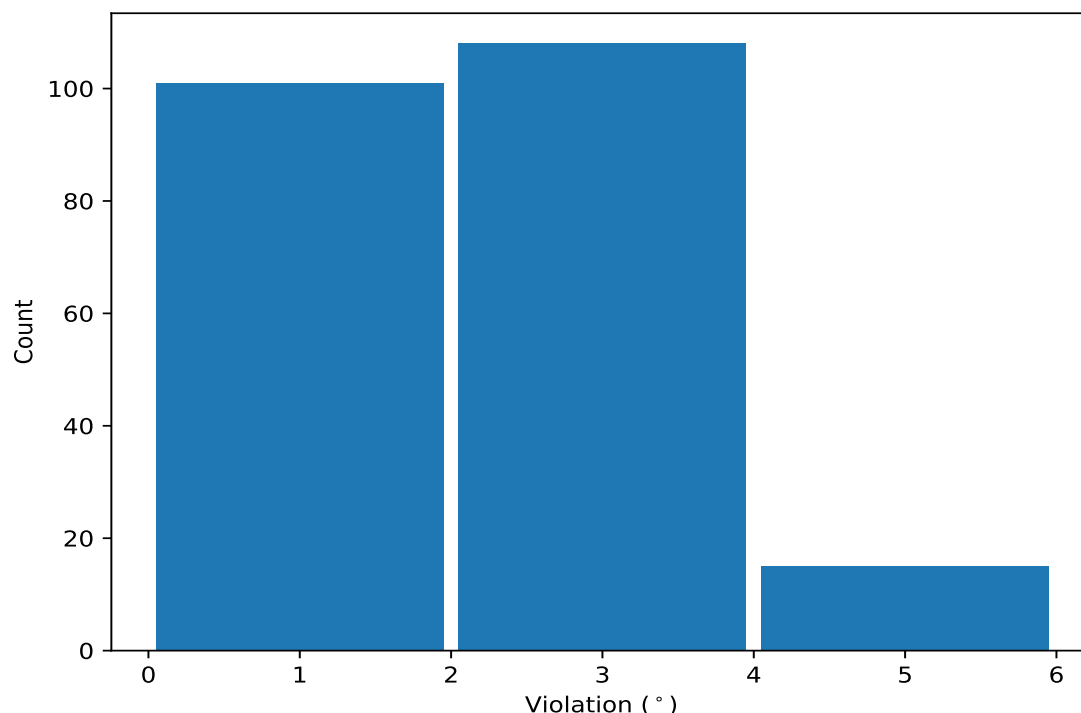
| Key     | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Models <sup>1</sup> | Mean | SD <sup>2</sup> | Median |
|---------|--------------|---------------|---------------|--------------|---------------------|------|-----------------|--------|
| (1,126) | 1:66:A:GLY:C | 1:67:A:ALA:N  | 1:67:A:ALA:CA | 1:67:A:ALA:C | 20                  | 4.1  | 0.23            | 4.09   |
| (1,128) | 1:67:A:ALA:C | 1:68:A:SER:N  | 1:68:A:SER:CA | 1:68:A:SER:C | 20                  | 3.23 | 0.52            | 3.26   |
| (1,50)  | 1:28:A:ILE:C | 1:29:A:GLN:N  | 1:29:A:GLN:CA | 1:29:A:GLN:C | 20                  | 2.49 | 0.37            | 2.52   |
| (1,125) | 1:67:A:ALA:N | 1:67:A:ALA:CA | 1:67:A:ALA:C  | 1:68:A:SER:N | 20                  | 2.47 | 0.49            | 2.37   |
| (1,129) | 1:69:A:GLY:N | 1:69:A:GLY:CA | 1:69:A:GLY:C  | 1:70:A:SER:N | 20                  | 1.95 | 0.31            | 1.96   |
| (1,115) | 1:62:A:THR:N | 1:62:A:THR:CA | 1:62:A:THR:C  | 1:63:A:LYS:N | 20                  | 1.73 | 0.24            | 1.76   |
| (1,123) | 1:66:A:GLY:N | 1:66:A:GLY:CA | 1:66:A:GLY:C  | 1:67:A:ALA:N | 20                  | 1.62 | 0.34            | 1.5    |
| (1,28)  | 1:18:A:LYS:N | 1:18:A:LYS:CA | 1:18:A:LYS:C  | 1:19:A:ASN:N | 16                  | 2.34 | 0.73            | 2.55   |
| (1,103) | 1:56:A:THR:N | 1:56:A:THR:CA | 1:56:A:THR:C  | 1:57:A:GLY:N | 11                  | 2.64 | 0.11            | 2.65   |
| (1,104) | 1:55:A:THR:C | 1:56:A:THR:N  | 1:56:A:THR:CA | 1:56:A:THR:C | 11                  | 2.58 | 0.19            | 2.58   |
| (1,5)   | 1:4:A:PRO:C  | 1:5:A:LYS:N   | 1:5:A:LYS:CA  | 1:5:A:LYS:C  | 11                  | 1.4  | 0.33            | 1.32   |
| (1,137) | 1:73:A:LEU:N | 1:73:A:LEU:CA | 1:73:A:LEU:C  | 1:74:A:ALA:N | 7                   | 1.29 | 0.26            | 1.24   |
| (1,3)   | 1:3:A:HIS:C  | 1:4:A:PRO:N   | 1:4:A:PRO:CA  | 1:4:A:PRO:C  | 6                   | 1.22 | 0.18            | 1.14   |
| (1,7)   | 1:5:A:LYS:C  | 1:6:A:TYR:N   | 1:6:A:TYR:CA  | 1:6:A:TYR:C  | 4                   | 1.65 | 0.25            | 1.66   |
| (1,75)  | 1:42:A:ALA:N | 1:42:A:ALA:CA | 1:42:A:ALA:C  | 1:43:A:ASP:N | 4                   | 1.3  | 0.17            | 1.38   |
| (1,111) | 1:60:A:LYS:N | 1:60:A:LYS:CA | 1:60:A:LYS:C  | 1:61:A:GLN:N | 4                   | 1.22 | 0.04            | 1.21   |
| (1,113) | 1:61:A:GLN:N | 1:61:A:GLN:CA | 1:61:A:GLN:C  | 1:62:A:THR:N | 3                   | 1.59 | 0.13            | 1.5    |
| (1,49)  | 1:29:A:GLN:N | 1:29:A:GLN:CA | 1:29:A:GLN:C  | 1:30:A:LYS:N | 2                   | 1.1  | 0.1             | 1.1    |

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

## 10.5 All violated dihedral-angle restraints [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 (°) |
|---------|--------------|--------------|---------------|--------------|----------|---------------|
| (1,126) | 1:66:A:GLY:C | 1:67:A:ALA:N | 1:67:A:ALA:CA | 1:67:A:ALA:C | 10       | 4.66          |
| (1,126) | 1:66:A:GLY:C | 1:67:A:ALA:N | 1:67:A:ALA:CA | 1:67:A:ALA:C | 3        | 4.51          |
| (1,126) | 1:66:A:GLY:C | 1:67:A:ALA:N | 1:67:A:ALA:CA | 1:67:A:ALA:C | 13       | 4.36          |
| (1,126) | 1:66:A:GLY:C | 1:67:A:ALA:N | 1:67:A:ALA:CA | 1:67:A:ALA:C | 12       | 4.27          |
| (1,126) | 1:66:A:GLY:C | 1:67:A:ALA:N | 1:67:A:ALA:CA | 1:67:A:ALA:C | 5        | 4.26          |
| (1,126) | 1:66:A:GLY:C | 1:67:A:ALA:N | 1:67:A:ALA:CA | 1:67:A:ALA:C | 11       | 4.21          |
| (1,126) | 1:66:A:GLY:C | 1:67:A:ALA:N | 1:67:A:ALA:CA | 1:67:A:ALA:C | 8        | 4.17          |
| (1,126) | 1:66:A:GLY:C | 1:67:A:ALA:N | 1:67:A:ALA:CA | 1:67:A:ALA:C | 9        | 4.15          |
| (1,128) | 1:67:A:ALA:C | 1:68:A:SER:N | 1:68:A:SER:CA | 1:68:A:SER:C | 8        | 4.12          |
| (1,126) | 1:66:A:GLY:C | 1:67:A:ALA:N | 1:67:A:ALA:CA | 1:67:A:ALA:C | 1        | 4.11          |
| (1,126) | 1:66:A:GLY:C | 1:67:A:ALA:N | 1:67:A:ALA:CA | 1:67:A:ALA:C | 2        | 4.09          |
| (1,126) | 1:66:A:GLY:C | 1:67:A:ALA:N | 1:67:A:ALA:CA | 1:67:A:ALA:C | 19       | 4.09          |
| (1,126) | 1:66:A:GLY:C | 1:67:A:ALA:N | 1:67:A:ALA:CA | 1:67:A:ALA:C | 20       | 4.09          |
| (1,128) | 1:67:A:ALA:C | 1:68:A:SER:N | 1:68:A:SER:CA | 1:68:A:SER:C | 13       | 4.08          |

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| Key     | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Model ID | Violation (°) |
|---------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,126) | 1:66:A:GLY:C | 1:67:A:ALA:N  | 1:67:A:ALA:CA | 1:67:A:ALA:C | 7        | 4.04          |
| (1,126) | 1:66:A:GLY:C | 1:67:A:ALA:N  | 1:67:A:ALA:CA | 1:67:A:ALA:C | 14       | 3.98          |
| (1,126) | 1:66:A:GLY:C | 1:67:A:ALA:N  | 1:67:A:ALA:CA | 1:67:A:ALA:C | 6        | 3.87          |
| (1,126) | 1:66:A:GLY:C | 1:67:A:ALA:N  | 1:67:A:ALA:CA | 1:67:A:ALA:C | 15       | 3.87          |
| (1,126) | 1:66:A:GLY:C | 1:67:A:ALA:N  | 1:67:A:ALA:CA | 1:67:A:ALA:C | 16       | 3.87          |
| (1,126) | 1:66:A:GLY:C | 1:67:A:ALA:N  | 1:67:A:ALA:CA | 1:67:A:ALA:C | 17       | 3.86          |
| (1,126) | 1:66:A:GLY:C | 1:67:A:ALA:N  | 1:67:A:ALA:CA | 1:67:A:ALA:C | 18       | 3.86          |
| (1,128) | 1:67:A:ALA:C | 1:68:A:SER:N  | 1:68:A:SER:CA | 1:68:A:SER:C | 5        | 3.81          |
| (1,126) | 1:66:A:GLY:C | 1:67:A:ALA:N  | 1:67:A:ALA:CA | 1:67:A:ALA:C | 4        | 3.77          |
| (1,128) | 1:67:A:ALA:C | 1:68:A:SER:N  | 1:68:A:SER:CA | 1:68:A:SER:C | 9        | 3.76          |
| (1,128) | 1:67:A:ALA:C | 1:68:A:SER:N  | 1:68:A:SER:CA | 1:68:A:SER:C | 14       | 3.72          |
| (1,128) | 1:67:A:ALA:C | 1:68:A:SER:N  | 1:68:A:SER:CA | 1:68:A:SER:C | 20       | 3.55          |
| (1,125) | 1:67:A:ALA:N | 1:67:A:ALA:CA | 1:67:A:ALA:C  | 1:68:A:SER:N | 13       | 3.44          |
| (1,128) | 1:67:A:ALA:C | 1:68:A:SER:N  | 1:68:A:SER:CA | 1:68:A:SER:C | 10       | 3.4           |
| (1,28)  | 1:18:A:LYS:N | 1:18:A:LYS:CA | 1:18:A:LYS:C  | 1:19:A:ASN:N | 5        | 3.36          |
| (1,128) | 1:67:A:ALA:C | 1:68:A:SER:N  | 1:68:A:SER:CA | 1:68:A:SER:C | 16       | 3.32          |
| (1,125) | 1:67:A:ALA:N | 1:67:A:ALA:CA | 1:67:A:ALA:C  | 1:68:A:SER:N | 20       | 3.29          |
| (1,128) | 1:67:A:ALA:C | 1:68:A:SER:N  | 1:68:A:SER:CA | 1:68:A:SER:C | 7        | 3.28          |
| (1,128) | 1:67:A:ALA:C | 1:68:A:SER:N  | 1:68:A:SER:CA | 1:68:A:SER:C | 2        | 3.26          |
| (1,128) | 1:67:A:ALA:C | 1:68:A:SER:N  | 1:68:A:SER:CA | 1:68:A:SER:C | 12       | 3.26          |
| (1,128) | 1:67:A:ALA:C | 1:68:A:SER:N  | 1:68:A:SER:CA | 1:68:A:SER:C | 11       | 3.24          |
| (1,28)  | 1:18:A:LYS:N | 1:18:A:LYS:CA | 1:18:A:LYS:C  | 1:19:A:ASN:N | 15       | 3.21          |
| (1,128) | 1:67:A:ALA:C | 1:68:A:SER:N  | 1:68:A:SER:CA | 1:68:A:SER:C | 1        | 3.18          |
| (1,50)  | 1:28:A:ILE:C | 1:29:A:GLN:N  | 1:29:A:GLN:CA | 1:29:A:GLN:C | 16       | 3.16          |
| (1,128) | 1:67:A:ALA:C | 1:68:A:SER:N  | 1:68:A:SER:CA | 1:68:A:SER:C | 15       | 3.14          |
| (1,28)  | 1:18:A:LYS:N | 1:18:A:LYS:CA | 1:18:A:LYS:C  | 1:19:A:ASN:N | 16       | 3.13          |
| (1,125) | 1:67:A:ALA:N | 1:67:A:ALA:CA | 1:67:A:ALA:C  | 1:68:A:SER:N | 8        | 3.06          |
| (1,28)  | 1:18:A:LYS:N | 1:18:A:LYS:CA | 1:18:A:LYS:C  | 1:19:A:ASN:N | 2        | 3.03          |
| (1,125) | 1:67:A:ALA:N | 1:67:A:ALA:CA | 1:67:A:ALA:C  | 1:68:A:SER:N | 14       | 3.02          |
| (1,125) | 1:67:A:ALA:N | 1:67:A:ALA:CA | 1:67:A:ALA:C  | 1:68:A:SER:N | 5        | 2.97          |
| (1,125) | 1:67:A:ALA:N | 1:67:A:ALA:CA | 1:67:A:ALA:C  | 1:68:A:SER:N | 9        | 2.96          |
| (1,50)  | 1:28:A:ILE:C | 1:29:A:GLN:N  | 1:29:A:GLN:CA | 1:29:A:GLN:C | 14       | 2.96          |
| (1,50)  | 1:28:A:ILE:C | 1:29:A:GLN:N  | 1:29:A:GLN:CA | 1:29:A:GLN:C | 15       | 2.94          |
| (1,104) | 1:55:A:THR:C | 1:56:A:THR:N  | 1:56:A:THR:CA | 1:56:A:THR:C | 6        | 2.89          |
| (1,128) | 1:67:A:ALA:C | 1:68:A:SER:N  | 1:68:A:SER:CA | 1:68:A:SER:C | 3        | 2.88          |
| (1,28)  | 1:18:A:LYS:N | 1:18:A:LYS:CA | 1:18:A:LYS:C  | 1:19:A:ASN:N | 11       | 2.88          |
| (1,128) | 1:67:A:ALA:C | 1:68:A:SER:N  | 1:68:A:SER:CA | 1:68:A:SER:C | 4        | 2.86          |
| (1,103) | 1:56:A:THR:N | 1:56:A:THR:CA | 1:56:A:THR:C  | 1:57:A:GLY:N | 10       | 2.85          |
| (1,104) | 1:55:A:THR:C | 1:56:A:THR:N  | 1:56:A:THR:CA | 1:56:A:THR:C | 4        | 2.8           |
| (1,104) | 1:55:A:THR:C | 1:56:A:THR:N  | 1:56:A:THR:CA | 1:56:A:THR:C | 8        | 2.8           |
| (1,103) | 1:56:A:THR:N | 1:56:A:THR:CA | 1:56:A:THR:C  | 1:57:A:GLY:N | 14       | 2.79          |
| (1,28)  | 1:18:A:LYS:N | 1:18:A:LYS:CA | 1:18:A:LYS:C  | 1:19:A:ASN:N | 18       | 2.77          |
| (1,50)  | 1:28:A:ILE:C | 1:29:A:GLN:N  | 1:29:A:GLN:CA | 1:29:A:GLN:C | 6        | 2.76          |
| (1,28)  | 1:18:A:LYS:N | 1:18:A:LYS:CA | 1:18:A:LYS:C  | 1:19:A:ASN:N | 4        | 2.76          |
| (1,50)  | 1:28:A:ILE:C | 1:29:A:GLN:N  | 1:29:A:GLN:CA | 1:29:A:GLN:C | 13       | 2.74          |
| (1,50)  | 1:28:A:ILE:C | 1:29:A:GLN:N  | 1:29:A:GLN:CA | 1:29:A:GLN:C | 4        | 2.72          |
| (1,50)  | 1:28:A:ILE:C | 1:29:A:GLN:N  | 1:29:A:GLN:CA | 1:29:A:GLN:C | 1        | 2.71          |
| (1,103) | 1:56:A:THR:N | 1:56:A:THR:CA | 1:56:A:THR:C  | 1:57:A:GLY:N | 4        | 2.7           |
| (1,103) | 1:56:A:THR:N | 1:56:A:THR:CA | 1:56:A:THR:C  | 1:57:A:GLY:N | 19       | 2.7           |
| (1,104) | 1:55:A:THR:C | 1:56:A:THR:N  | 1:56:A:THR:CA | 1:56:A:THR:C | 2        | 2.68          |
| (1,103) | 1:56:A:THR:N | 1:56:A:THR:CA | 1:56:A:THR:C  | 1:57:A:GLY:N | 2        | 2.68          |

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Continued from previous page...

| Key     | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Model ID | Violation (°) |
|---------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,28)  | 1:18:A:LYS:N | 1:18:A:LYS:CA | 1:18:A:LYS:C  | 1:19:A:ASN:N | 17       | 2.68          |
| (1,103) | 1:56:A:THR:N | 1:56:A:THR:CA | 1:56:A:THR:C  | 1:57:A:GLY:N | 11       | 2.65          |
| (1,50)  | 1:28:A:ILE:C | 1:29:A:GLN:N  | 1:29:A:GLN:CA | 1:29:A:GLN:C | 5        | 2.65          |
| (1,104) | 1:55:A:THR:C | 1:56:A:THR:N  | 1:56:A:THR:CA | 1:56:A:THR:C | 10       | 2.61          |
| (1,128) | 1:67:A:ALA:C | 1:68:A:SER:N  | 1:68:A:SER:CA | 1:68:A:SER:C | 19       | 2.59          |
| (1,104) | 1:55:A:THR:C | 1:56:A:THR:N  | 1:56:A:THR:CA | 1:56:A:THR:C | 7        | 2.58          |
| (1,103) | 1:56:A:THR:N | 1:56:A:THR:CA | 1:56:A:THR:C  | 1:57:A:GLY:N | 3        | 2.57          |
| (1,50)  | 1:28:A:ILE:C | 1:29:A:GLN:N  | 1:29:A:GLN:CA | 1:29:A:GLN:C | 12       | 2.56          |
| (1,103) | 1:56:A:THR:N | 1:56:A:THR:CA | 1:56:A:THR:C  | 1:57:A:GLY:N | 6        | 2.55          |
| (1,103) | 1:56:A:THR:N | 1:56:A:THR:CA | 1:56:A:THR:C  | 1:57:A:GLY:N | 8        | 2.55          |
| (1,128) | 1:67:A:ALA:C | 1:68:A:SER:N  | 1:68:A:SER:CA | 1:68:A:SER:C | 6        | 2.54          |
| (1,50)  | 1:28:A:ILE:C | 1:29:A:GLN:N  | 1:29:A:GLN:CA | 1:29:A:GLN:C | 8        | 2.54          |
| (1,103) | 1:56:A:THR:N | 1:56:A:THR:CA | 1:56:A:THR:C  | 1:57:A:GLY:N | 16       | 2.53          |
| (1,129) | 1:69:A:GLY:N | 1:69:A:GLY:CA | 1:69:A:GLY:C  | 1:70:A:SER:N | 11       | 2.52          |
| (1,125) | 1:67:A:ALA:N | 1:67:A:ALA:CA | 1:67:A:ALA:C  | 1:68:A:SER:N | 11       | 2.52          |
| (1,103) | 1:56:A:THR:N | 1:56:A:THR:CA | 1:56:A:THR:C  | 1:57:A:GLY:N | 7        | 2.52          |
| (1,50)  | 1:28:A:ILE:C | 1:29:A:GLN:N  | 1:29:A:GLN:CA | 1:29:A:GLN:C | 19       | 2.5           |
| (1,129) | 1:69:A:GLY:N | 1:69:A:GLY:CA | 1:69:A:GLY:C  | 1:70:A:SER:N | 16       | 2.49          |
| (1,50)  | 1:28:A:ILE:C | 1:29:A:GLN:N  | 1:29:A:GLN:CA | 1:29:A:GLN:C | 20       | 2.49          |
| (1,50)  | 1:28:A:ILE:C | 1:29:A:GLN:N  | 1:29:A:GLN:CA | 1:29:A:GLN:C | 7        | 2.48          |
| (1,125) | 1:67:A:ALA:N | 1:67:A:ALA:CA | 1:67:A:ALA:C  | 1:68:A:SER:N | 16       | 2.46          |
| (1,104) | 1:55:A:THR:C | 1:56:A:THR:N  | 1:56:A:THR:CA | 1:56:A:THR:C | 14       | 2.44          |
| (1,104) | 1:55:A:THR:C | 1:56:A:THR:N  | 1:56:A:THR:CA | 1:56:A:THR:C | 19       | 2.44          |
| (1,104) | 1:55:A:THR:C | 1:56:A:THR:N  | 1:56:A:THR:CA | 1:56:A:THR:C | 3        | 2.43          |
| (1,28)  | 1:18:A:LYS:N | 1:18:A:LYS:CA | 1:18:A:LYS:C  | 1:19:A:ASN:N | 9        | 2.42          |
| (1,50)  | 1:28:A:ILE:C | 1:29:A:GLN:N  | 1:29:A:GLN:CA | 1:29:A:GLN:C | 17       | 2.4           |
| (1,125) | 1:67:A:ALA:N | 1:67:A:ALA:CA | 1:67:A:ALA:C  | 1:68:A:SER:N | 10       | 2.39          |
| (1,125) | 1:67:A:ALA:N | 1:67:A:ALA:CA | 1:67:A:ALA:C  | 1:68:A:SER:N | 2        | 2.38          |
| (1,125) | 1:67:A:ALA:N | 1:67:A:ALA:CA | 1:67:A:ALA:C  | 1:68:A:SER:N | 7        | 2.36          |
| (1,123) | 1:66:A:GLY:N | 1:66:A:GLY:CA | 1:66:A:GLY:C  | 1:67:A:ALA:N | 3        | 2.36          |
| (1,104) | 1:55:A:THR:C | 1:56:A:THR:N  | 1:56:A:THR:CA | 1:56:A:THR:C | 16       | 2.35          |
| (1,50)  | 1:28:A:ILE:C | 1:29:A:GLN:N  | 1:29:A:GLN:CA | 1:29:A:GLN:C | 11       | 2.35          |
| (1,128) | 1:67:A:ALA:C | 1:68:A:SER:N  | 1:68:A:SER:CA | 1:68:A:SER:C | 17       | 2.34          |
| (1,125) | 1:67:A:ALA:N | 1:67:A:ALA:CA | 1:67:A:ALA:C  | 1:68:A:SER:N | 1        | 2.33          |
| (1,104) | 1:55:A:THR:C | 1:56:A:THR:N  | 1:56:A:THR:CA | 1:56:A:THR:C | 11       | 2.33          |
| (1,129) | 1:69:A:GLY:N | 1:69:A:GLY:CA | 1:69:A:GLY:C  | 1:70:A:SER:N | 10       | 2.32          |
| (1,125) | 1:67:A:ALA:N | 1:67:A:ALA:CA | 1:67:A:ALA:C  | 1:68:A:SER:N | 12       | 2.31          |
| (1,123) | 1:66:A:GLY:N | 1:66:A:GLY:CA | 1:66:A:GLY:C  | 1:67:A:ALA:N | 10       | 2.29          |
| (1,128) | 1:67:A:ALA:C | 1:68:A:SER:N  | 1:68:A:SER:CA | 1:68:A:SER:C | 18       | 2.26          |
| (1,50)  | 1:28:A:ILE:C | 1:29:A:GLN:N  | 1:29:A:GLN:CA | 1:29:A:GLN:C | 10       | 2.25          |
| (1,125) | 1:67:A:ALA:N | 1:67:A:ALA:CA | 1:67:A:ALA:C  | 1:68:A:SER:N | 3        | 2.21          |
| (1,125) | 1:67:A:ALA:N | 1:67:A:ALA:CA | 1:67:A:ALA:C  | 1:68:A:SER:N | 6        | 2.19          |
| (1,123) | 1:66:A:GLY:N | 1:66:A:GLY:CA | 1:66:A:GLY:C  | 1:67:A:ALA:N | 19       | 2.19          |
| (1,50)  | 1:28:A:ILE:C | 1:29:A:GLN:N  | 1:29:A:GLN:CA | 1:29:A:GLN:C | 2        | 2.19          |
| (1,129) | 1:69:A:GLY:N | 1:69:A:GLY:CA | 1:69:A:GLY:C  | 1:70:A:SER:N | 3        | 2.16          |
| (1,28)  | 1:18:A:LYS:N | 1:18:A:LYS:CA | 1:18:A:LYS:C  | 1:19:A:ASN:N | 19       | 2.16          |
| (1,129) | 1:69:A:GLY:N | 1:69:A:GLY:CA | 1:69:A:GLY:C  | 1:70:A:SER:N | 19       | 2.15          |
| (1,115) | 1:62:A:THR:N | 1:62:A:THR:CA | 1:62:A:THR:C  | 1:63:A:LYS:N | 8        | 2.13          |
| (1,129) | 1:69:A:GLY:N | 1:69:A:GLY:CA | 1:69:A:GLY:C  | 1:70:A:SER:N | 8        | 2.1           |
| (1,115) | 1:62:A:THR:N | 1:62:A:THR:CA | 1:62:A:THR:C  | 1:63:A:LYS:N | 7        | 2.1           |
| (1,5)   | 1:4:A:PRO:C  | 1:5:A:LYS:N   | 1:5:A:LYS:CA  | 1:5:A:LYS:C  | 12       | 2.09          |

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| Key     | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Model ID | Violation (°) |
|---------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,125) | 1:67:A:ALA:N | 1:67:A:ALA:CA | 1:67:A:ALA:C  | 1:68:A:SER:N | 4        | 2.07          |
| (1,129) | 1:69:A:GLY:N | 1:69:A:GLY:CA | 1:69:A:GLY:C  | 1:70:A:SER:N | 20       | 2.03          |
| (1,123) | 1:66:A:GLY:N | 1:66:A:GLY:CA | 1:66:A:GLY:C  | 1:67:A:ALA:N | 18       | 2.03          |
| (1,115) | 1:62:A:THR:N | 1:62:A:THR:CA | 1:62:A:THR:C  | 1:63:A:LYS:N | 12       | 2.03          |
| (1,125) | 1:67:A:ALA:N | 1:67:A:ALA:CA | 1:67:A:ALA:C  | 1:68:A:SER:N | 15       | 2.01          |
| (1,115) | 1:62:A:THR:N | 1:62:A:THR:CA | 1:62:A:THR:C  | 1:63:A:LYS:N | 19       | 2.0           |
| (1,50)  | 1:28:A:ILE:C | 1:29:A:GLN:N  | 1:29:A:GLN:CA | 1:29:A:GLN:C | 18       | 2.0           |
| (1,7)   | 1:5:A:LYS:C  | 1:6:A:TYR:N   | 1:6:A:TYR:CA  | 1:6:A:TYR:C  | 19       | 1.99          |
| (1,129) | 1:69:A:GLY:N | 1:69:A:GLY:CA | 1:69:A:GLY:C  | 1:70:A:SER:N | 12       | 1.98          |
| (1,129) | 1:69:A:GLY:N | 1:69:A:GLY:CA | 1:69:A:GLY:C  | 1:70:A:SER:N | 13       | 1.98          |
| (1,129) | 1:69:A:GLY:N | 1:69:A:GLY:CA | 1:69:A:GLY:C  | 1:70:A:SER:N | 7        | 1.96          |
| (1,129) | 1:69:A:GLY:N | 1:69:A:GLY:CA | 1:69:A:GLY:C  | 1:70:A:SER:N | 14       | 1.95          |
| (1,28)  | 1:18:A:LYS:N | 1:18:A:LYS:CA | 1:18:A:LYS:C  | 1:19:A:ASN:N | 13       | 1.95          |
| (1,129) | 1:69:A:GLY:N | 1:69:A:GLY:CA | 1:69:A:GLY:C  | 1:70:A:SER:N | 2        | 1.94          |
| (1,115) | 1:62:A:THR:N | 1:62:A:THR:CA | 1:62:A:THR:C  | 1:63:A:LYS:N | 1        | 1.9           |
| (1,125) | 1:67:A:ALA:N | 1:67:A:ALA:CA | 1:67:A:ALA:C  | 1:68:A:SER:N | 19       | 1.89          |
| (1,5)   | 1:4:A:PRO:C  | 1:5:A:LYS:N   | 1:5:A:LYS:CA  | 1:5:A:LYS:C  | 8        | 1.89          |
| (1,137) | 1:73:A:LEU:N | 1:73:A:LEU:CA | 1:73:A:LEU:C  | 1:74:A:ALA:N | 5        | 1.86          |
| (1,129) | 1:69:A:GLY:N | 1:69:A:GLY:CA | 1:69:A:GLY:C  | 1:70:A:SER:N | 4        | 1.85          |
| (1,129) | 1:69:A:GLY:N | 1:69:A:GLY:CA | 1:69:A:GLY:C  | 1:70:A:SER:N | 9        | 1.85          |
| (1,115) | 1:62:A:THR:N | 1:62:A:THR:CA | 1:62:A:THR:C  | 1:63:A:LYS:N | 3        | 1.85          |
| (1,115) | 1:62:A:THR:N | 1:62:A:THR:CA | 1:62:A:THR:C  | 1:63:A:LYS:N | 5        | 1.83          |
| (1,129) | 1:69:A:GLY:N | 1:69:A:GLY:CA | 1:69:A:GLY:C  | 1:70:A:SER:N | 5        | 1.82          |
| (1,125) | 1:67:A:ALA:N | 1:67:A:ALA:CA | 1:67:A:ALA:C  | 1:68:A:SER:N | 18       | 1.8           |
| (1,115) | 1:62:A:THR:N | 1:62:A:THR:CA | 1:62:A:THR:C  | 1:63:A:LYS:N | 15       | 1.8           |
| (1,115) | 1:62:A:THR:N | 1:62:A:THR:CA | 1:62:A:THR:C  | 1:63:A:LYS:N | 9        | 1.79          |
| (1,129) | 1:69:A:GLY:N | 1:69:A:GLY:CA | 1:69:A:GLY:C  | 1:70:A:SER:N | 1        | 1.78          |
| (1,115) | 1:62:A:THR:N | 1:62:A:THR:CA | 1:62:A:THR:C  | 1:63:A:LYS:N | 6        | 1.78          |
| (1,113) | 1:61:A:GLN:N | 1:61:A:GLN:CA | 1:61:A:GLN:C  | 1:62:A:THR:N | 17       | 1.78          |
| (1,28)  | 1:18:A:LYS:N | 1:18:A:LYS:CA | 1:18:A:LYS:C  | 1:19:A:ASN:N | 14       | 1.78          |
| (1,129) | 1:69:A:GLY:N | 1:69:A:GLY:CA | 1:69:A:GLY:C  | 1:70:A:SER:N | 6        | 1.74          |
| (1,115) | 1:62:A:THR:N | 1:62:A:THR:CA | 1:62:A:THR:C  | 1:63:A:LYS:N | 14       | 1.73          |
| (1,50)  | 1:28:A:ILE:C | 1:29:A:GLN:N  | 1:29:A:GLN:CA | 1:29:A:GLN:C | 9        | 1.73          |
| (1,123) | 1:66:A:GLY:N | 1:66:A:GLY:CA | 1:66:A:GLY:C  | 1:67:A:ALA:N | 2        | 1.71          |
| (1,28)  | 1:18:A:LYS:N | 1:18:A:LYS:CA | 1:18:A:LYS:C  | 1:19:A:ASN:N | 12       | 1.71          |
| (1,123) | 1:66:A:GLY:N | 1:66:A:GLY:CA | 1:66:A:GLY:C  | 1:67:A:ALA:N | 17       | 1.7           |
| (1,115) | 1:62:A:THR:N | 1:62:A:THR:CA | 1:62:A:THR:C  | 1:63:A:LYS:N | 17       | 1.7           |
| (1,129) | 1:69:A:GLY:N | 1:69:A:GLY:CA | 1:69:A:GLY:C  | 1:70:A:SER:N | 17       | 1.69          |
| (1,50)  | 1:28:A:ILE:C | 1:29:A:GLN:N  | 1:29:A:GLN:CA | 1:29:A:GLN:C | 3        | 1.68          |
| (1,7)   | 1:5:A:LYS:C  | 1:6:A:TYR:N   | 1:6:A:TYR:CA  | 1:6:A:TYR:C  | 11       | 1.68          |
| (1,125) | 1:67:A:ALA:N | 1:67:A:ALA:CA | 1:67:A:ALA:C  | 1:68:A:SER:N | 17       | 1.66          |
| (1,123) | 1:66:A:GLY:N | 1:66:A:GLY:CA | 1:66:A:GLY:C  | 1:67:A:ALA:N | 1        | 1.66          |
| (1,35)  | 1:20:A:ARG:C | 1:21:A:ALA:N  | 1:21:A:ALA:CA | 1:21:A:ALA:C | 10       | 1.66          |
| (1,123) | 1:66:A:GLY:N | 1:66:A:GLY:CA | 1:66:A:GLY:C  | 1:67:A:ALA:N | 11       | 1.65          |
| (1,123) | 1:66:A:GLY:N | 1:66:A:GLY:CA | 1:66:A:GLY:C  | 1:67:A:ALA:N | 12       | 1.65          |
| (1,115) | 1:62:A:THR:N | 1:62:A:THR:CA | 1:62:A:THR:C  | 1:63:A:LYS:N | 11       | 1.65          |
| (1,7)   | 1:5:A:LYS:C  | 1:6:A:TYR:N   | 1:6:A:TYR:CA  | 1:6:A:TYR:C  | 12       | 1.65          |
| (1,115) | 1:62:A:THR:N | 1:62:A:THR:CA | 1:62:A:THR:C  | 1:63:A:LYS:N | 2        | 1.64          |
| (1,115) | 1:62:A:THR:N | 1:62:A:THR:CA | 1:62:A:THR:C  | 1:63:A:LYS:N | 4        | 1.64          |
| (1,115) | 1:62:A:THR:N | 1:62:A:THR:CA | 1:62:A:THR:C  | 1:63:A:LYS:N | 18       | 1.59          |
| (1,5)   | 1:4:A:PRO:C  | 1:5:A:LYS:N   | 1:5:A:LYS:CA  | 1:5:A:LYS:C  | 5        | 1.57          |

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| Key     | Atom-1       | Atom-2        | Atom-3       | Atom-4       | Model ID | Violation (°) |
|---------|--------------|---------------|--------------|--------------|----------|---------------|
| (1,3)   | 1:3:A:HIS:C  | 1:4:A:PRO:N   | 1:4:A:PRO:CA | 1:4:A:PRO:C  | 2        | 1.52          |
| (1,123) | 1:66:A:GLY:N | 1:66:A:GLY:CA | 1:66:A:GLY:C | 1:67:A:ALA:N | 15       | 1.51          |
| (1,115) | 1:62:A:THR:N | 1:62:A:THR:CA | 1:62:A:THR:C | 1:63:A:LYS:N | 13       | 1.51          |
| (1,123) | 1:66:A:GLY:N | 1:66:A:GLY:CA | 1:66:A:GLY:C | 1:67:A:ALA:N | 6        | 1.5           |
| (1,113) | 1:61:A:GLN:N | 1:61:A:GLN:CA | 1:61:A:GLN:C | 1:62:A:THR:N | 16       | 1.5           |
| (1,123) | 1:66:A:GLY:N | 1:66:A:GLY:CA | 1:66:A:GLY:C | 1:67:A:ALA:N | 5        | 1.49          |
| (1,123) | 1:66:A:GLY:N | 1:66:A:GLY:CA | 1:66:A:GLY:C | 1:67:A:ALA:N | 7        | 1.49          |
| (1,123) | 1:66:A:GLY:N | 1:66:A:GLY:CA | 1:66:A:GLY:C | 1:67:A:ALA:N | 16       | 1.49          |
| (1,113) | 1:61:A:GLN:N | 1:61:A:GLN:CA | 1:61:A:GLN:C | 1:62:A:THR:N | 19       | 1.49          |
| (1,5)   | 1:4:A:PRO:C  | 1:5:A:LYS:N   | 1:5:A:LYS:CA | 1:5:A:LYS:C  | 11       | 1.49          |
| (1,123) | 1:66:A:GLY:N | 1:66:A:GLY:CA | 1:66:A:GLY:C | 1:67:A:ALA:N | 13       | 1.43          |
| (1,5)   | 1:4:A:PRO:C  | 1:5:A:LYS:N   | 1:5:A:LYS:CA | 1:5:A:LYS:C  | 15       | 1.42          |
| (1,75)  | 1:42:A:ALA:N | 1:42:A:ALA:CA | 1:42:A:ALA:C | 1:43:A:ASP:N | 5        | 1.41          |
| (1,3)   | 1:3:A:HIS:C  | 1:4:A:PRO:N   | 1:4:A:PRO:CA | 1:4:A:PRO:C  | 20       | 1.4           |
| (1,137) | 1:73:A:LEU:N | 1:73:A:LEU:CA | 1:73:A:LEU:C | 1:74:A:ALA:N | 2        | 1.39          |
| (1,75)  | 1:42:A:ALA:N | 1:42:A:ALA:CA | 1:42:A:ALA:C | 1:43:A:ASP:N | 13       | 1.39          |
| (1,28)  | 1:18:A:LYS:N | 1:18:A:LYS:CA | 1:18:A:LYS:C | 1:19:A:ASN:N | 7        | 1.38          |
| (1,75)  | 1:42:A:ALA:N | 1:42:A:ALA:CA | 1:42:A:ALA:C | 1:43:A:ASP:N | 4        | 1.37          |
| (1,115) | 1:62:A:THR:N | 1:62:A:THR:CA | 1:62:A:THR:C | 1:63:A:LYS:N | 20       | 1.34          |
| (1,91)  | 1:50:A:ILE:N | 1:50:A:ILE:CA | 1:50:A:ILE:C | 1:51:A:LYS:N | 9        | 1.34          |
| (1,129) | 1:69:A:GLY:N | 1:69:A:GLY:CA | 1:69:A:GLY:C | 1:70:A:SER:N | 15       | 1.33          |
| (1,5)   | 1:4:A:PRO:C  | 1:5:A:LYS:N   | 1:5:A:LYS:CA | 1:5:A:LYS:C  | 9        | 1.32          |
| (1,123) | 1:66:A:GLY:N | 1:66:A:GLY:CA | 1:66:A:GLY:C | 1:67:A:ALA:N | 20       | 1.31          |
| (1,115) | 1:62:A:THR:N | 1:62:A:THR:CA | 1:62:A:THR:C | 1:63:A:LYS:N | 16       | 1.31          |
| (1,129) | 1:69:A:GLY:N | 1:69:A:GLY:CA | 1:69:A:GLY:C | 1:70:A:SER:N | 18       | 1.29          |
| (1,123) | 1:66:A:GLY:N | 1:66:A:GLY:CA | 1:66:A:GLY:C | 1:67:A:ALA:N | 14       | 1.29          |
| (1,115) | 1:62:A:THR:N | 1:62:A:THR:CA | 1:62:A:THR:C | 1:63:A:LYS:N | 10       | 1.29          |
| (1,7)   | 1:5:A:LYS:C  | 1:6:A:TYR:N   | 1:6:A:TYR:CA | 1:6:A:TYR:C  | 8        | 1.29          |
| (1,111) | 1:60:A:LYS:N | 1:60:A:LYS:CA | 1:60:A:LYS:C | 1:61:A:GLN:N | 9        | 1.28          |
| (1,137) | 1:73:A:LEU:N | 1:73:A:LEU:CA | 1:73:A:LEU:C | 1:74:A:ALA:N | 3        | 1.26          |
| (1,123) | 1:66:A:GLY:N | 1:66:A:GLY:CA | 1:66:A:GLY:C | 1:67:A:ALA:N | 4        | 1.25          |
| (1,137) | 1:73:A:LEU:N | 1:73:A:LEU:CA | 1:73:A:LEU:C | 1:74:A:ALA:N | 10       | 1.24          |
| (1,123) | 1:66:A:GLY:N | 1:66:A:GLY:CA | 1:66:A:GLY:C | 1:67:A:ALA:N | 9        | 1.24          |
| (1,5)   | 1:4:A:PRO:C  | 1:5:A:LYS:N   | 1:5:A:LYS:CA | 1:5:A:LYS:C  | 14       | 1.22          |
| (1,111) | 1:60:A:LYS:N | 1:60:A:LYS:CA | 1:60:A:LYS:C | 1:61:A:GLN:N | 17       | 1.21          |
| (1,111) | 1:60:A:LYS:N | 1:60:A:LYS:CA | 1:60:A:LYS:C | 1:61:A:GLN:N | 20       | 1.21          |
| (1,49)  | 1:29:A:GLN:N | 1:29:A:GLN:CA | 1:29:A:GLN:C | 1:30:A:LYS:N | 2        | 1.2           |
| (1,3)   | 1:3:A:HIS:C  | 1:4:A:PRO:N   | 1:4:A:PRO:CA | 1:4:A:PRO:C  | 18       | 1.19          |
| (1,123) | 1:66:A:GLY:N | 1:66:A:GLY:CA | 1:66:A:GLY:C | 1:67:A:ALA:N | 8        | 1.18          |
| (1,111) | 1:60:A:LYS:N | 1:60:A:LYS:CA | 1:60:A:LYS:C | 1:61:A:GLN:N | 15       | 1.17          |
| (1,5)   | 1:4:A:PRO:C  | 1:5:A:LYS:N   | 1:5:A:LYS:CA | 1:5:A:LYS:C  | 16       | 1.17          |
| (1,137) | 1:73:A:LEU:N | 1:73:A:LEU:CA | 1:73:A:LEU:C | 1:74:A:ALA:N | 11       | 1.16          |
| (1,28)  | 1:18:A:LYS:N | 1:18:A:LYS:CA | 1:18:A:LYS:C | 1:19:A:ASN:N | 10       | 1.12          |
| (1,13)  | 1:8:A:ASP:C  | 1:9:A:MET:N   | 1:9:A:MET:CA | 1:9:A:MET:C  | 19       | 1.12          |
| (1,5)   | 1:4:A:PRO:C  | 1:5:A:LYS:N   | 1:5:A:LYS:CA | 1:5:A:LYS:C  | 3        | 1.1           |
| (1,3)   | 1:3:A:HIS:C  | 1:4:A:PRO:N   | 1:4:A:PRO:CA | 1:4:A:PRO:C  | 16       | 1.1           |
| (1,3)   | 1:3:A:HIS:C  | 1:4:A:PRO:N   | 1:4:A:PRO:CA | 1:4:A:PRO:C  | 4        | 1.09          |
| (1,1)   | 1:3:A:HIS:N  | 1:3:A:HIS:CA  | 1:3:A:HIS:C  | 1:4:A:PRO:N  | 11       | 1.09          |
| (1,137) | 1:73:A:LEU:N | 1:73:A:LEU:CA | 1:73:A:LEU:C | 1:74:A:ALA:N | 19       | 1.07          |
| (1,5)   | 1:4:A:PRO:C  | 1:5:A:LYS:N   | 1:5:A:LYS:CA | 1:5:A:LYS:C  | 6        | 1.06          |
| (1,28)  | 1:18:A:LYS:N | 1:18:A:LYS:CA | 1:18:A:LYS:C | 1:19:A:ASN:N | 20       | 1.05          |

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| Key     | Atom-1       | Atom-2        | Atom-3       | Atom-4       | Model ID | Violation (°) |
|---------|--------------|---------------|--------------|--------------|----------|---------------|
| (1,5)   | 1:4:A:PRO:C  | 1:5:A:LYS:N   | 1:5:A:LYS:CA | 1:5:A:LYS:C  | 7        | 1.04          |
| (1,137) | 1:73:A:LEU:N | 1:73:A:LEU:CA | 1:73:A:LEU:C | 1:74:A:ALA:N | 1        | 1.03          |
| (1,3)   | 1:3:A:HIS:C  | 1:4:A:PRO:N   | 1:4:A:PRO:CA | 1:4:A:PRO:C  | 9        | 1.02          |
| (1,135) | 1:72:A:ARG:N | 1:72:A:ARG:CA | 1:72:A:ARG:C | 1:73:A:LEU:N | 4        | 1.01          |
| (1,75)  | 1:42:A:ALA:N | 1:42:A:ALA:CA | 1:42:A:ALA:C | 1:43:A:ASP:N | 14       | 1.01          |
| (1,49)  | 1:29:A:GLN:N | 1:29:A:GLN:CA | 1:29:A:GLN:C | 1:30:A:LYS:N | 20       | 1.0           |