



# Full wwPDB NMR Structure Validation Report ⓘ

Mar 8, 2026 – 05:45 PM UTC

PDB ID : 2MJB / pdb\_00002mjb  
BMRB ID : 6457  
Title : Solution nmr structure of ubiquitin refined against dipolar couplings in 4 media  
Authors : Maltsev, A.; Grishaev, A.; Roche, J.; Zasloff, M.; Bax, A.  
Deposited on : 2014-01-02

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

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

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

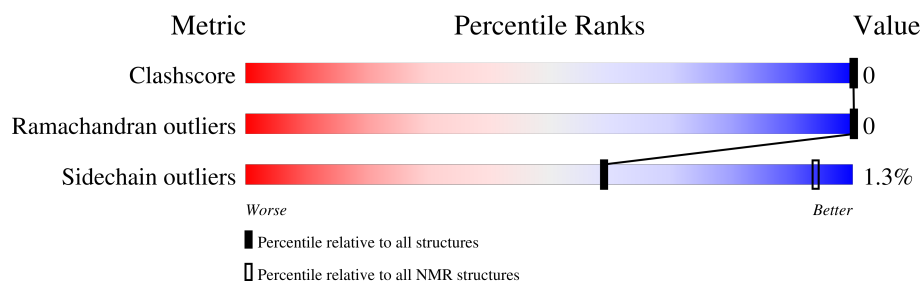
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 87%.

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     | 76     | <br>95% |

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 11 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

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:1-A:73 (73)         | 0.11              | 11           |

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 3 clusters and 1 single-model cluster was found.

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

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

There is only 1 type of molecule in this entry. The entry contains 1231 atoms, of which 629 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Ubiquitin-60S ribosomal protein L40.

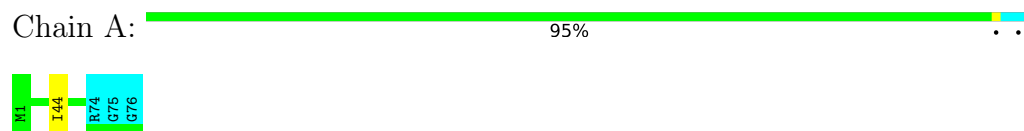
| Mol | Chain | Residues | Atoms |     |     |     |     |   |  | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|--|-------|
| 1   | A     | 76       | Total | C   | H   | N   | O   | S |  | 0     |
|     |       |          | 1231  | 378 | 629 | 105 | 118 | 1 |  |       |

## 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: Ubiquitin-60S ribosomal protein L40

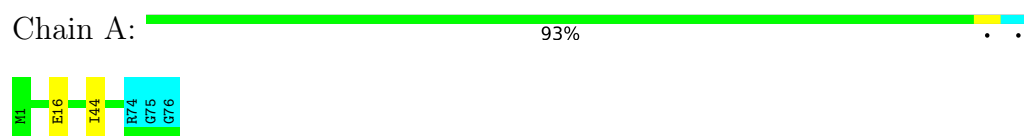


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

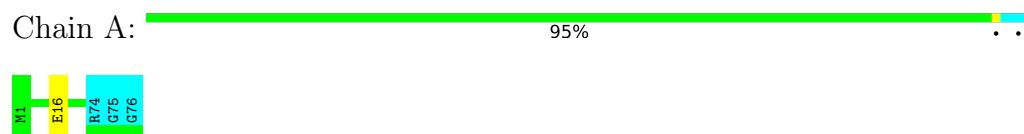
#### 4.2.1 Score per residue for model 1

- Molecule 1: Ubiquitin-60S ribosomal protein L40



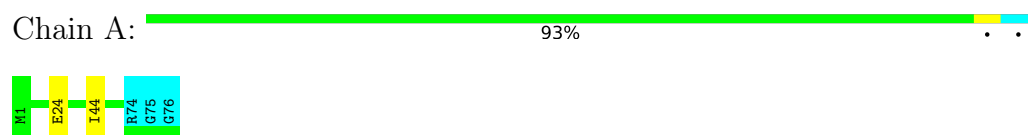
#### 4.2.2 Score per residue for model 2

- Molecule 1: Ubiquitin-60S ribosomal protein L40



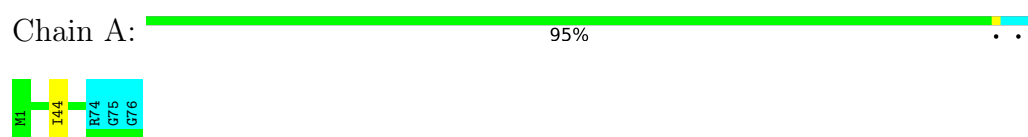
### 4.2.3 Score per residue for model 3

- Molecule 1: Ubiquitin-60S ribosomal protein L40



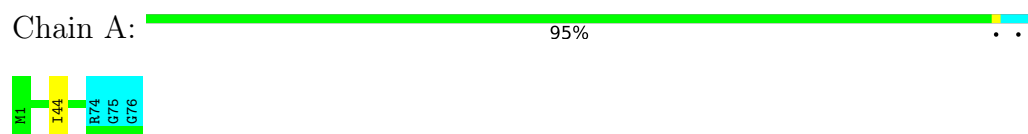
### 4.2.4 Score per residue for model 4

- Molecule 1: Ubiquitin-60S ribosomal protein L40



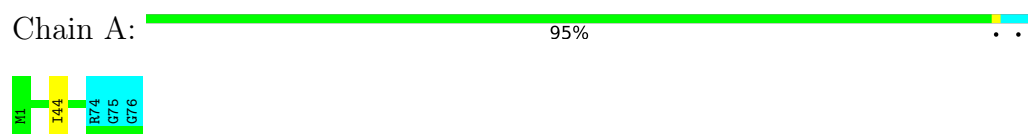
### 4.2.5 Score per residue for model 5

- Molecule 1: Ubiquitin-60S ribosomal protein L40



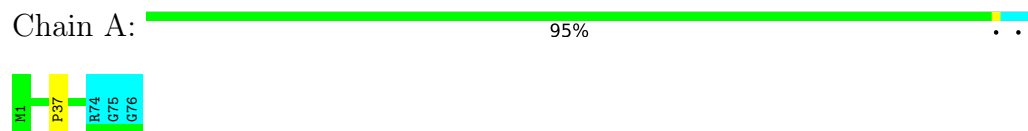
### 4.2.6 Score per residue for model 6

- Molecule 1: Ubiquitin-60S ribosomal protein L40



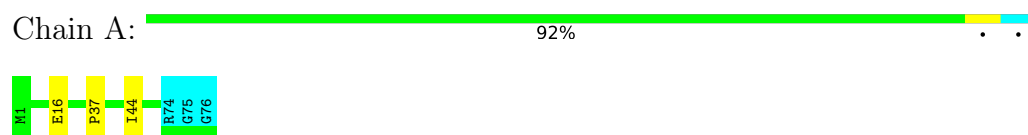
### 4.2.7 Score per residue for model 7

- Molecule 1: Ubiquitin-60S ribosomal protein L40



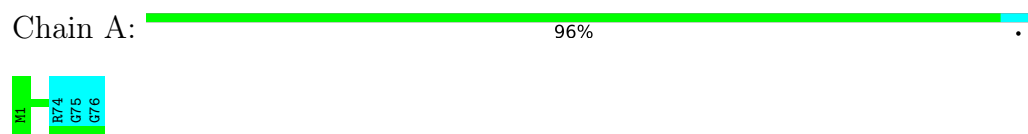
#### 4.2.8 Score per residue for model 8

- Molecule 1: Ubiquitin-60S ribosomal protein L40



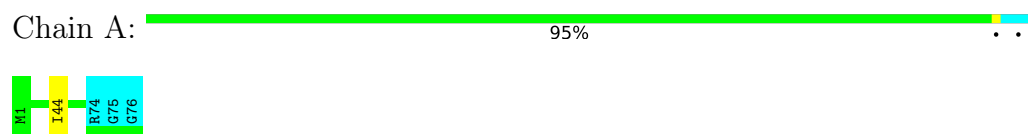
#### 4.2.9 Score per residue for model 9

- Molecule 1: Ubiquitin-60S ribosomal protein L40



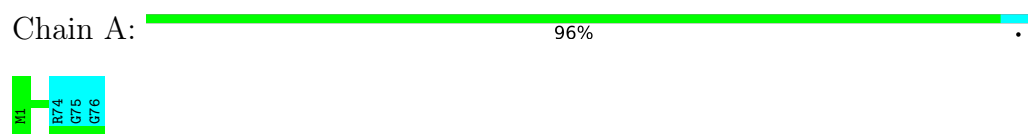
#### 4.2.10 Score per residue for model 10

- Molecule 1: Ubiquitin-60S ribosomal protein L40



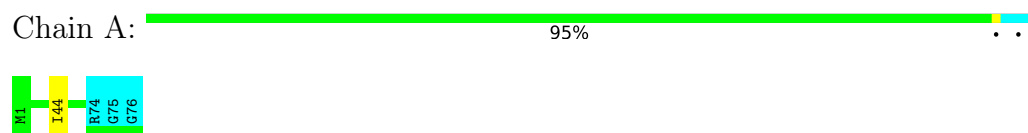
#### 4.2.11 Score per residue for model 11 (medoid)

- Molecule 1: Ubiquitin-60S ribosomal protein L40



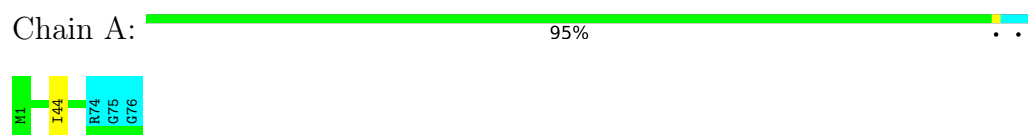
#### 4.2.12 Score per residue for model 12

- Molecule 1: Ubiquitin-60S ribosomal protein L40



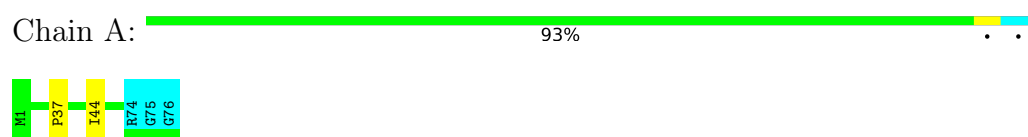
#### 4.2.13 Score per residue for model 13

- Molecule 1: Ubiquitin-60S ribosomal protein L40



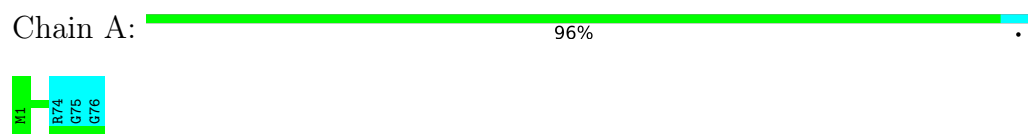
#### 4.2.14 Score per residue for model 14

- Molecule 1: Ubiquitin-60S ribosomal protein L40



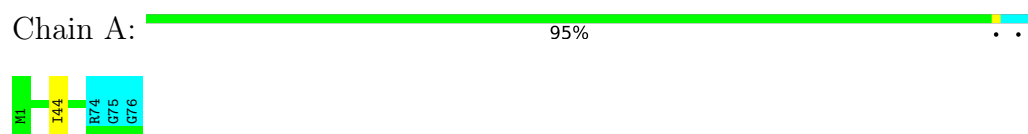
#### 4.2.15 Score per residue for model 15

- Molecule 1: Ubiquitin-60S ribosomal protein L40



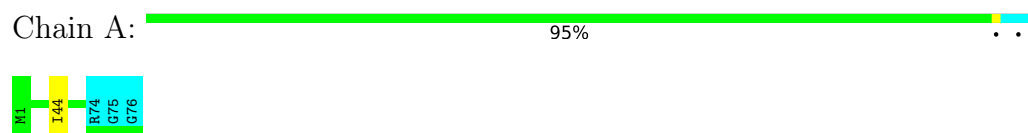
#### 4.2.16 Score per residue for model 16

- Molecule 1: Ubiquitin-60S ribosomal protein L40



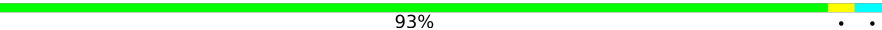
#### 4.2.17 Score per residue for model 17

- Molecule 1: Ubiquitin-60S ribosomal protein L40



#### 4.2.18 Score per residue for model 18

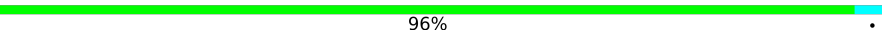
- Molecule 1: Ubiquitin-60S ribosomal protein L40

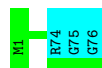
Chain A:  93% . .



#### 4.2.19 Score per residue for model 19

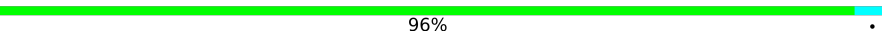
- Molecule 1: Ubiquitin-60S ribosomal protein L40

Chain A:  96% .



#### 4.2.20 Score per residue for model 20

- Molecule 1: Ubiquitin-60S ribosomal protein L40

Chain A:  96% .



## 5 Refinement protocol and experimental data overview

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

Of the 20 calculated structures, 20 were deposited, based on the following criterion: *all calculated structures submitted*.

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

| Software name | Classification | Version |
|---------------|----------------|---------|
| X-PLOR NIH    | refinement     |         |

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

|                                              |                |
|----------------------------------------------|----------------|
| Chemical shift file(s)                       | working_cs.cif |
| Number of chemical shift lists               | 1              |
| Total number of shifts                       | 922            |
| Number of shifts mapped to atoms             | 922            |
| Number of unparsed shifts                    | 0              |
| Number of shifts with mapping errors         | 0              |
| Number of shifts with mapping warnings       | 0              |
| Assignment completeness (well-defined parts) | 87%            |

## 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     | 1.21±0.01    | 0±0/589 ( 0.0± 0.1%) | 0.80±0.01   | 0±0/795 ( 0.0± 0.0%) |
| All | All   | 1.21         | 3/11780 ( 0.0%)      | 0.80        | 0/15900 ( 0.0%)      |

All unique bond outliers are listed below.

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) | Models |       |
|-----|-------|-----|------|-------|------|-------------|----------|--------|-------|
|     |       |     |      |       |      |             |          | Worst  | Total |
| 1   | A     | 37  | PRO  | CA-C  | 5.08 | 1.55        | 1.52     | 8      | 3     |

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes |
|-----|-------|-------|----------|----------|---------|
| All | All   | 11640 | 12200    | 12200    | -       |

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 -.

There are no clashes.

## 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     | 72/76 (95%)     | 72±0 (100±0%) | 0±0 (0±0%) | 0±0 (0±0%) | 100         | 100 |
| All | All   | 1440/1520 (95%) | 1440 (100%)   | 0 (0%)     | 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     | 67/68 (99%)     | 66±1 (99±1%) | 1±1 (1±1%) | 59          | 94 |
| All | All   | 1340/1360 (99%) | 1322 (99%)   | 18 (1%)    | 59          | 94 |

All 5 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     | 44  | ILE  | 12             |
| 1   | A     | 16  | GLU  | 3              |
| 1   | A     | 24  | GLU  | 1              |
| 1   | A     | 6   | LYS  | 1              |
| 1   | A     | 73  | 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

The completeness of assignment taking into account all chemical shift lists is 87% for the well-defined parts and 86% for the entire structure.

### 7.1 Chemical shift list 1

File name: working\_cs.cif

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

#### 7.1.1 Bookkeeping

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

|                                         |     |
|-----------------------------------------|-----|
| Total number of shifts                  | 922 |
| Number of shifts mapped to atoms        | 922 |
| Number of unparsed shifts               | 0   |
| Number of shifts with mapping errors    | 0   |
| Number of shifts with mapping warnings  | 0   |
| Number of shift outliers (ShiftChecker) | 1   |

#### 7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

| Nucleus                | # values | Correction $\pm$ precision, ppm | Suggested action           |
|------------------------|----------|---------------------------------|----------------------------|
| $^{13}\text{C}_\alpha$ | 76       | $-0.22 \pm 0.22$                | None needed ( $< 0.5$ ppm) |
| $^{13}\text{C}_\beta$  | 70       | $0.15 \pm 0.12$                 | None needed ( $< 0.5$ ppm) |
| $^{13}\text{C}'$       | 76       | $-0.33 \pm 0.13$                | None needed ( $< 0.5$ ppm) |
| $^{15}\text{N}$        | 75       | $0.98 \pm 0.39$                 | Should be applied          |

#### 7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 87%, i.e. 897 atoms were assigned a chemical shift out of a possible 1036. 0 out of 13 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total         | $^1\text{H}$  | $^{13}\text{C}$ | $^{15}\text{N}$ |
|-----------|---------------|---------------|-----------------|-----------------|
| Backbone  | 357/363 (98%) | 142/147 (97%) | 146/146 (100%)  | 69/70 (99%)     |
| Sidechain | 524/637 (82%) | 337/412 (82%) | 179/201 (89%)   | 8/24 (33%)      |

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|          | <b>Total</b>   | <b><sup>1</sup>H</b> | <b><sup>13</sup>C</b> | <b><sup>15</sup>N</b> |
|----------|----------------|----------------------|-----------------------|-----------------------|
| Aromatic | 16/36 (44%)    | 8/18 (44%)           | 8/17 (47%)            | 0/1 (0%)              |
| Overall  | 897/1036 (87%) | 487/577 (84%)        | 333/364 (91%)         | 77/95 (81%)           |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 86%, i.e. 919 atoms were assigned a chemical shift out of a possible 1071. 0 out of 13 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | <b>Total</b>   | <b><sup>1</sup>H</b> | <b><sup>13</sup>C</b> | <b><sup>15</sup>N</b> |
|-----------|----------------|----------------------|-----------------------|-----------------------|
| Backbone  | 372/380 (98%)  | 148/155 (95%)        | 152/152 (100%)        | 72/73 (99%)           |
| Sidechain | 531/655 (81%)  | 341/423 (81%)        | 182/205 (89%)         | 8/27 (30%)            |
| Aromatic  | 16/36 (44%)    | 8/18 (44%)           | 8/17 (47%)            | 0/1 (0%)              |
| Overall   | 919/1071 (86%) | 497/596 (83%)        | 342/374 (91%)         | 80/101 (79%)          |

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

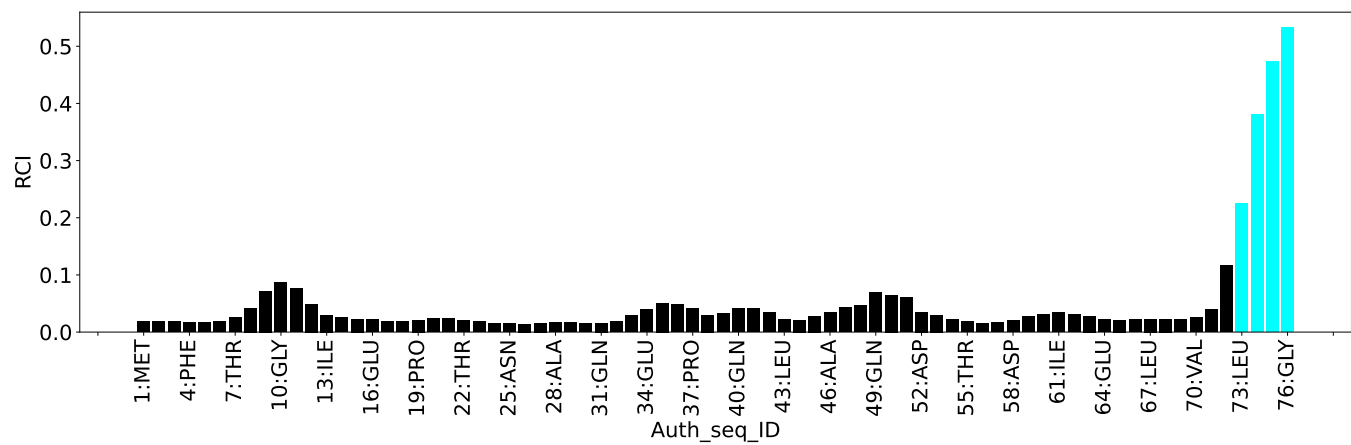
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

| List Id | Chain | Res | Type | Atom | Shift, ppm | Expected range, ppm | Z-score |
|---------|-------|-----|------|------|------------|---------------------|---------|
| 1       | A     | 68  | HIS  | CE1  | 119.48     | 126.08 – 149.12     | -7.9    |

#### 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                                | 2764  |
| Intra-residue ( $ i-j =0$ )                              | 652   |
| Sequential ( $ i-j =1$ )                                 | 446   |
| Medium range ( $ i-j >1$ and $ i-j <5$ )                 | 441   |
| Long range ( $ i-j \geq 5$ )                             | 1188  |
| Inter-chain                                              | 0     |
| Hydrogen bond restraints                                 | 37    |
| Disulfide bond restraints                                | 0     |
| Total dihedral-angle restraints                          | 63    |
| Number of unmapped restraints                            | 0     |
| Number of restraints per residue                         | 37.2  |
| Number of long range restraints per residue <sup>1</sup> | 15.9  |

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

### 8.2 Residual restraint violations

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

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

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

| Bins (Å)         | Average number of violations per model | Max (Å) |
|------------------|----------------------------------------|---------|
| 0.1-0.2 (Small)  | 22.5                                   | 0.2     |
| 0.2-0.5 (Medium) | 23.4                                   | 0.5     |
| >0.5 (Large)     | 13.8                                   | 1.47    |

### 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)   | 50.6                                   | 9.99    |
| 10.0-20.0 (Medium) | 4.0                                    | 17.67   |
| >20.0 (Large)      | 0.3                                    | 34.33   |

## 9 Distance violation analysis ⓘ

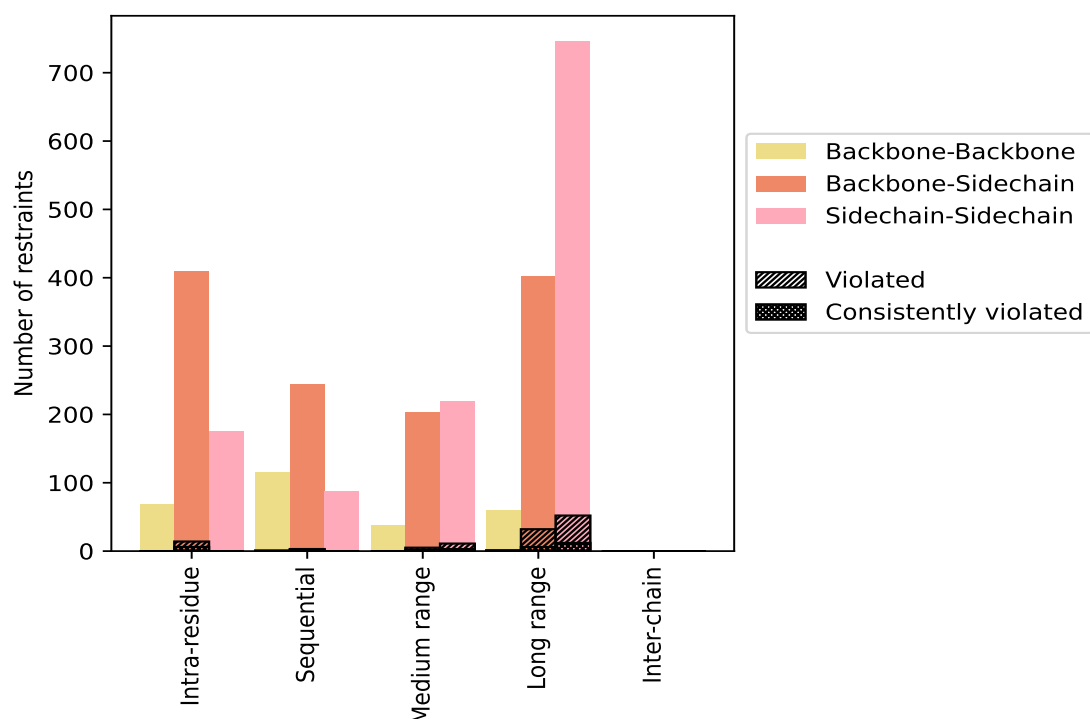
### 9.1 Summary of distance violations ⓘ

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>652</b>  | <b>23.6</b>    | <b>14</b>             | <b>2.1</b>     | <b>0.5</b>     | <b>6</b>                           | <b>0.9</b>     | <b>0.2</b>     |
| Backbone-Backbone                                                           | 68          | 2.5            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 409         | 14.8           | 14                    | 3.4            | 0.5            | 6                                  | 1.5            | 0.2            |
| Sidechain-Sidechain                                                         | 175         | 6.3            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| <b>Sequential (<math> i-j =1</math>)</b>                                    | <b>446</b>  | <b>16.1</b>    | <b>4</b>              | <b>0.9</b>     | <b>0.1</b>     | <b>2</b>                           | <b>0.4</b>     | <b>0.1</b>     |
| Backbone-Backbone                                                           | 115         | 4.2            | 1                     | 0.9            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 244         | 8.8            | 3                     | 1.2            | 0.1            | 2                                  | 0.8            | 0.1            |
| Sidechain-Sidechain                                                         | 87          | 3.1            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| <b>Medium range (<math> i-j &gt;1</math> &amp; <math> i-j &lt;5</math>)</b> | <b>441</b>  | <b>16.0</b>    | <b>16</b>             | <b>3.6</b>     | <b>0.6</b>     | <b>5</b>                           | <b>1.1</b>     | <b>0.2</b>     |
| Backbone-Backbone                                                           | 37          | 1.3            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 185         | 6.7            | 5                     | 2.7            | 0.2            | 2                                  | 1.1            | 0.1            |
| Sidechain-Sidechain                                                         | 219         | 7.9            | 11                    | 5.0            | 0.4            | 3                                  | 1.4            | 0.1            |
| <b>Long range (<math> i-j \geq 5</math>)</b>                                | <b>1188</b> | <b>43.0</b>    | <b>84</b>             | <b>7.1</b>     | <b>3.0</b>     | <b>19</b>                          | <b>1.6</b>     | <b>0.7</b>     |
| Backbone-Backbone                                                           | 59          | 2.1            | 1                     | 1.7            | 0.0            | 1                                  | 1.7            | 0.0            |
| Backbone-Sidechain                                                          | 383         | 13.9           | 31                    | 8.1            | 1.1            | 6                                  | 1.6            | 0.2            |
| Sidechain-Sidechain                                                         | 746         | 27.0           | 52                    | 7.0            | 1.9            | 12                                 | 1.6            | 0.4            |
| <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>37</b>   | <b>1.3</b>     | <b>1</b>              | <b>2.7</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>2764</b> | <b>100.0</b>   | <b>119</b>            | <b>4.3</b>     | <b>4.3</b>     | <b>32</b>                          | <b>1.2</b>     | <b>1.2</b>     |
| Backbone-Backbone                                                           | 279         | 10.1           | 2                     | 0.7            | 0.1            | 1                                  | 0.4            | 0.0            |
| Backbone-Sidechain                                                          | 1258        | 45.5           | 54                    | 4.3            | 2.0            | 16                                 | 1.3            | 0.6            |
| Sidechain-Sidechain                                                         | 1227        | 44.4           | 63                    | 5.1            | 2.3            | 15                                 | 1.2            | 0.5            |

<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        | 8                    | 3               | 7               | 38              | 0               | 56    | 0.36     | 1.09    | 0.26                | 0.26       |
| 2        | 10                   | 2               | 6               | 42              | 0               | 60    | 0.36     | 1.19    | 0.26                | 0.26       |
| 3        | 10                   | 2               | 7               | 44              | 0               | 63    | 0.36     | 1.27    | 0.28                | 0.26       |
| 4        | 11                   | 3               | 11              | 37              | 0               | 62    | 0.37     | 1.4     | 0.28                | 0.28       |
| 5        | 8                    | 3               | 7               | 40              | 0               | 58    | 0.35     | 1.22    | 0.26                | 0.26       |
| 6        | 10                   | 2               | 9               | 43              | 0               | 64    | 0.37     | 1.12    | 0.27                | 0.26       |
| 7        | 10                   | 3               | 8               | 42              | 0               | 63    | 0.33     | 1.09    | 0.26                | 0.21       |
| 8        | 10                   | 2               | 11              | 35              | 0               | 58    | 0.4      | 1.47    | 0.32                | 0.28       |
| 9        | 10                   | 2               | 10              | 41              | 0               | 63    | 0.33     | 1.05    | 0.23                | 0.24       |
| 10       | 9                    | 2               | 8               | 42              | 0               | 61    | 0.32     | 1.1     | 0.24                | 0.22       |

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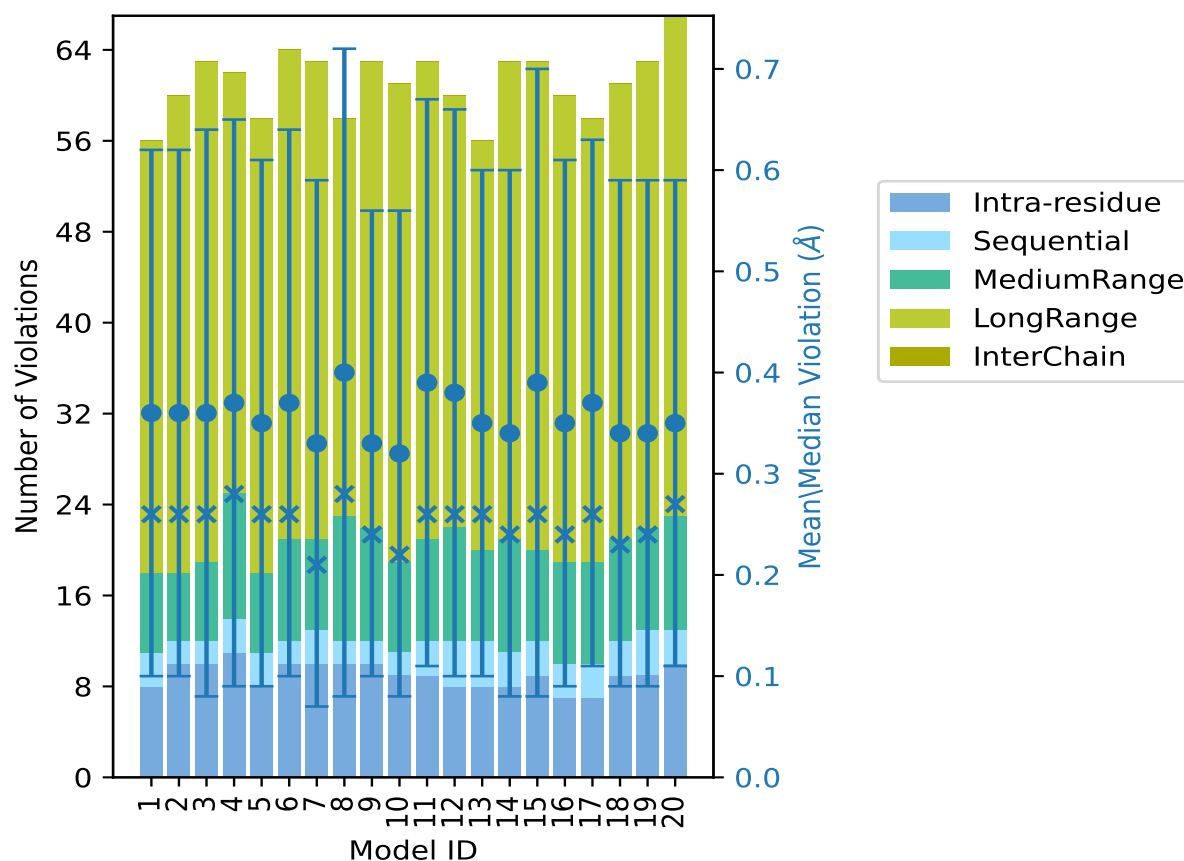
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| Model ID | Number of violations |                 |                 |                 |                 |       | Mean (Å) | Max (Å) | SD <sup>6</sup> (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
|          | IR <sup>1</sup>      | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total |          |         |                     |            |
| 11       | 9                    | 3               | 9               | 42              | 0               | 63    | 0.39     | 1.23    | 0.28                | 0.26       |
| 12       | 8                    | 4               | 10              | 38              | 0               | 60    | 0.38     | 1.24    | 0.28                | 0.26       |
| 13       | 8                    | 4               | 8               | 36              | 0               | 56    | 0.35     | 1.28    | 0.25                | 0.26       |
| 14       | 8                    | 3               | 10              | 42              | 0               | 63    | 0.34     | 1.2     | 0.26                | 0.24       |
| 15       | 9                    | 3               | 8               | 43              | 0               | 63    | 0.39     | 1.44    | 0.31                | 0.26       |
| 16       | 7                    | 3               | 9               | 41              | 0               | 60    | 0.35     | 1.12    | 0.26                | 0.24       |
| 17       | 7                    | 3               | 9               | 39              | 0               | 58    | 0.37     | 1.13    | 0.26                | 0.26       |
| 18       | 9                    | 3               | 9               | 40              | 0               | 61    | 0.34     | 1.14    | 0.25                | 0.23       |
| 19       | 9                    | 4               | 9               | 41              | 0               | 63    | 0.34     | 1.21    | 0.25                | 0.24       |
| 20       | 10                   | 3               | 10              | 44              | 0               | 67    | 0.35     | 1.16    | 0.24                | 0.27       |

<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

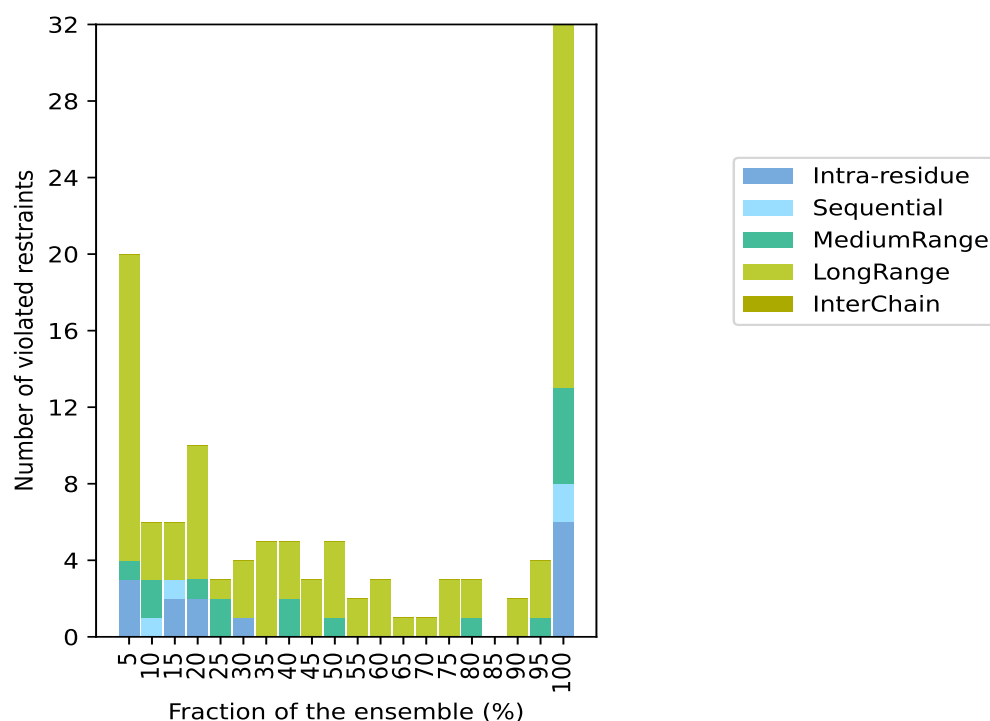
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 2609(IR:638, SQ:442, MR:425, LR:1104, IC:0) restraints are 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                             | 0               | 1               | 16              | 0               | 20    | 1                        | 5.0   |
| 0                             | 1               | 2               | 3               | 0               | 6     | 2                        | 10.0  |
| 2                             | 1               | 0               | 3               | 0               | 6     | 3                        | 15.0  |
| 2                             | 0               | 1               | 7               | 0               | 10    | 4                        | 20.0  |
| 0                             | 0               | 2               | 1               | 0               | 3     | 5                        | 25.0  |
| 1                             | 0               | 0               | 3               | 0               | 4     | 6                        | 30.0  |
| 0                             | 0               | 0               | 5               | 0               | 5     | 7                        | 35.0  |
| 0                             | 0               | 2               | 3               | 0               | 5     | 8                        | 40.0  |
| 0                             | 0               | 0               | 3               | 0               | 3     | 9                        | 45.0  |
| 0                             | 0               | 1               | 4               | 0               | 5     | 10                       | 50.0  |
| 0                             | 0               | 0               | 2               | 0               | 2     | 11                       | 55.0  |
| 0                             | 0               | 0               | 3               | 0               | 3     | 12                       | 60.0  |
| 0                             | 0               | 0               | 1               | 0               | 1     | 13                       | 65.0  |
| 0                             | 0               | 0               | 1               | 0               | 1     | 14                       | 70.0  |
| 0                             | 0               | 0               | 3               | 0               | 3     | 15                       | 75.0  |
| 0                             | 0               | 1               | 2               | 0               | 3     | 16                       | 80.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 17                       | 85.0  |
| 0                             | 0               | 0               | 2               | 0               | 2     | 18                       | 90.0  |
| 0                             | 0               | 1               | 3               | 0               | 4     | 19                       | 95.0  |
| 6                             | 2               | 5               | 19              | 0               | 32    | 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

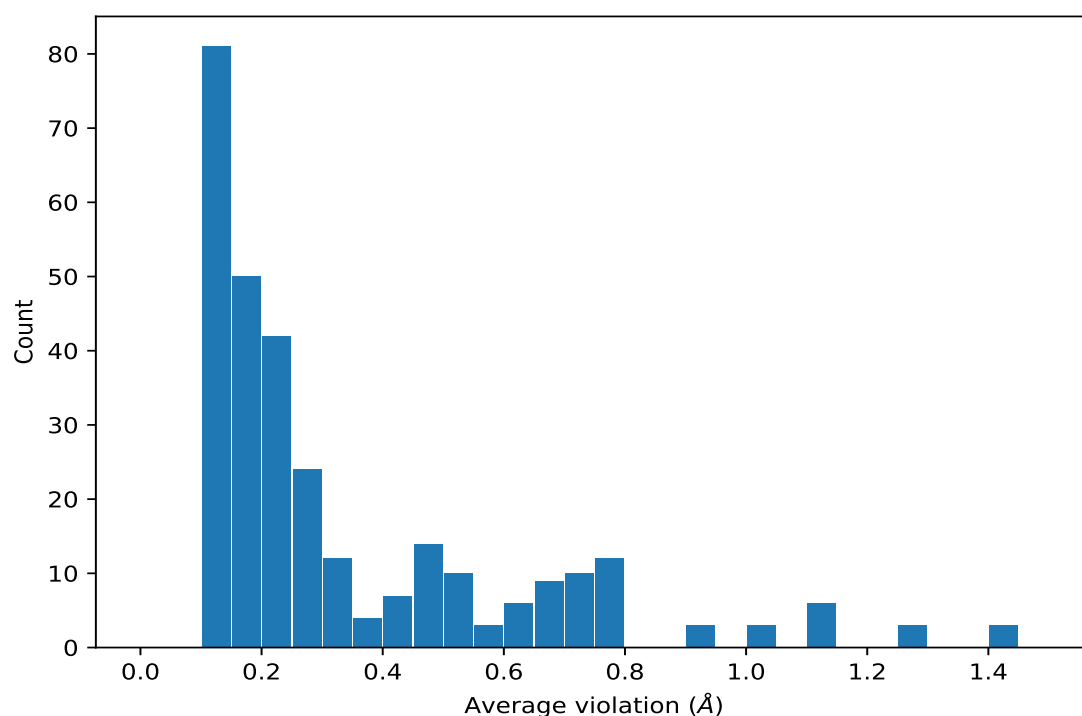
### 9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



## 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) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,36)   | 1:1:A:MET:HE2   | 1:17:A:VAL:HG12 | 20                  | 1.15     | 0.07                | 1.15       |
| (1,36)   | 1:1:A:MET:HE3   | 1:17:A:VAL:HG12 | 20                  | 1.15     | 0.07                | 1.15       |
| (1,36)   | 1:1:A:MET:HE1   | 1:17:A:VAL:HG12 | 20                  | 1.15     | 0.07                | 1.15       |
| (1,36)   | 1:1:A:MET:HE2   | 1:17:A:VAL:HG13 | 20                  | 1.15     | 0.07                | 1.15       |
| (1,36)   | 1:1:A:MET:HE2   | 1:17:A:VAL:HG11 | 20                  | 1.15     | 0.07                | 1.15       |
| (1,36)   | 1:1:A:MET:HE3   | 1:17:A:VAL:HG11 | 20                  | 1.15     | 0.07                | 1.15       |
| (1,2473) | 1:66:A:THR:HG23 | 1:68:A:HIS:HB3  | 20                  | 1.0      | 0.03                | 0.99       |
| (1,2473) | 1:66:A:THR:HG22 | 1:68:A:HIS:HB3  | 20                  | 1.0      | 0.03                | 0.99       |
| (1,2473) | 1:66:A:THR:HG21 | 1:68:A:HIS:HB3  | 20                  | 1.0      | 0.03                | 0.99       |
| (1,2483) | 1:67:A:LEU:HD11 | 1:67:A:LEU:HA   | 20                  | 0.78     | 0.0                 | 0.78       |
| (1,2483) | 1:67:A:LEU:HD12 | 1:67:A:LEU:HA   | 20                  | 0.78     | 0.0                 | 0.78       |
| (1,2483) | 1:67:A:LEU:HD13 | 1:67:A:LEU:HA   | 20                  | 0.78     | 0.0                 | 0.78       |
| (1,35)   | 1:1:A:MET:HE2   | 1:17:A:VAL:HG12 | 20                  | 0.78     | 0.07                | 0.77       |
| (1,35)   | 1:1:A:MET:HE3   | 1:17:A:VAL:HG12 | 20                  | 0.78     | 0.07                | 0.77       |
| (1,35)   | 1:1:A:MET:HE1   | 1:17:A:VAL:HG12 | 20                  | 0.78     | 0.07                | 0.77       |
| (1,35)   | 1:1:A:MET:HE2   | 1:17:A:VAL:HG13 | 20                  | 0.78     | 0.07                | 0.77       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,35)   | 1:1:A:MET:HE2   | 1:17:A:VAL:HG11 | 20                  | 0.78     | 0.07                | 0.77       |
| (1,35)   | 1:1:A:MET:HE3   | 1:17:A:VAL:HG11 | 20                  | 0.78     | 0.07                | 0.77       |
| (1,156)  | 1:3:A:ILE:HD11  | 1:3:A:ILE:HA    | 20                  | 0.77     | 0.02                | 0.76       |
| (1,156)  | 1:3:A:ILE:HD13  | 1:3:A:ILE:HA    | 20                  | 0.77     | 0.02                | 0.76       |
| (1,156)  | 1:3:A:ILE:HD12  | 1:3:A:ILE:HA    | 20                  | 0.77     | 0.02                | 0.76       |
| (1,2478) | 1:67:A:LEU:HA   | 1:67:A:LEU:HD11 | 20                  | 0.51     | 0.01                | 0.51       |
| (1,2478) | 1:67:A:LEU:HA   | 1:67:A:LEU:HD12 | 20                  | 0.51     | 0.01                | 0.51       |
| (1,2478) | 1:67:A:LEU:HA   | 1:67:A:LEU:HD13 | 20                  | 0.51     | 0.01                | 0.51       |
| (1,98)   | 1:1:A:MET:HE2   | 1:67:A:LEU:HD12 | 20                  | 0.51     | 0.05                | 0.5        |
| (1,98)   | 1:1:A:MET:HE2   | 1:67:A:LEU:HD13 | 20                  | 0.51     | 0.05                | 0.5        |
| (1,98)   | 1:1:A:MET:HE1   | 1:67:A:LEU:HD12 | 20                  | 0.51     | 0.05                | 0.5        |
| (1,98)   | 1:1:A:MET:HE2   | 1:67:A:LEU:HD11 | 20                  | 0.51     | 0.05                | 0.5        |
| (1,1768) | 1:42:A:ARG:HD2  | 1:70:A:VAL:HG23 | 20                  | 0.5      | 0.05                | 0.5        |
| (1,1768) | 1:42:A:ARG:HD2  | 1:70:A:VAL:HG21 | 20                  | 0.5      | 0.05                | 0.5        |
| (1,1768) | 1:42:A:ARG:HD2  | 1:70:A:VAL:HG22 | 20                  | 0.5      | 0.05                | 0.5        |
| (1,149)  | 1:3:A:ILE:HA    | 1:3:A:ILE:HD11  | 20                  | 0.49     | 0.02                | 0.48       |
| (1,149)  | 1:3:A:ILE:HA    | 1:3:A:ILE:HD13  | 20                  | 0.49     | 0.02                | 0.48       |
| (1,149)  | 1:3:A:ILE:HA    | 1:3:A:ILE:HD12  | 20                  | 0.49     | 0.02                | 0.48       |
| (1,2547) | 1:70:A:VAL:HB   | 1:71:A:LEU:H    | 20                  | 0.48     | 0.02                | 0.48       |
| (1,1758) | 1:42:A:ARG:HA   | 1:70:A:VAL:HG21 | 20                  | 0.44     | 0.01                | 0.44       |
| (1,1758) | 1:42:A:ARG:HA   | 1:70:A:VAL:HG22 | 20                  | 0.44     | 0.01                | 0.44       |
| (1,1758) | 1:42:A:ARG:HA   | 1:70:A:VAL:HG23 | 20                  | 0.44     | 0.01                | 0.44       |
| (1,1726) | 1:42:A:ARG:HA   | 1:42:A:ARG:HD3  | 20                  | 0.36     | 0.03                | 0.36       |
| (1,551)  | 1:8:A:LEU:HG    | 1:70:A:VAL:HA   | 20                  | 0.36     | 0.03                | 0.35       |
| (1,292)  | 1:4:A:PHE:HB3   | 1:66:A:THR:HA   | 20                  | 0.29     | 0.02                | 0.29       |
| (1,378)  | 1:5:A:VAL:HG21  | 1:67:A:LEU:HG   | 20                  | 0.28     | 0.03                | 0.27       |
| (1,378)  | 1:5:A:VAL:HG22  | 1:67:A:LEU:HG   | 20                  | 0.28     | 0.03                | 0.27       |
| (1,378)  | 1:5:A:VAL:HG23  | 1:67:A:LEU:HG   | 20                  | 0.28     | 0.03                | 0.27       |
| (1,387)  | 1:5:A:VAL:HG11  | 1:69:A:LEU:HG   | 20                  | 0.27     | 0.01                | 0.26       |
| (1,387)  | 1:5:A:VAL:HG12  | 1:69:A:LEU:HG   | 20                  | 0.27     | 0.01                | 0.26       |
| (1,387)  | 1:5:A:VAL:HG13  | 1:69:A:LEU:HG   | 20                  | 0.27     | 0.01                | 0.26       |
| (1,634)  | 1:13:A:ILE:HG12 | 1:30:A:ILE:HD11 | 20                  | 0.26     | 0.02                | 0.26       |
| (1,634)  | 1:13:A:ILE:HG12 | 1:30:A:ILE:HD12 | 20                  | 0.26     | 0.02                | 0.26       |
| (1,634)  | 1:13:A:ILE:HG12 | 1:30:A:ILE:HD13 | 20                  | 0.26     | 0.02                | 0.26       |
| (1,634)  | 1:13:A:ILE:HG13 | 1:30:A:ILE:HD11 | 20                  | 0.26     | 0.02                | 0.26       |
| (1,634)  | 1:13:A:ILE:HG13 | 1:30:A:ILE:HD12 | 20                  | 0.26     | 0.02                | 0.26       |
| (1,634)  | 1:13:A:ILE:HG13 | 1:30:A:ILE:HD13 | 20                  | 0.26     | 0.02                | 0.26       |
| (1,1370) | 1:30:A:ILE:HA   | 1:33:A:LYS:HB3  | 20                  | 0.26     | 0.01                | 0.26       |
| (1,264)  | 1:4:A:PHE:HA    | 1:14:A:THR:HG22 | 20                  | 0.24     | 0.09                | 0.24       |
| (1,264)  | 1:4:A:PHE:HA    | 1:14:A:THR:HG23 | 20                  | 0.24     | 0.09                | 0.24       |
| (1,264)  | 1:4:A:PHE:HA    | 1:14:A:THR:HG21 | 20                  | 0.24     | 0.09                | 0.24       |
| (1,264)  | 1:4:A:PHE:HA    | 1:12:A:THR:HG21 | 20                  | 0.24     | 0.09                | 0.24       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,264)  | 1:4:A:PHE:HA    | 1:12:A:THR:HG22 | 20                  | 0.24     | 0.09                | 0.24       |
| (1,264)  | 1:4:A:PHE:HA    | 1:12:A:THR:HG23 | 20                  | 0.24     | 0.09                | 0.24       |
| (1,1294) | 1:27:A:LYS:HE2  | 1:52:A:ASP:HB3  | 20                  | 0.24     | 0.03                | 0.23       |
| (1,1294) | 1:27:A:LYS:HE3  | 1:52:A:ASP:HB3  | 20                  | 0.24     | 0.03                | 0.23       |
| (1,318)  | 1:5:A:VAL:HG11  | 1:7:A:THR:HG22  | 20                  | 0.22     | 0.06                | 0.21       |
| (1,318)  | 1:5:A:VAL:HG12  | 1:7:A:THR:HG21  | 20                  | 0.22     | 0.06                | 0.21       |
| (1,318)  | 1:5:A:VAL:HG11  | 1:7:A:THR:HG21  | 20                  | 0.22     | 0.06                | 0.21       |
| (1,318)  | 1:5:A:VAL:HG12  | 1:7:A:THR:HG23  | 20                  | 0.22     | 0.06                | 0.21       |
| (1,318)  | 1:5:A:VAL:HG13  | 1:7:A:THR:HG23  | 20                  | 0.22     | 0.06                | 0.21       |
| (1,318)  | 1:5:A:VAL:HG11  | 1:7:A:THR:HG23  | 20                  | 0.22     | 0.06                | 0.21       |
| (1,177)  | 1:29:A:LYS:HA   | 1:15:A:LEU:HD22 | 20                  | 0.21     | 0.04                | 0.22       |
| (1,177)  | 1:29:A:LYS:HA   | 1:15:A:LEU:HD21 | 20                  | 0.21     | 0.04                | 0.22       |
| (1,177)  | 1:29:A:LYS:HA   | 1:15:A:LEU:HD23 | 20                  | 0.21     | 0.04                | 0.22       |
| (2,7)    | 1:2:A:GLN:HG2   | 1:3:A:ILE:HA    | 20                  | 0.21     | 0.01                | 0.21       |
| (1,15)   | 1:1:A:MET:HB3   | 1:3:A:ILE:HG21  | 20                  | 0.21     | 0.01                | 0.21       |
| (1,15)   | 1:1:A:MET:HB3   | 1:3:A:ILE:HG22  | 20                  | 0.21     | 0.01                | 0.21       |
| (1,15)   | 1:1:A:MET:HB3   | 1:3:A:ILE:HG23  | 20                  | 0.21     | 0.01                | 0.21       |
| (1,1511) | 1:34:A:GLU:HG3  | 1:69:A:LEU:HD21 | 20                  | 0.18     | 0.06                | 0.18       |
| (1,1511) | 1:34:A:GLU:HG3  | 1:69:A:LEU:HD22 | 20                  | 0.18     | 0.06                | 0.18       |
| (1,1511) | 1:34:A:GLU:HG3  | 1:69:A:LEU:HD23 | 20                  | 0.18     | 0.06                | 0.18       |
| (1,386)  | 1:5:A:VAL:HG11  | 1:69:A:LEU:HG   | 20                  | 0.18     | 0.01                | 0.18       |
| (1,386)  | 1:5:A:VAL:HG12  | 1:69:A:LEU:HG   | 20                  | 0.18     | 0.01                | 0.18       |
| (1,386)  | 1:5:A:VAL:HG13  | 1:69:A:LEU:HG   | 20                  | 0.18     | 0.01                | 0.18       |
| (1,97)   | 1:1:A:MET:HG3   | 1:63:A:LYS:HA   | 20                  | 0.18     | 0.01                | 0.18       |
| (1,865)  | 1:19:A:PRO:HA   | 1:56:A:LEU:HA   | 20                  | 0.18     | 0.01                | 0.18       |
| (1,604)  | 1:14:A:THR:HG22 | 1:14:A:THR:H    | 20                  | 0.16     | 0.01                | 0.16       |
| (1,604)  | 1:14:A:THR:HG21 | 1:14:A:THR:H    | 20                  | 0.16     | 0.01                | 0.16       |
| (1,604)  | 1:14:A:THR:HG23 | 1:14:A:THR:H    | 20                  | 0.16     | 0.01                | 0.16       |
| (1,1350) | 1:30:A:ILE:HA   | 1:30:A:ILE:HD11 | 20                  | 0.16     | 0.01                | 0.16       |
| (1,1350) | 1:30:A:ILE:HA   | 1:30:A:ILE:HD12 | 20                  | 0.16     | 0.01                | 0.16       |
| (1,1350) | 1:30:A:ILE:HA   | 1:30:A:ILE:HD13 | 20                  | 0.16     | 0.01                | 0.16       |
| (1,1990) | 1:45:A:PHE:HB3  | 1:67:A:LEU:HD11 | 20                  | 0.14     | 0.01                | 0.14       |
| (1,1990) | 1:45:A:PHE:HB3  | 1:67:A:LEU:HD12 | 20                  | 0.14     | 0.01                | 0.14       |
| (1,1990) | 1:45:A:PHE:HB3  | 1:67:A:LEU:HD13 | 20                  | 0.14     | 0.01                | 0.14       |
| (1,1990) | 1:45:A:PHE:HB3  | 1:67:A:LEU:HD21 | 20                  | 0.14     | 0.01                | 0.14       |
| (1,1990) | 1:45:A:PHE:HB3  | 1:67:A:LEU:HD22 | 20                  | 0.14     | 0.01                | 0.14       |
| (1,1990) | 1:45:A:PHE:HB3  | 1:67:A:LEU:HD23 | 20                  | 0.14     | 0.01                | 0.14       |
| (1,1887) | 1:44:A:ILE:HD13 | 1:70:A:VAL:HG11 | 20                  | 0.14     | 0.02                | 0.14       |
| (1,1887) | 1:44:A:ILE:HD11 | 1:70:A:VAL:HG12 | 20                  | 0.14     | 0.02                | 0.14       |
| (1,1887) | 1:44:A:ILE:HD11 | 1:70:A:VAL:HG11 | 20                  | 0.14     | 0.02                | 0.14       |
| (1,1887) | 1:44:A:ILE:HD13 | 1:70:A:VAL:HG13 | 20                  | 0.14     | 0.02                | 0.14       |
| (1,1887) | 1:44:A:ILE:HD12 | 1:70:A:VAL:HG11 | 20                  | 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) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1887) | 1:44:A:ILE:HD11 | 1:70:A:VAL:HG13 | 20                  | 0.14     | 0.02                | 0.14       |
| (1,1691) | 1:40:A:GLN:HG3  | 1:71:A:LEU:HD23 | 19                  | 0.74     | 0.08                | 0.74       |
| (1,1691) | 1:40:A:GLN:HG2  | 1:71:A:LEU:HD23 | 19                  | 0.74     | 0.08                | 0.74       |
| (1,1691) | 1:40:A:GLN:HG3  | 1:71:A:LEU:HD21 | 19                  | 0.74     | 0.08                | 0.74       |
| (1,1691) | 1:40:A:GLN:HG2  | 1:71:A:LEU:HD21 | 19                  | 0.74     | 0.08                | 0.74       |
| (1,357)  | 1:17:A:VAL:HG11 | 1:29:A:LYS:HG3  | 19                  | 0.41     | 0.05                | 0.41       |
| (1,357)  | 1:17:A:VAL:HG11 | 1:29:A:LYS:HG2  | 19                  | 0.41     | 0.05                | 0.41       |
| (1,357)  | 1:17:A:VAL:HG12 | 1:29:A:LYS:HG3  | 19                  | 0.41     | 0.05                | 0.41       |
| (1,357)  | 1:17:A:VAL:HG13 | 1:29:A:LYS:HG3  | 19                  | 0.41     | 0.05                | 0.41       |
| (1,38)   | 1:1:A:MET:HE2   | 1:17:A:VAL:HG22 | 19                  | 0.32     | 0.13                | 0.34       |
| (1,38)   | 1:1:A:MET:HE3   | 1:17:A:VAL:HG23 | 19                  | 0.32     | 0.13                | 0.34       |
| (1,38)   | 1:1:A:MET:HE3   | 1:17:A:VAL:HG21 | 19                  | 0.32     | 0.13                | 0.34       |
| (1,38)   | 1:1:A:MET:HE1   | 1:17:A:VAL:HG23 | 19                  | 0.32     | 0.13                | 0.34       |
| (1,38)   | 1:1:A:MET:HE3   | 1:17:A:VAL:HG22 | 19                  | 0.32     | 0.13                | 0.34       |
| (1,38)   | 1:1:A:MET:HE2   | 1:17:A:VAL:HG21 | 19                  | 0.32     | 0.13                | 0.34       |
| (1,1560) | 1:36:A:ILE:HG21 | 1:40:A:GLN:HG2  | 19                  | 0.22     | 0.02                | 0.21       |
| (1,1560) | 1:36:A:ILE:HG21 | 1:40:A:GLN:HG3  | 19                  | 0.22     | 0.02                | 0.21       |
| (1,1560) | 1:36:A:ILE:HG22 | 1:40:A:GLN:HG2  | 19                  | 0.22     | 0.02                | 0.21       |
| (1,1560) | 1:36:A:ILE:HG22 | 1:40:A:GLN:HG3  | 19                  | 0.22     | 0.02                | 0.21       |
| (1,1560) | 1:36:A:ILE:HG23 | 1:40:A:GLN:HG2  | 19                  | 0.22     | 0.02                | 0.21       |
| (1,1560) | 1:36:A:ILE:HG23 | 1:40:A:GLN:HG3  | 19                  | 0.22     | 0.02                | 0.21       |
| (1,1775) | 1:72:A:ARG:HD2  | 1:72:A:ARG:HA   | 18                  | 0.68     | 0.09                | 0.68       |
| (1,1775) | 1:72:A:ARG:HD3  | 1:72:A:ARG:HA   | 18                  | 0.68     | 0.09                | 0.68       |
| (2,72)   | 1:27:A:LYS:HE3  | 1:69:A:LEU:HD12 | 18                  | 0.23     | 0.05                | 0.24       |
| (2,72)   | 1:27:A:LYS:HE3  | 1:69:A:LEU:HD13 | 18                  | 0.23     | 0.05                | 0.24       |
| (2,72)   | 1:27:A:LYS:HE3  | 1:69:A:LEU:HD11 | 18                  | 0.23     | 0.05                | 0.24       |
| (1,459)  | 1:6:A:LYS:HE3   | 1:66:A:THR:HG21 | 16                  | 0.48     | 0.22                | 0.54       |
| (1,459)  | 1:6:A:LYS:HE2   | 1:66:A:THR:HG23 | 16                  | 0.48     | 0.22                | 0.54       |
| (1,459)  | 1:6:A:LYS:HE3   | 1:66:A:THR:HG23 | 16                  | 0.48     | 0.22                | 0.54       |
| (1,459)  | 1:6:A:LYS:HE2   | 1:66:A:THR:HG22 | 16                  | 0.48     | 0.22                | 0.54       |
| (1,459)  | 1:6:A:LYS:HE2   | 1:66:A:THR:HG21 | 16                  | 0.48     | 0.22                | 0.54       |
| (1,319)  | 1:5:A:VAL:HG11  | 1:7:A:THR:HG22  | 16                  | 0.17     | 0.06                | 0.15       |
| (1,319)  | 1:5:A:VAL:HG12  | 1:7:A:THR:HG21  | 16                  | 0.17     | 0.06                | 0.15       |
| (1,319)  | 1:5:A:VAL:HG11  | 1:7:A:THR:HG21  | 16                  | 0.17     | 0.06                | 0.15       |
| (1,319)  | 1:5:A:VAL:HG13  | 1:7:A:THR:HG23  | 16                  | 0.17     | 0.06                | 0.15       |
| (1,319)  | 1:5:A:VAL:HG12  | 1:7:A:THR:HG23  | 16                  | 0.17     | 0.06                | 0.15       |
| (1,319)  | 1:5:A:VAL:HG11  | 1:7:A:THR:HG23  | 16                  | 0.17     | 0.06                | 0.15       |
| (1,1861) | 1:44:A:ILE:HD11 | 1:49:A:GLN:HA   | 16                  | 0.17     | 0.02                | 0.18       |
| (1,1861) | 1:44:A:ILE:HD12 | 1:49:A:GLN:HA   | 16                  | 0.17     | 0.02                | 0.18       |
| (1,1861) | 1:44:A:ILE:HD13 | 1:49:A:GLN:HA   | 16                  | 0.17     | 0.02                | 0.18       |
| (1,1920) | 1:44:A:ILE:HG12 | 1:70:A:VAL:HG23 | 15                  | 0.73     | 0.03                | 0.72       |
| (1,1920) | 1:44:A:ILE:HG12 | 1:70:A:VAL:HG21 | 15                  | 0.73     | 0.03                | 0.72       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1920) | 1:44:A:ILE:HG12 | 1:70:A:VAL:HG22 | 15                  | 0.73     | 0.03                | 0.72       |
| (1,1888) | 1:44:A:ILE:HG12 | 1:70:A:VAL:HG11 | 15                  | 0.62     | 0.02                | 0.62       |
| (1,1888) | 1:44:A:ILE:HG12 | 1:70:A:VAL:HG12 | 15                  | 0.62     | 0.02                | 0.62       |
| (1,1888) | 1:44:A:ILE:HG12 | 1:70:A:VAL:HG13 | 15                  | 0.62     | 0.02                | 0.62       |
| (1,1776) | 1:42:A:ARG:HG3  | 1:72:A:ARG:H    | 15                  | 0.32     | 0.08                | 0.33       |
| (1,1817) | 1:43:A:LEU:HD22 | 1:67:A:LEU:HB3  | 14                  | 0.16     | 0.04                | 0.16       |
| (1,1817) | 1:43:A:LEU:HD21 | 1:67:A:LEU:HB3  | 14                  | 0.16     | 0.04                | 0.16       |
| (1,1817) | 1:43:A:LEU:HD23 | 1:67:A:LEU:HB3  | 14                  | 0.16     | 0.04                | 0.16       |
| (1,1860) | 1:44:A:ILE:HD11 | 1:49:A:GLN:HA   | 13                  | 0.12     | 0.01                | 0.12       |
| (1,1860) | 1:44:A:ILE:HD12 | 1:49:A:GLN:HA   | 13                  | 0.12     | 0.01                | 0.12       |
| (1,1860) | 1:44:A:ILE:HD13 | 1:49:A:GLN:HA   | 13                  | 0.12     | 0.01                | 0.12       |
| (1,1692) | 1:40:A:GLN:HG2  | 1:73:A:LEU:HD22 | 12                  | 0.67     | 0.3                 | 0.7        |
| (1,1692) | 1:40:A:GLN:HG2  | 1:73:A:LEU:HD13 | 12                  | 0.67     | 0.3                 | 0.7        |
| (1,1692) | 1:40:A:GLN:HG3  | 1:71:A:LEU:HD23 | 12                  | 0.67     | 0.3                 | 0.7        |
| (1,1692) | 1:40:A:GLN:HG2  | 1:73:A:LEU:HD12 | 12                  | 0.67     | 0.3                 | 0.7        |
| (1,1692) | 1:40:A:GLN:HG2  | 1:73:A:LEU:HD11 | 12                  | 0.67     | 0.3                 | 0.7        |
| (1,1692) | 1:40:A:GLN:HG2  | 1:71:A:LEU:HD21 | 12                  | 0.67     | 0.3                 | 0.7        |
| (1,1692) | 1:40:A:GLN:HG2  | 1:73:A:LEU:HD23 | 12                  | 0.67     | 0.3                 | 0.7        |
| (1,458)  | 1:6:A:LYS:HD2   | 1:66:A:THR:HG21 | 12                  | 0.47     | 0.17                | 0.4        |
| (1,458)  | 1:6:A:LYS:HD3   | 1:66:A:THR:HG22 | 12                  | 0.47     | 0.17                | 0.4        |
| (1,458)  | 1:6:A:LYS:HD2   | 1:66:A:THR:HG23 | 12                  | 0.47     | 0.17                | 0.4        |
| (1,458)  | 1:6:A:LYS:HD3   | 1:66:A:THR:HG23 | 12                  | 0.47     | 0.17                | 0.4        |
| (1,458)  | 1:6:A:LYS:HD3   | 1:66:A:THR:HG21 | 12                  | 0.47     | 0.17                | 0.4        |
| (1,148)  | 1:68:A:HIS:HA   | 1:66:A:THR:HG21 | 12                  | 0.16     | 0.02                | 0.16       |
| (1,148)  | 1:68:A:HIS:HA   | 1:66:A:THR:HG22 | 12                  | 0.16     | 0.02                | 0.16       |
| (1,148)  | 1:68:A:HIS:HA   | 1:66:A:THR:HG23 | 12                  | 0.16     | 0.02                | 0.16       |
| (1,356)  | 1:17:A:VAL:HG11 | 1:29:A:LYS:HG3  | 11                  | 0.14     | 0.03                | 0.12       |
| (1,356)  | 1:17:A:VAL:HG12 | 1:29:A:LYS:HG3  | 11                  | 0.14     | 0.03                | 0.12       |
| (1,356)  | 1:17:A:VAL:HG11 | 1:29:A:LYS:HG2  | 11                  | 0.14     | 0.03                | 0.12       |
| (1,356)  | 1:17:A:VAL:HG13 | 1:29:A:LYS:HG3  | 11                  | 0.14     | 0.03                | 0.12       |
| (1,973)  | 1:22:A:THR:HA   | 1:55:A:THR:HB   | 11                  | 0.11     | 0.01                | 0.1        |
| (1,19)   | 1:1:A:MET:HE2   | 1:3:A:ILE:HD13  | 10                  | 0.28     | 0.07                | 0.3        |
| (1,19)   | 1:1:A:MET:HE2   | 1:3:A:ILE:HD12  | 10                  | 0.28     | 0.07                | 0.3        |
| (1,19)   | 1:1:A:MET:HE2   | 1:3:A:ILE:HD11  | 10                  | 0.28     | 0.07                | 0.3        |
| (1,19)   | 1:1:A:MET:HE1   | 1:3:A:ILE:HD12  | 10                  | 0.28     | 0.07                | 0.3        |
| (1,439)  | 1:6:A:LYS:HD2   | 1:12:A:THR:HA   | 10                  | 0.25     | 0.05                | 0.26       |
| (1,439)  | 1:6:A:LYS:HD3   | 1:12:A:THR:HA   | 10                  | 0.25     | 0.05                | 0.26       |
| (1,37)   | 1:1:A:MET:HE2   | 1:17:A:VAL:HG22 | 10                  | 0.22     | 0.06                | 0.22       |
| (1,37)   | 1:1:A:MET:HE3   | 1:17:A:VAL:HG23 | 10                  | 0.22     | 0.06                | 0.22       |
| (1,37)   | 1:1:A:MET:HE1   | 1:17:A:VAL:HG23 | 10                  | 0.22     | 0.06                | 0.22       |
| (1,37)   | 1:1:A:MET:HE3   | 1:17:A:VAL:HG21 | 10                  | 0.22     | 0.06                | 0.22       |
| (1,37)   | 1:1:A:MET:HE2   | 1:17:A:VAL:HG21 | 10                  | 0.22     | 0.06                | 0.22       |

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| Key      | Atom-1         | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,60)   | 1:28:A:ALA:HB1 | 1:25:A:ASN:HA   | 10                  | 0.16     | 0.01                | 0.16       |
| (1,66)   | 1:28:A:ALA:HB1 | 1:27:A:LYS:HA   | 10                  | 0.13     | 0.0                 | 0.13       |
| (1,463)  | 1:6:A:LYS:HG3  | 1:66:A:THR:HG21 | 9                   | 0.94     | 0.32                | 1.11       |
| (1,463)  | 1:6:A:LYS:HG3  | 1:66:A:THR:HG22 | 9                   | 0.94     | 0.32                | 1.11       |
| (1,463)  | 1:6:A:LYS:HG2  | 1:66:A:THR:HG21 | 9                   | 0.94     | 0.32                | 1.11       |
| (1,339)  | 1:5:A:VAL:HG21 | 1:13:A:ILE:HG13 | 9                   | 0.23     | 0.07                | 0.27       |
| (1,339)  | 1:5:A:VAL:HG23 | 1:13:A:ILE:HG13 | 9                   | 0.23     | 0.07                | 0.27       |
| (1,339)  | 1:5:A:VAL:HG22 | 1:13:A:ILE:HG13 | 9                   | 0.23     | 0.07                | 0.27       |
| (1,1770) | 1:42:A:ARG:HG2 | 1:70:A:VAL:HG21 | 9                   | 0.12     | 0.01                | 0.12       |
| (1,1770) | 1:42:A:ARG:HG2 | 1:70:A:VAL:HG22 | 9                   | 0.12     | 0.01                | 0.12       |
| (1,1770) | 1:42:A:ARG:HG2 | 1:70:A:VAL:HG23 | 9                   | 0.12     | 0.01                | 0.12       |
| (1,1770) | 1:42:A:ARG:HG3 | 1:70:A:VAL:HG21 | 9                   | 0.12     | 0.01                | 0.12       |
| (1,1770) | 1:42:A:ARG:HG3 | 1:70:A:VAL:HG22 | 9                   | 0.12     | 0.01                | 0.12       |
| (1,1770) | 1:42:A:ARG:HG3 | 1:70:A:VAL:HG23 | 9                   | 0.12     | 0.01                | 0.12       |
| (1,461)  | 1:6:A:LYS:HG3  | 1:66:A:THR:HG21 | 8                   | 0.74     | 0.12                | 0.8        |
| (1,461)  | 1:6:A:LYS:HG3  | 1:66:A:THR:HG22 | 8                   | 0.74     | 0.12                | 0.8        |
| (1,461)  | 1:6:A:LYS:HG2  | 1:66:A:THR:HG21 | 8                   | 0.74     | 0.12                | 0.8        |
| (1,462)  | 1:6:A:LYS:HG3  | 1:66:A:THR:HG21 | 8                   | 0.63     | 0.12                | 0.69       |
| (1,462)  | 1:6:A:LYS:HG3  | 1:66:A:THR:HG22 | 8                   | 0.63     | 0.12                | 0.69       |
| (1,462)  | 1:6:A:LYS:HG2  | 1:66:A:THR:HG21 | 8                   | 0.63     | 0.12                | 0.69       |
| (1,269)  | 1:4:A:PHE:HB2  | 1:12:A:THR:HG21 | 8                   | 0.17     | 0.03                | 0.18       |
| (1,269)  | 1:4:A:PHE:HB2  | 1:12:A:THR:HG22 | 8                   | 0.17     | 0.03                | 0.18       |
| (1,269)  | 1:4:A:PHE:HB2  | 1:12:A:THR:HG23 | 8                   | 0.17     | 0.03                | 0.18       |
| (1,914)  | 1:52:A:ASP:HB2 | 1:24:A:GLU:HB2  | 8                   | 0.12     | 0.04                | 0.11       |
| (1,914)  | 1:52:A:ASP:HB2 | 1:24:A:GLU:HB3  | 8                   | 0.12     | 0.04                | 0.11       |
| (1,562)  | 1:9:A:THR:HG21 | 1:11:A:LYS:HD2  | 8                   | 0.11     | 0.01                | 0.11       |
| (1,562)  | 1:9:A:THR:HG21 | 1:11:A:LYS:HD3  | 8                   | 0.11     | 0.01                | 0.11       |
| (1,562)  | 1:9:A:THR:HG22 | 1:11:A:LYS:HD2  | 8                   | 0.11     | 0.01                | 0.11       |
| (1,562)  | 1:9:A:THR:HG22 | 1:11:A:LYS:HD3  | 8                   | 0.11     | 0.01                | 0.11       |
| (1,562)  | 1:9:A:THR:HG23 | 1:11:A:LYS:HD2  | 8                   | 0.11     | 0.01                | 0.11       |
| (1,562)  | 1:9:A:THR:HG23 | 1:11:A:LYS:HD3  | 8                   | 0.11     | 0.01                | 0.11       |
| (1,460)  | 1:6:A:LYS:HG3  | 1:66:A:THR:HG21 | 7                   | 0.34     | 0.08                | 0.37       |
| (1,460)  | 1:6:A:LYS:HG3  | 1:66:A:THR:HG22 | 7                   | 0.34     | 0.08                | 0.37       |
| (1,45)   | 1:1:A:MET:HE3  | 1:18:A:GLU:HA   | 7                   | 0.18     | 0.04                | 0.18       |
| (1,45)   | 1:1:A:MET:HE2  | 1:18:A:GLU:HA   | 7                   | 0.18     | 0.04                | 0.18       |
| (1,1512) | 1:34:A:GLU:HG3 | 1:69:A:LEU:HD23 | 7                   | 0.15     | 0.03                | 0.14       |
| (1,1512) | 1:34:A:GLU:HG3 | 1:69:A:LEU:HD21 | 7                   | 0.15     | 0.03                | 0.14       |
| (1,1512) | 1:34:A:GLU:HG3 | 1:69:A:LEU:HD22 | 7                   | 0.15     | 0.03                | 0.14       |
| (1,506)  | 1:7:A:THR:HA   | 1:69:A:LEU:HD21 | 7                   | 0.13     | 0.01                | 0.13       |
| (1,506)  | 1:7:A:THR:HA   | 1:69:A:LEU:HD22 | 7                   | 0.13     | 0.01                | 0.13       |
| (1,506)  | 1:7:A:THR:HA   | 1:69:A:LEU:HD23 | 7                   | 0.13     | 0.01                | 0.13       |
| (1,1149) | 1:24:A:GLU:HA  | 1:52:A:ASP:HB3  | 7                   | 0.1      | 0.0                 | 0.1        |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1696) | 1:40:A:GLN:HG2  | 1:74:A:ARG:HG3  | 6                   | 0.57     | 0.27                | 0.5        |
| (1,1696) | 1:40:A:GLN:HG2  | 1:74:A:ARG:HG2  | 6                   | 0.57     | 0.27                | 0.5        |
| (1,1696) | 1:40:A:GLN:HG2  | 1:73:A:LEU:HG   | 6                   | 0.57     | 0.27                | 0.5        |
| (1,1675) | 1:40:A:GLN:HA   | 1:72:A:ARG:HD2  | 6                   | 0.21     | 0.04                | 0.22       |
| (1,1675) | 1:40:A:GLN:HA   | 1:72:A:ARG:HD3  | 6                   | 0.21     | 0.04                | 0.22       |
| (1,532)  | 1:8:A:LEU:HG    | 1:8:A:LEU:H     | 6                   | 0.12     | 0.01                | 0.12       |
| (1,1863) | 1:44:A:ILE:HD11 | 1:49:A:GLN:HB2  | 6                   | 0.11     | 0.0                 | 0.11       |
| (1,1863) | 1:44:A:ILE:HD11 | 1:49:A:GLN:HB3  | 6                   | 0.11     | 0.0                 | 0.11       |
| (1,1863) | 1:44:A:ILE:HD12 | 1:49:A:GLN:HB2  | 6                   | 0.11     | 0.0                 | 0.11       |
| (1,1863) | 1:44:A:ILE:HD12 | 1:49:A:GLN:HB3  | 6                   | 0.11     | 0.0                 | 0.11       |
| (1,1863) | 1:44:A:ILE:HD13 | 1:49:A:GLN:HB2  | 6                   | 0.11     | 0.0                 | 0.11       |
| (1,1863) | 1:44:A:ILE:HD13 | 1:49:A:GLN:HB3  | 6                   | 0.11     | 0.0                 | 0.11       |
| (1,1744) | 1:42:A:ARG:HG2  | 1:44:A:ILE:HD11 | 5                   | 0.36     | 0.29                | 0.26       |
| (1,1744) | 1:42:A:ARG:HG2  | 1:44:A:ILE:HD12 | 5                   | 0.36     | 0.29                | 0.26       |
| (1,341)  | 1:5:A:VAL:HG21  | 1:13:A:ILE:HG13 | 5                   | 0.15     | 0.02                | 0.15       |
| (1,341)  | 1:5:A:VAL:HG22  | 1:13:A:ILE:HG13 | 5                   | 0.15     | 0.02                | 0.15       |
| (1,341)  | 1:5:A:VAL:HG23  | 1:13:A:ILE:HG13 | 5                   | 0.15     | 0.02                | 0.15       |
| (1,420)  | 1:6:A:LYS:HE2   | 1:10:A:GLY:HA2  | 5                   | 0.13     | 0.02                | 0.14       |
| (1,420)  | 1:6:A:LYS:HE2   | 1:10:A:GLY:HA3  | 5                   | 0.13     | 0.02                | 0.14       |
| (1,420)  | 1:6:A:LYS:HE3   | 1:10:A:GLY:HA2  | 5                   | 0.13     | 0.02                | 0.14       |
| (1,420)  | 1:6:A:LYS:HE3   | 1:10:A:GLY:HA3  | 5                   | 0.13     | 0.02                | 0.14       |
| (1,457)  | 1:6:A:LYS:HD3   | 1:66:A:THR:HG23 | 4                   | 0.27     | 0.04                | 0.25       |
| (1,457)  | 1:6:A:LYS:HD3   | 1:66:A:THR:HG21 | 4                   | 0.27     | 0.04                | 0.25       |
| (1,457)  | 1:6:A:LYS:HD3   | 1:66:A:THR:HG22 | 4                   | 0.27     | 0.04                | 0.25       |
| (1,1916) | 1:44:A:ILE:HD11 | 1:70:A:VAL:HG21 | 4                   | 0.17     | 0.0                 | 0.17       |
| (1,1916) | 1:44:A:ILE:HD11 | 1:70:A:VAL:HG22 | 4                   | 0.17     | 0.0                 | 0.17       |
| (1,1916) | 1:44:A:ILE:HD11 | 1:70:A:VAL:HG23 | 4                   | 0.17     | 0.0                 | 0.17       |
| (1,1916) | 1:44:A:ILE:HD12 | 1:70:A:VAL:HG21 | 4                   | 0.17     | 0.0                 | 0.17       |
| (1,1916) | 1:44:A:ILE:HD12 | 1:70:A:VAL:HG22 | 4                   | 0.17     | 0.0                 | 0.17       |
| (1,1916) | 1:44:A:ILE:HD12 | 1:70:A:VAL:HG23 | 4                   | 0.17     | 0.0                 | 0.17       |
| (1,1916) | 1:44:A:ILE:HD13 | 1:70:A:VAL:HG21 | 4                   | 0.17     | 0.0                 | 0.17       |
| (1,1916) | 1:44:A:ILE:HD13 | 1:70:A:VAL:HG22 | 4                   | 0.17     | 0.0                 | 0.17       |
| (1,1916) | 1:44:A:ILE:HD13 | 1:70:A:VAL:HG23 | 4                   | 0.17     | 0.0                 | 0.17       |
| (1,1869) | 1:44:A:ILE:HG12 | 1:49:A:GLN:HA   | 4                   | 0.16     | 0.02                | 0.16       |
| (1,1869) | 1:44:A:ILE:HG13 | 1:49:A:GLN:HA   | 4                   | 0.16     | 0.02                | 0.16       |
| (1,2564) | 1:72:A:ARG:HA   | 1:72:A:ARG:HD2  | 4                   | 0.15     | 0.02                | 0.15       |
| (1,2564) | 1:72:A:ARG:HA   | 1:72:A:ARG:HD3  | 4                   | 0.15     | 0.02                | 0.15       |
| (1,630)  | 1:13:A:ILE:HG21 | 1:15:A:LEU:HD23 | 4                   | 0.15     | 0.02                | 0.15       |
| (1,630)  | 1:13:A:ILE:HG22 | 1:15:A:LEU:HD23 | 4                   | 0.15     | 0.02                | 0.15       |
| (1,1722) | 1:41:A:GLN:H    | 1:71:A:LEU:HD23 | 4                   | 0.12     | 0.02                | 0.12       |
| (1,1867) | 1:44:A:ILE:HG12 | 1:49:A:GLN:HA   | 4                   | 0.12     | 0.02                | 0.12       |
| (1,1867) | 1:44:A:ILE:HG13 | 1:49:A:GLN:HA   | 4                   | 0.12     | 0.02                | 0.12       |

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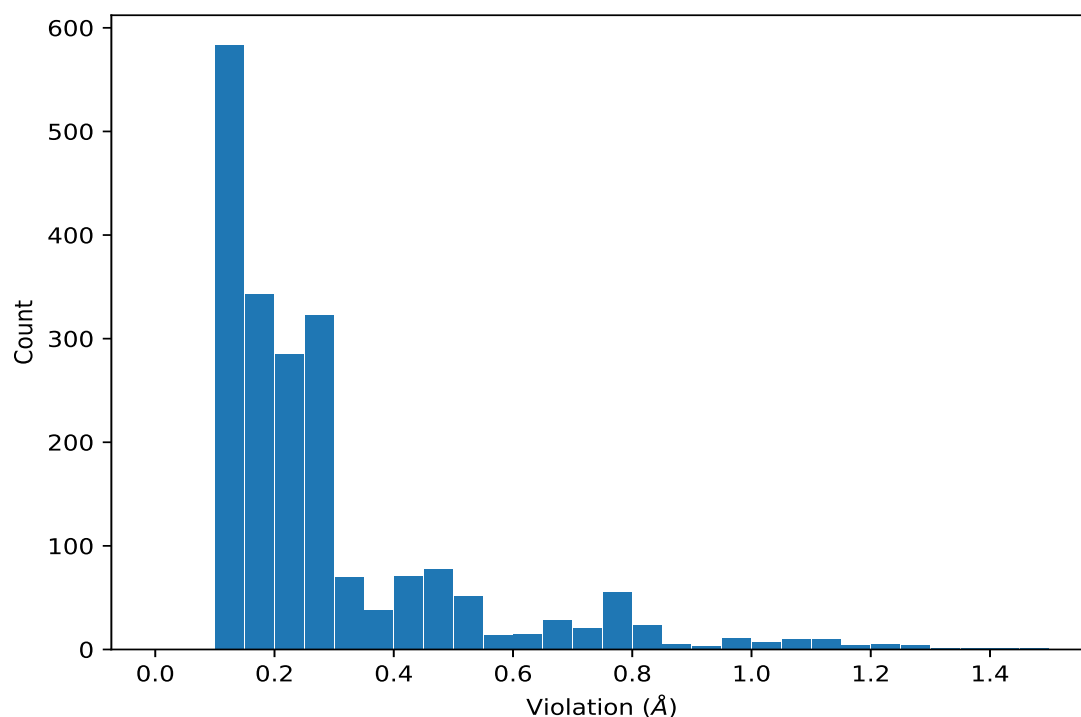
| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,48)   | 1:1:A:MET:HE3   | 1:19:A:PRO:HA   | 4                   | 0.12     | 0.02                | 0.12       |
| (1,1475) | 1:33:A:LYS:HD2  | 1:33:A:LYS:HA   | 4                   | 0.12     | 0.01                | 0.12       |
| (1,1475) | 1:33:A:LYS:HD3  | 1:33:A:LYS:HA   | 4                   | 0.12     | 0.01                | 0.12       |
| (1,1903) | 1:44:A:ILE:HG21 | 1:68:A:HIS:HB3  | 4                   | 0.12     | 0.01                | 0.12       |
| (1,1903) | 1:44:A:ILE:HG22 | 1:68:A:HIS:HB3  | 4                   | 0.12     | 0.01                | 0.12       |
| (1,1903) | 1:44:A:ILE:HG23 | 1:68:A:HIS:HB3  | 4                   | 0.12     | 0.01                | 0.12       |
| (1,340)  | 1:5:A:VAL:HG23  | 1:13:A:ILE:HG13 | 3                   | 1.44     | 0.03                | 1.44       |
| (1,340)  | 1:5:A:VAL:HG21  | 1:15:A:LEU:HG   | 3                   | 1.44     | 0.03                | 1.44       |
| (1,340)  | 1:5:A:VAL:HG21  | 1:13:A:ILE:HG13 | 3                   | 1.44     | 0.03                | 1.44       |
| (1,338)  | 1:5:A:VAL:HG23  | 1:13:A:ILE:HG13 | 3                   | 1.28     | 0.02                | 1.28       |
| (1,338)  | 1:5:A:VAL:HG21  | 1:15:A:LEU:HG   | 3                   | 1.28     | 0.02                | 1.28       |
| (1,338)  | 1:5:A:VAL:HG21  | 1:13:A:ILE:HG13 | 3                   | 1.28     | 0.02                | 1.28       |
| (1,684)  | 1:15:A:LEU:HA   | 1:15:A:LEU:HD12 | 3                   | 0.34     | 0.0                 | 0.34       |
| (1,684)  | 1:15:A:LEU:HA   | 1:15:A:LEU:HD13 | 3                   | 0.34     | 0.0                 | 0.34       |
| (1,2028) | 1:48:A:LYS:HG2  | 1:48:A:LYS:HA   | 3                   | 0.18     | 0.0                 | 0.18       |
| (1,2028) | 1:48:A:LYS:HG3  | 1:48:A:LYS:HA   | 3                   | 0.18     | 0.0                 | 0.18       |
| (1,126)  | 1:2:A:GLN:HA    | 1:14:A:THR:HG22 | 3                   | 0.14     | 0.01                | 0.13       |
| (1,126)  | 1:2:A:GLN:HA    | 1:14:A:THR:HG23 | 3                   | 0.14     | 0.01                | 0.13       |
| (1,598)  | 1:12:A:THR:HA   | 1:13:A:ILE:HG21 | 3                   | 0.1      | 0.0                 | 0.1        |
| (1,598)  | 1:12:A:THR:HA   | 1:13:A:ILE:HG22 | 3                   | 0.1      | 0.0                 | 0.1        |
| (1,598)  | 1:12:A:THR:HA   | 1:13:A:ILE:HG23 | 3                   | 0.1      | 0.0                 | 0.1        |
| (1,1392) | 1:30:A:ILE:HB   | 1:41:A:GLN:HE22 | 2                   | 0.35     | 0.0                 | 0.35       |
| (1,2591) | 1:74:A:ARG:HA   | 1:75:A:GLY:H    | 2                   | 0.3      | 0.01                | 0.3        |
| (1,738)  | 1:15:A:LEU:HD13 | 1:33:A:LYS:HD2  | 2                   | 0.2      | 0.05                | 0.2        |
| (1,738)  | 1:15:A:LEU:HD11 | 1:33:A:LYS:HD2  | 2                   | 0.2      | 0.05                | 0.2        |
| (1,1134) | 1:24:A:GLU:HA   | 1:27:A:LYS:HD2  | 2                   | 0.16     | 0.01                | 0.16       |
| (1,1134) | 1:24:A:GLU:HA   | 1:27:A:LYS:HD3  | 2                   | 0.16     | 0.01                | 0.16       |
| (1,1659) | 1:38:A:PRO:HA   | 1:41:A:GLN:HE21 | 2                   | 0.14     | 0.01                | 0.14       |
| (1,1878) | 1:44:A:ILE:HG21 | 1:49:A:GLN:HB2  | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1878) | 1:44:A:ILE:HG21 | 1:49:A:GLN:HB3  | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1878) | 1:44:A:ILE:HG22 | 1:49:A:GLN:HB2  | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1878) | 1:44:A:ILE:HG22 | 1:49:A:GLN:HB3  | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1878) | 1:44:A:ILE:HG23 | 1:49:A:GLN:HB2  | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1878) | 1:44:A:ILE:HG23 | 1:49:A:GLN:HB3  | 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) |
|----------|----------------|-----------------|----------|---------------|
| (1,340)  | 1:5:A:VAL:HG23 | 1:13:A:ILE:HG13 | 8        | 1.47          |
| (1,340)  | 1:5:A:VAL:HG21 | 1:13:A:ILE:HG13 | 15       | 1.44          |
| (1,340)  | 1:5:A:VAL:HG21 | 1:15:A:LEU:HG   | 4        | 1.4           |
| (1,338)  | 1:5:A:VAL:HG23 | 1:13:A:ILE:HG13 | 8        | 1.31          |
| (1,338)  | 1:5:A:VAL:HG21 | 1:13:A:ILE:HG13 | 15       | 1.28          |
| (1,36)   | 1:1:A:MET:HE2  | 1:17:A:VAL:HG12 | 13       | 1.28          |
| (1,36)   | 1:1:A:MET:HE2  | 1:17:A:VAL:HG12 | 3        | 1.27          |
| (1,338)  | 1:5:A:VAL:HG21 | 1:15:A:LEU:HG   | 4        | 1.25          |
| (1,1692) | 1:40:A:GLN:HG3 | 1:71:A:LEU:HD23 | 3        | 1.24          |
| (1,36)   | 1:1:A:MET:HE3  | 1:17:A:VAL:HG12 | 12       | 1.24          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,36)   | 1:1:A:MET:HE2   | 1:17:A:VAL:HG13 | 11       | 1.23          |
| (1,36)   | 1:1:A:MET:HE1   | 1:17:A:VAL:HG12 | 5        | 1.22          |
| (1,36)   | 1:1:A:MET:HE2   | 1:17:A:VAL:HG13 | 19       | 1.21          |
| (1,36)   | 1:1:A:MET:HE2   | 1:17:A:VAL:HG13 | 14       | 1.2           |
| (1,36)   | 1:1:A:MET:HE2   | 1:17:A:VAL:HG12 | 2        | 1.19          |
| (1,36)   | 1:1:A:MET:HE2   | 1:17:A:VAL:HG11 | 15       | 1.17          |
| (1,36)   | 1:1:A:MET:HE3   | 1:17:A:VAL:HG12 | 20       | 1.16          |
| (1,36)   | 1:1:A:MET:HE3   | 1:17:A:VAL:HG11 | 18       | 1.14          |
| (1,463)  | 1:6:A:LYS:HG3   | 1:66:A:THR:HG21 | 12       | 1.13          |
| (1,36)   | 1:1:A:MET:HE2   | 1:17:A:VAL:HG11 | 17       | 1.13          |
| (1,463)  | 1:6:A:LYS:HG3   | 1:66:A:THR:HG21 | 6        | 1.12          |
| (1,463)  | 1:6:A:LYS:HG3   | 1:66:A:THR:HG21 | 14       | 1.12          |
| (1,463)  | 1:6:A:LYS:HG3   | 1:66:A:THR:HG21 | 16       | 1.12          |
| (1,463)  | 1:6:A:LYS:HG3   | 1:66:A:THR:HG21 | 11       | 1.11          |
| (1,463)  | 1:6:A:LYS:HG3   | 1:66:A:THR:HG21 | 17       | 1.11          |
| (1,36)   | 1:1:A:MET:HE2   | 1:17:A:VAL:HG12 | 16       | 1.11          |
| (1,36)   | 1:1:A:MET:HE3   | 1:17:A:VAL:HG12 | 10       | 1.1           |
| (1,36)   | 1:1:A:MET:HE2   | 1:17:A:VAL:HG12 | 1        | 1.09          |
| (1,36)   | 1:1:A:MET:HE3   | 1:17:A:VAL:HG12 | 4        | 1.09          |
| (1,36)   | 1:1:A:MET:HE3   | 1:17:A:VAL:HG12 | 7        | 1.09          |
| (1,2473) | 1:66:A:THR:HG23 | 1:68:A:HIS:HB3  | 1        | 1.07          |
| (1,2473) | 1:66:A:THR:HG23 | 1:68:A:HIS:HB3  | 2        | 1.07          |
| (1,1692) | 1:40:A:GLN:HG2  | 1:71:A:LEU:HD21 | 15       | 1.07          |
| (1,1696) | 1:40:A:GLN:HG2  | 1:74:A:ARG:HG3  | 1        | 1.06          |
| (1,36)   | 1:1:A:MET:HE3   | 1:17:A:VAL:HG12 | 8        | 1.06          |
| (1,36)   | 1:1:A:MET:HE3   | 1:17:A:VAL:HG12 | 6        | 1.05          |
| (1,36)   | 1:1:A:MET:HE3   | 1:17:A:VAL:HG12 | 9        | 1.05          |
| (1,2473) | 1:66:A:THR:HG23 | 1:68:A:HIS:HB3  | 13       | 1.02          |
| (1,2473) | 1:66:A:THR:HG23 | 1:68:A:HIS:HB3  | 18       | 1.01          |
| (1,2473) | 1:66:A:THR:HG23 | 1:68:A:HIS:HB3  | 14       | 1.0           |
| (1,2473) | 1:66:A:THR:HG23 | 1:68:A:HIS:HB3  | 15       | 1.0           |
| (1,2473) | 1:66:A:THR:HG23 | 1:68:A:HIS:HB3  | 16       | 1.0           |
| (1,2473) | 1:66:A:THR:HG23 | 1:68:A:HIS:HB3  | 17       | 1.0           |
| (1,2473) | 1:66:A:THR:HG23 | 1:68:A:HIS:HB3  | 20       | 1.0           |
| (1,2473) | 1:66:A:THR:HG21 | 1:68:A:HIS:HB3  | 4        | 0.99          |
| (1,2473) | 1:66:A:THR:HG22 | 1:68:A:HIS:HB3  | 9        | 0.99          |
| (1,2473) | 1:66:A:THR:HG23 | 1:68:A:HIS:HB3  | 11       | 0.99          |
| (1,2473) | 1:66:A:THR:HG23 | 1:68:A:HIS:HB3  | 19       | 0.99          |
| (1,2473) | 1:66:A:THR:HG22 | 1:68:A:HIS:HB3  | 3        | 0.98          |
| (1,2473) | 1:66:A:THR:HG22 | 1:68:A:HIS:HB3  | 7        | 0.98          |
| (1,2473) | 1:66:A:THR:HG23 | 1:68:A:HIS:HB3  | 12       | 0.98          |
| (1,2473) | 1:66:A:THR:HG22 | 1:68:A:HIS:HB3  | 5        | 0.97          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2473) | 1:66:A:THR:HG22 | 1:68:A:HIS:HB3  | 8        | 0.97          |
| (1,2473) | 1:66:A:THR:HG22 | 1:68:A:HIS:HB3  | 10       | 0.97          |
| (1,2473) | 1:66:A:THR:HG22 | 1:68:A:HIS:HB3  | 6        | 0.96          |
| (1,1744) | 1:42:A:ARG:HG2  | 1:44:A:ILE:HD12 | 8        | 0.93          |
| (1,1691) | 1:40:A:GLN:HG3  | 1:71:A:LEU:HD23 | 8        | 0.9           |
| (1,35)   | 1:1:A:MET:HE2   | 1:17:A:VAL:HG12 | 13       | 0.9           |
| (1,35)   | 1:1:A:MET:HE2   | 1:17:A:VAL:HG12 | 3        | 0.89          |
| (1,1691) | 1:40:A:GLN:HG3  | 1:71:A:LEU:HD23 | 3        | 0.88          |
| (1,463)  | 1:6:A:LYS:HG3   | 1:66:A:THR:HG22 | 18       | 0.88          |
| (1,35)   | 1:1:A:MET:HE2   | 1:17:A:VAL:HG13 | 11       | 0.86          |
| (1,35)   | 1:1:A:MET:HE3   | 1:17:A:VAL:HG12 | 12       | 0.86          |
| (1,35)   | 1:1:A:MET:HE1   | 1:17:A:VAL:HG12 | 5        | 0.85          |
| (1,1775) | 1:72:A:ARG:HD3  | 1:72:A:ARG:HA   | 2        | 0.84          |
| (1,459)  | 1:6:A:LYS:HE2   | 1:66:A:THR:HG21 | 11       | 0.84          |
| (1,1692) | 1:40:A:GLN:HG2  | 1:73:A:LEU:HD12 | 7        | 0.83          |
| (1,35)   | 1:1:A:MET:HE2   | 1:17:A:VAL:HG13 | 19       | 0.83          |
| (1,461)  | 1:6:A:LYS:HG3   | 1:66:A:THR:HG21 | 12       | 0.82          |
| (1,459)  | 1:6:A:LYS:HE2   | 1:66:A:THR:HG21 | 12       | 0.82          |
| (1,35)   | 1:1:A:MET:HE2   | 1:17:A:VAL:HG12 | 2        | 0.82          |
| (1,35)   | 1:1:A:MET:HE2   | 1:17:A:VAL:HG13 | 14       | 0.82          |
| (1,1775) | 1:72:A:ARG:HD2  | 1:72:A:ARG:HA   | 6        | 0.81          |
| (1,1692) | 1:40:A:GLN:HG2  | 1:73:A:LEU:HD13 | 2        | 0.81          |
| (1,1692) | 1:40:A:GLN:HG2  | 1:73:A:LEU:HD13 | 9        | 0.81          |
| (1,1691) | 1:40:A:GLN:HG2  | 1:71:A:LEU:HD23 | 12       | 0.81          |
| (1,461)  | 1:6:A:LYS:HG3   | 1:66:A:THR:HG21 | 6        | 0.81          |
| (1,461)  | 1:6:A:LYS:HG3   | 1:66:A:THR:HG21 | 14       | 0.81          |
| (1,156)  | 1:3:A:ILE:HD13  | 1:3:A:ILE:HA    | 9        | 0.81          |
| (1,156)  | 1:3:A:ILE:HD11  | 1:3:A:ILE:HA    | 20       | 0.81          |
| (1,1775) | 1:72:A:ARG:HD2  | 1:72:A:ARG:HA   | 19       | 0.8           |
| (1,1692) | 1:40:A:GLN:HG2  | 1:73:A:LEU:HD13 | 11       | 0.8           |
| (1,1691) | 1:40:A:GLN:HG3  | 1:71:A:LEU:HD23 | 1        | 0.8           |
| (1,1691) | 1:40:A:GLN:HG2  | 1:71:A:LEU:HD23 | 2        | 0.8           |
| (1,461)  | 1:6:A:LYS:HG3   | 1:66:A:THR:HG21 | 11       | 0.8           |
| (1,461)  | 1:6:A:LYS:HG3   | 1:66:A:THR:HG21 | 16       | 0.8           |
| (1,461)  | 1:6:A:LYS:HG3   | 1:66:A:THR:HG21 | 17       | 0.8           |
| (1,2483) | 1:67:A:LEU:HD13 | 1:67:A:LEU:HA   | 8        | 0.79          |
| (1,2483) | 1:67:A:LEU:HD11 | 1:67:A:LEU:HA   | 15       | 0.79          |
| (1,1920) | 1:44:A:ILE:HG12 | 1:70:A:VAL:HG23 | 17       | 0.79          |
| (1,1691) | 1:40:A:GLN:HG2  | 1:71:A:LEU:HD21 | 18       | 0.79          |
| (1,463)  | 1:6:A:LYS:HG2   | 1:66:A:THR:HG21 | 20       | 0.79          |
| (1,35)   | 1:1:A:MET:HE2   | 1:17:A:VAL:HG11 | 15       | 0.79          |
| (1,2483) | 1:67:A:LEU:HD11 | 1:67:A:LEU:HA   | 1        | 0.78          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2483) | 1:67:A:LEU:HD11 | 1:67:A:LEU:HA   | 2        | 0.78          |
| (1,2483) | 1:67:A:LEU:HD12 | 1:67:A:LEU:HA   | 3        | 0.78          |
| (1,2483) | 1:67:A:LEU:HD12 | 1:67:A:LEU:HA   | 4        | 0.78          |
| (1,2483) | 1:67:A:LEU:HD11 | 1:67:A:LEU:HA   | 5        | 0.78          |
| (1,2483) | 1:67:A:LEU:HD13 | 1:67:A:LEU:HA   | 7        | 0.78          |
| (1,2483) | 1:67:A:LEU:HD13 | 1:67:A:LEU:HA   | 10       | 0.78          |
| (1,2483) | 1:67:A:LEU:HD13 | 1:67:A:LEU:HA   | 11       | 0.78          |
| (1,2483) | 1:67:A:LEU:HD13 | 1:67:A:LEU:HA   | 12       | 0.78          |
| (1,2483) | 1:67:A:LEU:HD13 | 1:67:A:LEU:HA   | 13       | 0.78          |
| (1,2483) | 1:67:A:LEU:HD13 | 1:67:A:LEU:HA   | 14       | 0.78          |
| (1,2483) | 1:67:A:LEU:HD13 | 1:67:A:LEU:HA   | 16       | 0.78          |
| (1,2483) | 1:67:A:LEU:HD11 | 1:67:A:LEU:HA   | 17       | 0.78          |
| (1,2483) | 1:67:A:LEU:HD13 | 1:67:A:LEU:HA   | 18       | 0.78          |
| (1,2483) | 1:67:A:LEU:HD11 | 1:67:A:LEU:HA   | 19       | 0.78          |
| (1,1920) | 1:44:A:ILE:HG12 | 1:70:A:VAL:HG21 | 7        | 0.78          |
| (1,1920) | 1:44:A:ILE:HG12 | 1:70:A:VAL:HG22 | 11       | 0.78          |
| (1,1691) | 1:40:A:GLN:HG3  | 1:71:A:LEU:HD23 | 7        | 0.78          |
| (1,156)  | 1:3:A:ILE:HD12  | 1:3:A:ILE:HA    | 8        | 0.78          |
| (1,35)   | 1:1:A:MET:HE3   | 1:17:A:VAL:HG12 | 20       | 0.78          |
| (1,2483) | 1:67:A:LEU:HD12 | 1:67:A:LEU:HA   | 6        | 0.77          |
| (1,2483) | 1:67:A:LEU:HD12 | 1:67:A:LEU:HA   | 9        | 0.77          |
| (1,2483) | 1:67:A:LEU:HD11 | 1:67:A:LEU:HA   | 20       | 0.77          |
| (1,458)  | 1:6:A:LYS:HD3   | 1:66:A:THR:HG21 | 20       | 0.77          |
| (1,156)  | 1:3:A:ILE:HD11  | 1:3:A:ILE:HA    | 11       | 0.77          |
| (1,156)  | 1:3:A:ILE:HD11  | 1:3:A:ILE:HA    | 13       | 0.77          |
| (1,156)  | 1:3:A:ILE:HD11  | 1:3:A:ILE:HA    | 1        | 0.76          |
| (1,156)  | 1:3:A:ILE:HD11  | 1:3:A:ILE:HA    | 2        | 0.76          |
| (1,156)  | 1:3:A:ILE:HD13  | 1:3:A:ILE:HA    | 3        | 0.76          |
| (1,156)  | 1:3:A:ILE:HD13  | 1:3:A:ILE:HA    | 4        | 0.76          |
| (1,156)  | 1:3:A:ILE:HD11  | 1:3:A:ILE:HA    | 5        | 0.76          |
| (1,156)  | 1:3:A:ILE:HD13  | 1:3:A:ILE:HA    | 6        | 0.76          |
| (1,156)  | 1:3:A:ILE:HD13  | 1:3:A:ILE:HA    | 7        | 0.76          |
| (1,156)  | 1:3:A:ILE:HD11  | 1:3:A:ILE:HA    | 10       | 0.76          |
| (1,156)  | 1:3:A:ILE:HD11  | 1:3:A:ILE:HA    | 12       | 0.76          |
| (1,156)  | 1:3:A:ILE:HD13  | 1:3:A:ILE:HA    | 14       | 0.76          |
| (1,156)  | 1:3:A:ILE:HD13  | 1:3:A:ILE:HA    | 15       | 0.76          |
| (1,156)  | 1:3:A:ILE:HD11  | 1:3:A:ILE:HA    | 16       | 0.76          |
| (1,156)  | 1:3:A:ILE:HD12  | 1:3:A:ILE:HA    | 17       | 0.76          |
| (1,156)  | 1:3:A:ILE:HD12  | 1:3:A:ILE:HA    | 18       | 0.76          |
| (1,156)  | 1:3:A:ILE:HD12  | 1:3:A:ILE:HA    | 19       | 0.76          |
| (1,35)   | 1:1:A:MET:HE3   | 1:17:A:VAL:HG11 | 18       | 0.76          |
| (1,1920) | 1:44:A:ILE:HG12 | 1:70:A:VAL:HG23 | 5        | 0.75          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1920) | 1:44:A:ILE:HG12 | 1:70:A:VAL:HG23 | 18       | 0.75          |
| (1,1775) | 1:72:A:ARG:HD2  | 1:72:A:ARG:HA   | 8        | 0.75          |
| (1,1775) | 1:72:A:ARG:HD3  | 1:72:A:ARG:HA   | 18       | 0.75          |
| (1,1691) | 1:40:A:GLN:HG2  | 1:71:A:LEU:HD23 | 14       | 0.75          |
| (1,1691) | 1:40:A:GLN:HG2  | 1:71:A:LEU:HD21 | 20       | 0.75          |
| (1,35)   | 1:1:A:MET:HE2   | 1:17:A:VAL:HG11 | 17       | 0.75          |
| (1,1691) | 1:40:A:GLN:HG2  | 1:71:A:LEU:HD21 | 6        | 0.74          |
| (1,1920) | 1:44:A:ILE:HG12 | 1:70:A:VAL:HG23 | 12       | 0.73          |
| (1,1920) | 1:44:A:ILE:HG12 | 1:70:A:VAL:HG22 | 19       | 0.73          |
| (1,1696) | 1:40:A:GLN:HG2  | 1:73:A:LEU:HG   | 3        | 0.73          |
| (1,1691) | 1:40:A:GLN:HG3  | 1:71:A:LEU:HD21 | 4        | 0.73          |
| (1,35)   | 1:1:A:MET:HE2   | 1:17:A:VAL:HG12 | 16       | 0.73          |
| (1,1920) | 1:44:A:ILE:HG12 | 1:70:A:VAL:HG23 | 4        | 0.72          |
| (1,1920) | 1:44:A:ILE:HG12 | 1:70:A:VAL:HG22 | 15       | 0.72          |
| (1,1775) | 1:72:A:ARG:HD3  | 1:72:A:ARG:HA   | 20       | 0.72          |
| (1,1691) | 1:40:A:GLN:HG3  | 1:71:A:LEU:HD21 | 10       | 0.72          |
| (1,35)   | 1:1:A:MET:HE3   | 1:17:A:VAL:HG12 | 10       | 0.72          |
| (1,1920) | 1:44:A:ILE:HG12 | 1:70:A:VAL:HG23 | 1        | 0.71          |
| (1,1920) | 1:44:A:ILE:HG12 | 1:70:A:VAL:HG21 | 16       | 0.71          |
| (1,1920) | 1:44:A:ILE:HG12 | 1:70:A:VAL:HG21 | 20       | 0.71          |
| (1,1775) | 1:72:A:ARG:HD2  | 1:72:A:ARG:HA   | 5        | 0.71          |
| (1,1775) | 1:72:A:ARG:HD2  | 1:72:A:ARG:HA   | 11       | 0.71          |
| (1,1691) | 1:40:A:GLN:HG2  | 1:71:A:LEU:HD21 | 15       | 0.71          |
| (1,462)  | 1:6:A:LYS:HG3   | 1:66:A:THR:HG21 | 12       | 0.71          |
| (1,35)   | 1:1:A:MET:HE2   | 1:17:A:VAL:HG12 | 1        | 0.71          |
| (1,35)   | 1:1:A:MET:HE3   | 1:17:A:VAL:HG12 | 4        | 0.71          |
| (1,35)   | 1:1:A:MET:HE3   | 1:17:A:VAL:HG12 | 7        | 0.71          |
| (1,1920) | 1:44:A:ILE:HG12 | 1:70:A:VAL:HG23 | 6        | 0.7           |
| (1,1920) | 1:44:A:ILE:HG12 | 1:70:A:VAL:HG23 | 9        | 0.7           |
| (1,1691) | 1:40:A:GLN:HG2  | 1:71:A:LEU:HD21 | 5        | 0.7           |
| (1,1691) | 1:40:A:GLN:HG2  | 1:71:A:LEU:HD21 | 19       | 0.7           |
| (1,462)  | 1:6:A:LYS:HG3   | 1:66:A:THR:HG21 | 6        | 0.7           |
| (1,462)  | 1:6:A:LYS:HG3   | 1:66:A:THR:HG21 | 14       | 0.7           |
| (1,1920) | 1:44:A:ILE:HG12 | 1:70:A:VAL:HG23 | 2        | 0.69          |
| (1,462)  | 1:6:A:LYS:HG3   | 1:66:A:THR:HG21 | 11       | 0.69          |
| (1,462)  | 1:6:A:LYS:HG3   | 1:66:A:THR:HG21 | 16       | 0.69          |
| (1,462)  | 1:6:A:LYS:HG3   | 1:66:A:THR:HG21 | 17       | 0.69          |
| (1,1775) | 1:72:A:ARG:HD2  | 1:72:A:ARG:HA   | 1        | 0.68          |
| (1,459)  | 1:6:A:LYS:HE2   | 1:66:A:THR:HG23 | 3        | 0.68          |
| (1,458)  | 1:6:A:LYS:HD3   | 1:66:A:THR:HG22 | 4        | 0.68          |
| (1,458)  | 1:6:A:LYS:HD3   | 1:66:A:THR:HG23 | 9        | 0.68          |
| (1,35)   | 1:1:A:MET:HE3   | 1:17:A:VAL:HG12 | 8        | 0.68          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,35)   | 1:1:A:MET:HE3   | 1:17:A:VAL:HG12 | 9        | 0.68          |
| (1,1775) | 1:72:A:ARG:HD2  | 1:72:A:ARG:HA   | 3        | 0.67          |
| (1,1775) | 1:72:A:ARG:HD2  | 1:72:A:ARG:HA   | 12       | 0.67          |
| (1,1691) | 1:40:A:GLN:HG2  | 1:71:A:LEU:HD23 | 11       | 0.67          |
| (1,35)   | 1:1:A:MET:HE3   | 1:17:A:VAL:HG12 | 6        | 0.67          |
| (1,1775) | 1:72:A:ARG:HD2  | 1:72:A:ARG:HA   | 13       | 0.66          |
| (1,1775) | 1:72:A:ARG:HD2  | 1:72:A:ARG:HA   | 15       | 0.66          |
| (1,459)  | 1:6:A:LYS:HE2   | 1:66:A:THR:HG22 | 6        | 0.66          |
| (1,459)  | 1:6:A:LYS:HE3   | 1:66:A:THR:HG21 | 20       | 0.66          |
| (1,1888) | 1:44:A:ILE:HG12 | 1:70:A:VAL:HG11 | 4        | 0.65          |
| (1,1888) | 1:44:A:ILE:HG12 | 1:70:A:VAL:HG11 | 12       | 0.65          |
| (1,915)  | 1:52:A:ASP:HB2  | 1:24:A:GLU:HG2  | 3        | 0.65          |
| (1,458)  | 1:6:A:LYS:HD3   | 1:66:A:THR:HG21 | 13       | 0.65          |
| (1,1888) | 1:44:A:ILE:HG12 | 1:70:A:VAL:HG13 | 15       | 0.64          |
| (1,1888) | 1:44:A:ILE:HG12 | 1:70:A:VAL:HG13 | 16       | 0.64          |
| (1,1768) | 1:42:A:ARG:HD2  | 1:70:A:VAL:HG23 | 2        | 0.64          |
| (1,1691) | 1:40:A:GLN:HG2  | 1:71:A:LEU:HD21 | 16       | 0.64          |
| (1,1888) | 1:44:A:ILE:HG12 | 1:70:A:VAL:HG11 | 1        | 0.63          |
| (1,1888) | 1:44:A:ILE:HG12 | 1:70:A:VAL:HG13 | 5        | 0.63          |
| (1,1888) | 1:44:A:ILE:HG12 | 1:70:A:VAL:HG13 | 11       | 0.63          |
| (1,1888) | 1:44:A:ILE:HG12 | 1:70:A:VAL:HG11 | 17       | 0.62          |
| (1,1888) | 1:44:A:ILE:HG12 | 1:70:A:VAL:HG13 | 18       | 0.62          |
| (1,1888) | 1:44:A:ILE:HG12 | 1:70:A:VAL:HG11 | 19       | 0.62          |
| (1,1775) | 1:72:A:ARG:HD2  | 1:72:A:ARG:HA   | 7        | 0.62          |
| (1,1775) | 1:72:A:ARG:HD2  | 1:72:A:ARG:HA   | 9        | 0.62          |
| (1,1775) | 1:72:A:ARG:HD2  | 1:72:A:ARG:HA   | 14       | 0.62          |
| (1,1888) | 1:44:A:ILE:HG12 | 1:70:A:VAL:HG13 | 9        | 0.61          |
| (1,1691) | 1:40:A:GLN:HG3  | 1:71:A:LEU:HD21 | 9        | 0.61          |
| (1,1888) | 1:44:A:ILE:HG12 | 1:70:A:VAL:HG12 | 6        | 0.6           |
| (1,1888) | 1:44:A:ILE:HG12 | 1:70:A:VAL:HG11 | 20       | 0.6           |
| (1,98)   | 1:1:A:MET:HE1   | 1:67:A:LEU:HD12 | 5        | 0.6           |
| (1,1888) | 1:44:A:ILE:HG12 | 1:70:A:VAL:HG12 | 2        | 0.59          |
| (1,1888) | 1:44:A:ILE:HG12 | 1:70:A:VAL:HG12 | 7        | 0.59          |
| (1,1692) | 1:40:A:GLN:HG2  | 1:73:A:LEU:HD13 | 19       | 0.59          |
| (1,98)   | 1:1:A:MET:HE2   | 1:67:A:LEU:HD12 | 1        | 0.58          |
| (1,1691) | 1:40:A:GLN:HG2  | 1:71:A:LEU:HD21 | 17       | 0.57          |
| (1,461)  | 1:6:A:LYS:HG3   | 1:66:A:THR:HG22 | 18       | 0.57          |
| (1,1692) | 1:40:A:GLN:HG2  | 1:73:A:LEU:HD22 | 17       | 0.55          |
| (1,98)   | 1:1:A:MET:HE2   | 1:67:A:LEU:HD13 | 9        | 0.55          |
| (1,98)   | 1:1:A:MET:HE2   | 1:67:A:LEU:HD11 | 14       | 0.55          |
| (1,98)   | 1:1:A:MET:HE2   | 1:67:A:LEU:HD12 | 20       | 0.55          |
| (1,38)   | 1:1:A:MET:HE3   | 1:17:A:VAL:HG21 | 13       | 0.55          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1768) | 1:42:A:ARG:HD2  | 1:70:A:VAL:HG21 | 7        | 0.54          |
| (1,1768) | 1:42:A:ARG:HD2  | 1:70:A:VAL:HG23 | 9        | 0.54          |
| (1,1768) | 1:42:A:ARG:HD2  | 1:70:A:VAL:HG23 | 10       | 0.54          |
| (1,1768) | 1:42:A:ARG:HD2  | 1:70:A:VAL:HG22 | 11       | 0.54          |
| (1,1696) | 1:40:A:GLN:HG2  | 1:73:A:LEU:HG   | 6        | 0.54          |
| (1,459)  | 1:6:A:LYS:HE2   | 1:66:A:THR:HG23 | 14       | 0.54          |
| (1,459)  | 1:6:A:LYS:HE2   | 1:66:A:THR:HG23 | 16       | 0.54          |
| (1,459)  | 1:6:A:LYS:HE2   | 1:66:A:THR:HG23 | 17       | 0.54          |
| (1,149)  | 1:3:A:ILE:HA    | 1:3:A:ILE:HD11  | 20       | 0.54          |
| (1,98)   | 1:1:A:MET:HE2   | 1:67:A:LEU:HD13 | 6        | 0.54          |
| (1,98)   | 1:1:A:MET:HE2   | 1:67:A:LEU:HD11 | 16       | 0.54          |
| (1,1768) | 1:42:A:ARG:HD2  | 1:70:A:VAL:HG23 | 5        | 0.53          |
| (1,1768) | 1:42:A:ARG:HD2  | 1:70:A:VAL:HG23 | 12       | 0.53          |
| (1,1768) | 1:42:A:ARG:HD2  | 1:70:A:VAL:HG22 | 14       | 0.53          |
| (1,459)  | 1:6:A:LYS:HE3   | 1:66:A:THR:HG21 | 18       | 0.53          |
| (1,149)  | 1:3:A:ILE:HA    | 1:3:A:ILE:HD13  | 9        | 0.53          |
| (1,2547) | 1:70:A:VAL:HB   | 1:71:A:LEU:H    | 20       | 0.52          |
| (1,2478) | 1:67:A:LEU:HA   | 1:67:A:LEU:HD12 | 4        | 0.52          |
| (1,2478) | 1:67:A:LEU:HA   | 1:67:A:LEU:HD13 | 8        | 0.52          |
| (1,2478) | 1:67:A:LEU:HA   | 1:67:A:LEU:HD13 | 10       | 0.52          |
| (1,2478) | 1:67:A:LEU:HA   | 1:67:A:LEU:HD11 | 15       | 0.52          |
| (1,1775) | 1:72:A:ARG:HD2  | 1:72:A:ARG:HA   | 4        | 0.52          |
| (1,1768) | 1:42:A:ARG:HD2  | 1:70:A:VAL:HG22 | 15       | 0.52          |
| (1,357)  | 1:17:A:VAL:HG11 | 1:29:A:LYS:HG2  | 13       | 0.52          |
| (1,98)   | 1:1:A:MET:HE2   | 1:67:A:LEU:HD11 | 8        | 0.52          |
| (1,98)   | 1:1:A:MET:HE2   | 1:67:A:LEU:HD11 | 11       | 0.52          |
| (1,2547) | 1:70:A:VAL:HB   | 1:71:A:LEU:H    | 3        | 0.51          |
| (1,2547) | 1:70:A:VAL:HB   | 1:71:A:LEU:H    | 18       | 0.51          |
| (1,2478) | 1:67:A:LEU:HA   | 1:67:A:LEU:HD11 | 1        | 0.51          |
| (1,2478) | 1:67:A:LEU:HA   | 1:67:A:LEU:HD11 | 2        | 0.51          |
| (1,2478) | 1:67:A:LEU:HA   | 1:67:A:LEU:HD12 | 3        | 0.51          |
| (1,2478) | 1:67:A:LEU:HA   | 1:67:A:LEU:HD11 | 5        | 0.51          |
| (1,2478) | 1:67:A:LEU:HA   | 1:67:A:LEU:HD12 | 6        | 0.51          |
| (1,2478) | 1:67:A:LEU:HA   | 1:67:A:LEU:HD13 | 7        | 0.51          |
| (1,2478) | 1:67:A:LEU:HA   | 1:67:A:LEU:HD13 | 11       | 0.51          |
| (1,2478) | 1:67:A:LEU:HA   | 1:67:A:LEU:HD13 | 12       | 0.51          |
| (1,2478) | 1:67:A:LEU:HA   | 1:67:A:LEU:HD13 | 13       | 0.51          |
| (1,2478) | 1:67:A:LEU:HA   | 1:67:A:LEU:HD13 | 14       | 0.51          |
| (1,2478) | 1:67:A:LEU:HA   | 1:67:A:LEU:HD13 | 16       | 0.51          |
| (1,2478) | 1:67:A:LEU:HA   | 1:67:A:LEU:HD11 | 17       | 0.51          |
| (1,2478) | 1:67:A:LEU:HA   | 1:67:A:LEU:HD13 | 18       | 0.51          |
| (1,2478) | 1:67:A:LEU:HA   | 1:67:A:LEU:HD11 | 19       | 0.51          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1768) | 1:42:A:ARG:HD2  | 1:70:A:VAL:HG22 | 19       | 0.51          |
| (1,98)   | 1:1:A:MET:HE2   | 1:67:A:LEU:HD11 | 12       | 0.51          |
| (1,2547) | 1:70:A:VAL:HB   | 1:71:A:LEU:H    | 4        | 0.5           |
| (1,2547) | 1:70:A:VAL:HB   | 1:71:A:LEU:H    | 10       | 0.5           |
| (1,2478) | 1:67:A:LEU:HA   | 1:67:A:LEU:HD12 | 9        | 0.5           |
| (1,2478) | 1:67:A:LEU:HA   | 1:67:A:LEU:HD11 | 20       | 0.5           |
| (1,1768) | 1:42:A:ARG:HD2  | 1:70:A:VAL:HG23 | 4        | 0.5           |
| (1,1146) | 1:40:A:GLN:HG2  | 1:39:A:ASP:H    | 13       | 0.5           |
| (1,357)  | 1:17:A:VAL:HG13 | 1:29:A:LYS:HG3  | 15       | 0.5           |
| (1,149)  | 1:3:A:ILE:HA    | 1:3:A:ILE:HD12  | 8        | 0.5           |
| (1,2547) | 1:70:A:VAL:HB   | 1:71:A:LEU:H    | 6        | 0.49          |
| (1,2547) | 1:70:A:VAL:HB   | 1:71:A:LEU:H    | 12       | 0.49          |
| (1,2547) | 1:70:A:VAL:HB   | 1:71:A:LEU:H    | 14       | 0.49          |
| (1,149)  | 1:3:A:ILE:HA    | 1:3:A:ILE:HD11  | 11       | 0.49          |
| (1,149)  | 1:3:A:ILE:HA    | 1:3:A:ILE:HD11  | 13       | 0.49          |
| (1,149)  | 1:3:A:ILE:HA    | 1:3:A:ILE:HD11  | 16       | 0.49          |
| (1,98)   | 1:1:A:MET:HE2   | 1:67:A:LEU:HD11 | 7        | 0.49          |
| (1,98)   | 1:1:A:MET:HE2   | 1:67:A:LEU:HD11 | 10       | 0.49          |
| (1,98)   | 1:1:A:MET:HE2   | 1:67:A:LEU:HD11 | 18       | 0.49          |
| (1,2547) | 1:70:A:VAL:HB   | 1:71:A:LEU:H    | 2        | 0.48          |
| (1,2547) | 1:70:A:VAL:HB   | 1:71:A:LEU:H    | 7        | 0.48          |
| (1,2547) | 1:70:A:VAL:HB   | 1:71:A:LEU:H    | 8        | 0.48          |
| (1,2547) | 1:70:A:VAL:HB   | 1:71:A:LEU:H    | 13       | 0.48          |
| (1,2547) | 1:70:A:VAL:HB   | 1:71:A:LEU:H    | 16       | 0.48          |
| (1,1768) | 1:42:A:ARG:HD2  | 1:70:A:VAL:HG23 | 1        | 0.48          |
| (1,1768) | 1:42:A:ARG:HD2  | 1:70:A:VAL:HG23 | 17       | 0.48          |
| (1,461)  | 1:6:A:LYS:HG2   | 1:66:A:THR:HG21 | 20       | 0.48          |
| (1,149)  | 1:3:A:ILE:HA    | 1:3:A:ILE:HD11  | 1        | 0.48          |
| (1,149)  | 1:3:A:ILE:HA    | 1:3:A:ILE:HD11  | 2        | 0.48          |
| (1,149)  | 1:3:A:ILE:HA    | 1:3:A:ILE:HD13  | 3        | 0.48          |
| (1,149)  | 1:3:A:ILE:HA    | 1:3:A:ILE:HD13  | 4        | 0.48          |
| (1,149)  | 1:3:A:ILE:HA    | 1:3:A:ILE:HD11  | 5        | 0.48          |
| (1,149)  | 1:3:A:ILE:HA    | 1:3:A:ILE:HD13  | 6        | 0.48          |
| (1,149)  | 1:3:A:ILE:HA    | 1:3:A:ILE:HD13  | 7        | 0.48          |
| (1,149)  | 1:3:A:ILE:HA    | 1:3:A:ILE:HD11  | 10       | 0.48          |
| (1,149)  | 1:3:A:ILE:HA    | 1:3:A:ILE:HD11  | 12       | 0.48          |
| (1,149)  | 1:3:A:ILE:HA    | 1:3:A:ILE:HD13  | 14       | 0.48          |
| (1,149)  | 1:3:A:ILE:HA    | 1:3:A:ILE:HD13  | 15       | 0.48          |
| (1,149)  | 1:3:A:ILE:HA    | 1:3:A:ILE:HD12  | 17       | 0.48          |
| (1,149)  | 1:3:A:ILE:HA    | 1:3:A:ILE:HD12  | 18       | 0.48          |
| (1,149)  | 1:3:A:ILE:HA    | 1:3:A:ILE:HD12  | 19       | 0.48          |
| (1,98)   | 1:1:A:MET:HE2   | 1:67:A:LEU:HD12 | 19       | 0.48          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,38)   | 1:1:A:MET:HE3   | 1:17:A:VAL:HG23 | 3        | 0.48          |
| (1,2547) | 1:70:A:VAL:HB   | 1:71:A:LEU:H    | 1        | 0.47          |
| (1,2547) | 1:70:A:VAL:HB   | 1:71:A:LEU:H    | 5        | 0.47          |
| (1,2547) | 1:70:A:VAL:HB   | 1:71:A:LEU:H    | 19       | 0.47          |
| (1,1768) | 1:42:A:ARG:HD2  | 1:70:A:VAL:HG23 | 8        | 0.47          |
| (1,1768) | 1:42:A:ARG:HD2  | 1:70:A:VAL:HG22 | 13       | 0.47          |
| (1,98)   | 1:1:A:MET:HE2   | 1:67:A:LEU:HD12 | 2        | 0.47          |
| (1,98)   | 1:1:A:MET:HE2   | 1:67:A:LEU:HD13 | 4        | 0.47          |
| (1,98)   | 1:1:A:MET:HE2   | 1:67:A:LEU:HD12 | 15       | 0.47          |
| (1,38)   | 1:1:A:MET:HE2   | 1:17:A:VAL:HG21 | 15       | 0.47          |
| (1,2547) | 1:70:A:VAL:HB   | 1:71:A:LEU:H    | 9        | 0.46          |
| (1,2547) | 1:70:A:VAL:HB   | 1:71:A:LEU:H    | 11       | 0.46          |
| (1,2547) | 1:70:A:VAL:HB   | 1:71:A:LEU:H    | 15       | 0.46          |
| (1,1768) | 1:42:A:ARG:HD2  | 1:70:A:VAL:HG23 | 3        | 0.46          |
| (1,1768) | 1:42:A:ARG:HD2  | 1:70:A:VAL:HG23 | 18       | 0.46          |
| (1,1758) | 1:42:A:ARG:HA   | 1:70:A:VAL:HG21 | 6        | 0.46          |
| (1,1758) | 1:42:A:ARG:HA   | 1:70:A:VAL:HG22 | 6        | 0.46          |
| (1,1758) | 1:42:A:ARG:HA   | 1:70:A:VAL:HG23 | 6        | 0.46          |
| (1,1758) | 1:42:A:ARG:HA   | 1:70:A:VAL:HG21 | 8        | 0.46          |
| (1,1758) | 1:42:A:ARG:HA   | 1:70:A:VAL:HG22 | 8        | 0.46          |
| (1,1758) | 1:42:A:ARG:HA   | 1:70:A:VAL:HG23 | 8        | 0.46          |
| (1,1758) | 1:42:A:ARG:HA   | 1:70:A:VAL:HG21 | 17       | 0.46          |
| (1,1758) | 1:42:A:ARG:HA   | 1:70:A:VAL:HG22 | 17       | 0.46          |
| (1,1758) | 1:42:A:ARG:HA   | 1:70:A:VAL:HG23 | 17       | 0.46          |
| (1,1758) | 1:42:A:ARG:HA   | 1:70:A:VAL:HG21 | 20       | 0.46          |
| (1,1758) | 1:42:A:ARG:HA   | 1:70:A:VAL:HG22 | 20       | 0.46          |
| (1,1758) | 1:42:A:ARG:HA   | 1:70:A:VAL:HG23 | 20       | 0.46          |
| (1,1696) | 1:40:A:GLN:HG2  | 1:74:A:ARG:HG2  | 2        | 0.46          |
| (1,462)  | 1:6:A:LYS:HG3   | 1:66:A:THR:HG22 | 18       | 0.46          |
| (1,458)  | 1:6:A:LYS:HD2   | 1:66:A:THR:HG21 | 19       | 0.46          |
| (1,357)  | 1:17:A:VAL:HG11 | 1:29:A:LYS:HG3  | 8        | 0.46          |
| (1,98)   | 1:1:A:MET:HE1   | 1:67:A:LEU:HD12 | 17       | 0.46          |
| (1,1776) | 1:42:A:ARG:HG3  | 1:72:A:ARG:H    | 10       | 0.45          |
| (1,1775) | 1:72:A:ARG:HD2  | 1:72:A:ARG:HA   | 10       | 0.45          |
| (1,1768) | 1:42:A:ARG:HD2  | 1:70:A:VAL:HG21 | 16       | 0.45          |
| (1,1758) | 1:42:A:ARG:HA   | 1:70:A:VAL:HG21 | 5        | 0.45          |
| (1,1758) | 1:42:A:ARG:HA   | 1:70:A:VAL:HG22 | 5        | 0.45          |
| (1,1758) | 1:42:A:ARG:HA   | 1:70:A:VAL:HG23 | 5        | 0.45          |
| (1,1758) | 1:42:A:ARG:HA   | 1:70:A:VAL:HG21 | 11       | 0.45          |
| (1,1758) | 1:42:A:ARG:HA   | 1:70:A:VAL:HG22 | 11       | 0.45          |
| (1,1758) | 1:42:A:ARG:HA   | 1:70:A:VAL:HG23 | 11       | 0.45          |
| (1,1758) | 1:42:A:ARG:HA   | 1:70:A:VAL:HG21 | 16       | 0.45          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1758) | 1:42:A:ARG:HA   | 1:70:A:VAL:HG22 | 16       | 0.45          |
| (1,1758) | 1:42:A:ARG:HA   | 1:70:A:VAL:HG23 | 16       | 0.45          |
| (1,1692) | 1:40:A:GLN:HG2  | 1:73:A:LEU:HD22 | 1        | 0.45          |
| (1,98)   | 1:1:A:MET:HE2   | 1:67:A:LEU:HD11 | 13       | 0.45          |
| (1,2547) | 1:70:A:VAL:HB   | 1:71:A:LEU:H    | 17       | 0.44          |
| (1,1758) | 1:42:A:ARG:HA   | 1:70:A:VAL:HG21 | 1        | 0.44          |
| (1,1758) | 1:42:A:ARG:HA   | 1:70:A:VAL:HG22 | 1        | 0.44          |
| (1,1758) | 1:42:A:ARG:HA   | 1:70:A:VAL:HG23 | 1        | 0.44          |
| (1,1758) | 1:42:A:ARG:HA   | 1:70:A:VAL:HG21 | 2        | 0.44          |
| (1,1758) | 1:42:A:ARG:HA   | 1:70:A:VAL:HG22 | 2        | 0.44          |
| (1,1758) | 1:42:A:ARG:HA   | 1:70:A:VAL:HG23 | 2        | 0.44          |
| (1,1758) | 1:42:A:ARG:HA   | 1:70:A:VAL:HG21 | 7        | 0.44          |
| (1,1758) | 1:42:A:ARG:HA   | 1:70:A:VAL:HG22 | 7        | 0.44          |
| (1,1758) | 1:42:A:ARG:HA   | 1:70:A:VAL:HG23 | 7        | 0.44          |
| (1,1758) | 1:42:A:ARG:HA   | 1:70:A:VAL:HG21 | 15       | 0.44          |
| (1,1758) | 1:42:A:ARG:HA   | 1:70:A:VAL:HG22 | 15       | 0.44          |
| (1,1758) | 1:42:A:ARG:HA   | 1:70:A:VAL:HG23 | 15       | 0.44          |
| (1,1758) | 1:42:A:ARG:HA   | 1:70:A:VAL:HG21 | 18       | 0.44          |
| (1,1758) | 1:42:A:ARG:HA   | 1:70:A:VAL:HG22 | 18       | 0.44          |
| (1,1758) | 1:42:A:ARG:HA   | 1:70:A:VAL:HG23 | 18       | 0.44          |
| (1,1758) | 1:42:A:ARG:HA   | 1:70:A:VAL:HG21 | 19       | 0.44          |
| (1,1758) | 1:42:A:ARG:HA   | 1:70:A:VAL:HG22 | 19       | 0.44          |
| (1,1758) | 1:42:A:ARG:HA   | 1:70:A:VAL:HG23 | 19       | 0.44          |
| (1,1726) | 1:42:A:ARG:HA   | 1:42:A:ARG:HD3  | 18       | 0.44          |
| (1,1696) | 1:40:A:GLN:HG2  | 1:73:A:LEU:HG   | 4        | 0.44          |
| (1,357)  | 1:17:A:VAL:HG11 | 1:29:A:LYS:HG3  | 5        | 0.44          |
| (1,38)   | 1:1:A:MET:HE2   | 1:17:A:VAL:HG21 | 19       | 0.44          |
| (1,1758) | 1:42:A:ARG:HA   | 1:70:A:VAL:HG21 | 3        | 0.43          |
| (1,1758) | 1:42:A:ARG:HA   | 1:70:A:VAL:HG22 | 3        | 0.43          |
| (1,1758) | 1:42:A:ARG:HA   | 1:70:A:VAL:HG23 | 3        | 0.43          |
| (1,1758) | 1:42:A:ARG:HA   | 1:70:A:VAL:HG21 | 4        | 0.43          |
| (1,1758) | 1:42:A:ARG:HA   | 1:70:A:VAL:HG22 | 4        | 0.43          |
| (1,1758) | 1:42:A:ARG:HA   | 1:70:A:VAL:HG23 | 4        | 0.43          |
| (1,1758) | 1:42:A:ARG:HA   | 1:70:A:VAL:HG21 | 9        | 0.43          |
| (1,1758) | 1:42:A:ARG:HA   | 1:70:A:VAL:HG22 | 9        | 0.43          |
| (1,1758) | 1:42:A:ARG:HA   | 1:70:A:VAL:HG23 | 9        | 0.43          |
| (1,1758) | 1:42:A:ARG:HA   | 1:70:A:VAL:HG21 | 12       | 0.43          |
| (1,1758) | 1:42:A:ARG:HA   | 1:70:A:VAL:HG22 | 12       | 0.43          |
| (1,1758) | 1:42:A:ARG:HA   | 1:70:A:VAL:HG23 | 12       | 0.43          |
| (1,1758) | 1:42:A:ARG:HA   | 1:70:A:VAL:HG21 | 13       | 0.43          |
| (1,1758) | 1:42:A:ARG:HA   | 1:70:A:VAL:HG22 | 13       | 0.43          |
| (1,1758) | 1:42:A:ARG:HA   | 1:70:A:VAL:HG23 | 13       | 0.43          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,459)  | 1:6:A:LYS:HE2   | 1:66:A:THR:HG23 | 8        | 0.43          |
| (1,447)  | 1:6:A:LYS:HG2   | 1:12:A:THR:HG23 | 20       | 0.43          |
| (1,357)  | 1:17:A:VAL:HG11 | 1:29:A:LYS:HG3  | 1        | 0.43          |
| (1,357)  | 1:17:A:VAL:HG12 | 1:29:A:LYS:HG3  | 11       | 0.43          |
| (1,357)  | 1:17:A:VAL:HG12 | 1:29:A:LYS:HG3  | 14       | 0.43          |
| (1,354)  | 1:17:A:VAL:HG11 | 1:29:A:LYS:HE2  | 16       | 0.43          |
| (1,38)   | 1:1:A:MET:HE2   | 1:17:A:VAL:HG21 | 16       | 0.43          |
| (1,1768) | 1:42:A:ARG:HD2  | 1:70:A:VAL:HG21 | 20       | 0.42          |
| (1,551)  | 1:8:A:LEU:HG    | 1:70:A:VAL:HA   | 9        | 0.42          |
| (1,551)  | 1:8:A:LEU:HG    | 1:70:A:VAL:HA   | 13       | 0.42          |
| (1,357)  | 1:17:A:VAL:HG11 | 1:29:A:LYS:HG3  | 6        | 0.42          |
| (1,357)  | 1:17:A:VAL:HG12 | 1:29:A:LYS:HG3  | 19       | 0.42          |
| (1,264)  | 1:4:A:PHE:HA    | 1:14:A:THR:HG21 | 13       | 0.42          |
| (1,38)   | 1:1:A:MET:HE3   | 1:17:A:VAL:HG21 | 12       | 0.42          |
| (1,1768) | 1:42:A:ARG:HD2  | 1:70:A:VAL:HG23 | 6        | 0.41          |
| (1,1758) | 1:42:A:ARG:HA   | 1:70:A:VAL:HG21 | 10       | 0.41          |
| (1,1758) | 1:42:A:ARG:HA   | 1:70:A:VAL:HG22 | 10       | 0.41          |
| (1,1758) | 1:42:A:ARG:HA   | 1:70:A:VAL:HG23 | 10       | 0.41          |
| (1,1758) | 1:42:A:ARG:HA   | 1:70:A:VAL:HG21 | 14       | 0.41          |
| (1,1758) | 1:42:A:ARG:HA   | 1:70:A:VAL:HG22 | 14       | 0.41          |
| (1,1758) | 1:42:A:ARG:HA   | 1:70:A:VAL:HG23 | 14       | 0.41          |
| (1,1726) | 1:42:A:ARG:HA   | 1:42:A:ARG:HD3  | 11       | 0.41          |
| (1,551)  | 1:8:A:LEU:HG    | 1:70:A:VAL:HA   | 17       | 0.41          |
| (1,458)  | 1:6:A:LYS:HD2   | 1:66:A:THR:HG23 | 8        | 0.41          |
| (1,357)  | 1:17:A:VAL:HG11 | 1:29:A:LYS:HG3  | 2        | 0.41          |
| (1,357)  | 1:17:A:VAL:HG11 | 1:29:A:LYS:HG3  | 12       | 0.41          |
| (1,357)  | 1:17:A:VAL:HG11 | 1:29:A:LYS:HG3  | 20       | 0.41          |
| (1,1726) | 1:42:A:ARG:HA   | 1:42:A:ARG:HD3  | 12       | 0.4           |
| (1,458)  | 1:6:A:LYS:HD2   | 1:66:A:THR:HG23 | 5        | 0.4           |
| (1,357)  | 1:17:A:VAL:HG11 | 1:29:A:LYS:HG3  | 4        | 0.4           |
| (1,357)  | 1:17:A:VAL:HG11 | 1:29:A:LYS:HG3  | 10       | 0.4           |
| (1,264)  | 1:4:A:PHE:HA    | 1:14:A:THR:HG23 | 10       | 0.4           |
| (1,38)   | 1:1:A:MET:HE2   | 1:17:A:VAL:HG21 | 14       | 0.4           |
| (1,1726) | 1:42:A:ARG:HA   | 1:42:A:ARG:HD3  | 6        | 0.39          |
| (1,357)  | 1:17:A:VAL:HG11 | 1:29:A:LYS:HG2  | 3        | 0.39          |
| (1,357)  | 1:17:A:VAL:HG11 | 1:29:A:LYS:HG3  | 9        | 0.39          |
| (1,98)   | 1:1:A:MET:HE2   | 1:67:A:LEU:HD13 | 3        | 0.39          |
| (1,1776) | 1:42:A:ARG:HG3  | 1:72:A:ARG:H    | 4        | 0.38          |
| (1,1776) | 1:42:A:ARG:HG3  | 1:72:A:ARG:H    | 14       | 0.38          |
| (1,460)  | 1:6:A:LYS:HG3   | 1:66:A:THR:HG21 | 12       | 0.38          |
| (1,459)  | 1:6:A:LYS:HE3   | 1:66:A:THR:HG21 | 1        | 0.38          |
| (1,458)  | 1:6:A:LYS:HD2   | 1:66:A:THR:HG23 | 7        | 0.38          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,357)  | 1:17:A:VAL:HG11 | 1:29:A:LYS:HG3  | 7        | 0.38          |
| (1,357)  | 1:17:A:VAL:HG13 | 1:29:A:LYS:HG3  | 17       | 0.38          |
| (1,264)  | 1:4:A:PHE:HA    | 1:14:A:THR:HG23 | 2        | 0.38          |
| (1,1776) | 1:42:A:ARG:HG3  | 1:72:A:ARG:H    | 11       | 0.37          |
| (1,1726) | 1:42:A:ARG:HA   | 1:42:A:ARG:HD3  | 13       | 0.37          |
| (1,1726) | 1:42:A:ARG:HA   | 1:42:A:ARG:HD3  | 14       | 0.37          |
| (1,1726) | 1:42:A:ARG:HA   | 1:42:A:ARG:HD3  | 19       | 0.37          |
| (1,551)  | 1:8:A:LEU:HG    | 1:70:A:VAL:HA   | 20       | 0.37          |
| (1,462)  | 1:6:A:LYS:HG2   | 1:66:A:THR:HG21 | 20       | 0.37          |
| (1,460)  | 1:6:A:LYS:HG3   | 1:66:A:THR:HG21 | 6        | 0.37          |
| (1,460)  | 1:6:A:LYS:HG3   | 1:66:A:THR:HG21 | 11       | 0.37          |
| (1,460)  | 1:6:A:LYS:HG3   | 1:66:A:THR:HG21 | 14       | 0.37          |
| (1,460)  | 1:6:A:LYS:HG3   | 1:66:A:THR:HG21 | 16       | 0.37          |
| (1,460)  | 1:6:A:LYS:HG3   | 1:66:A:THR:HG21 | 17       | 0.37          |
| (1,318)  | 1:5:A:VAL:HG11  | 1:7:A:THR:HG21  | 12       | 0.37          |
| (1,38)   | 1:1:A:MET:HE1   | 1:17:A:VAL:HG23 | 5        | 0.37          |
| (1,1776) | 1:42:A:ARG:HG3  | 1:72:A:ARG:H    | 12       | 0.36          |
| (1,1776) | 1:42:A:ARG:HG3  | 1:72:A:ARG:H    | 13       | 0.36          |
| (1,1726) | 1:42:A:ARG:HA   | 1:42:A:ARG:HD3  | 2        | 0.36          |
| (1,1726) | 1:42:A:ARG:HA   | 1:42:A:ARG:HD3  | 5        | 0.36          |
| (1,1726) | 1:42:A:ARG:HA   | 1:42:A:ARG:HD3  | 15       | 0.36          |
| (1,551)  | 1:8:A:LEU:HG    | 1:70:A:VAL:HA   | 12       | 0.36          |
| (1,459)  | 1:6:A:LYS:HE3   | 1:66:A:THR:HG21 | 2        | 0.36          |
| (1,458)  | 1:6:A:LYS:HD2   | 1:66:A:THR:HG23 | 10       | 0.36          |
| (1,458)  | 1:6:A:LYS:HD2   | 1:66:A:THR:HG21 | 15       | 0.36          |
| (1,378)  | 1:5:A:VAL:HG21  | 1:67:A:LEU:HG   | 4        | 0.36          |
| (1,378)  | 1:5:A:VAL:HG22  | 1:67:A:LEU:HG   | 4        | 0.36          |
| (1,378)  | 1:5:A:VAL:HG23  | 1:67:A:LEU:HG   | 4        | 0.36          |
| (1,19)   | 1:1:A:MET:HE2   | 1:3:A:ILE:HD13  | 6        | 0.36          |
| (1,1726) | 1:42:A:ARG:HA   | 1:42:A:ARG:HD3  | 8        | 0.35          |
| (1,1726) | 1:42:A:ARG:HA   | 1:42:A:ARG:HD3  | 16       | 0.35          |
| (1,1726) | 1:42:A:ARG:HA   | 1:42:A:ARG:HD3  | 17       | 0.35          |
| (1,1726) | 1:42:A:ARG:HA   | 1:42:A:ARG:HD3  | 20       | 0.35          |
| (1,1392) | 1:30:A:ILE:HB   | 1:41:A:GLN:HE22 | 9        | 0.35          |
| (1,1392) | 1:30:A:ILE:HB   | 1:41:A:GLN:HE22 | 20       | 0.35          |
| (1,684)  | 1:15:A:LEU:HA   | 1:15:A:LEU:HD13 | 15       | 0.35          |
| (1,551)  | 1:8:A:LEU:HG    | 1:70:A:VAL:HA   | 1        | 0.35          |
| (1,551)  | 1:8:A:LEU:HG    | 1:70:A:VAL:HA   | 3        | 0.35          |
| (1,551)  | 1:8:A:LEU:HG    | 1:70:A:VAL:HA   | 5        | 0.35          |
| (1,551)  | 1:8:A:LEU:HG    | 1:70:A:VAL:HA   | 11       | 0.35          |
| (1,551)  | 1:8:A:LEU:HG    | 1:70:A:VAL:HA   | 15       | 0.35          |
| (1,551)  | 1:8:A:LEU:HG    | 1:70:A:VAL:HA   | 18       | 0.35          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,459)  | 1:6:A:LYS:HE2  | 1:66:A:THR:HG21 | 19       | 0.35          |
| (1,378)  | 1:5:A:VAL:HG21 | 1:67:A:LEU:HG   | 8        | 0.35          |
| (1,378)  | 1:5:A:VAL:HG22 | 1:67:A:LEU:HG   | 8        | 0.35          |
| (1,378)  | 1:5:A:VAL:HG23 | 1:67:A:LEU:HG   | 8        | 0.35          |
| (1,378)  | 1:5:A:VAL:HG21 | 1:67:A:LEU:HG   | 15       | 0.35          |
| (1,378)  | 1:5:A:VAL:HG22 | 1:67:A:LEU:HG   | 15       | 0.35          |
| (1,378)  | 1:5:A:VAL:HG23 | 1:67:A:LEU:HG   | 15       | 0.35          |
| (1,38)   | 1:1:A:MET:HE2  | 1:17:A:VAL:HG22 | 2        | 0.35          |
| (1,1776) | 1:42:A:ARG:HG3 | 1:72:A:ARG:H    | 19       | 0.34          |
| (1,1726) | 1:42:A:ARG:HA  | 1:42:A:ARG:HD3  | 1        | 0.34          |
| (1,1692) | 1:40:A:GLN:HG2 | 1:73:A:LEU:HD11 | 14       | 0.34          |
| (1,684)  | 1:15:A:LEU:HA  | 1:15:A:LEU:HD12 | 4        | 0.34          |
| (1,684)  | 1:15:A:LEU:HA  | 1:15:A:LEU:HD12 | 8        | 0.34          |
| (1,551)  | 1:8:A:LEU:HG   | 1:70:A:VAL:HA   | 6        | 0.34          |
| (1,551)  | 1:8:A:LEU:HG   | 1:70:A:VAL:HA   | 8        | 0.34          |
| (1,551)  | 1:8:A:LEU:HG   | 1:70:A:VAL:HA   | 10       | 0.34          |
| (1,551)  | 1:8:A:LEU:HG   | 1:70:A:VAL:HA   | 16       | 0.34          |
| (1,551)  | 1:8:A:LEU:HG   | 1:70:A:VAL:HA   | 19       | 0.34          |
| (1,457)  | 1:6:A:LYS:HD3  | 1:66:A:THR:HG21 | 20       | 0.34          |
| (1,318)  | 1:5:A:VAL:HG11 | 1:7:A:THR:HG21  | 11       | 0.34          |
| (1,264)  | 1:4:A:PHE:HA   | 1:14:A:THR:HG22 | 17       | 0.34          |
| (1,38)   | 1:1:A:MET:HE2  | 1:17:A:VAL:HG22 | 11       | 0.34          |
| (1,37)   | 1:1:A:MET:HE3  | 1:17:A:VAL:HG21 | 13       | 0.34          |
| (1,1776) | 1:42:A:ARG:HG3 | 1:72:A:ARG:H    | 18       | 0.33          |
| (1,1726) | 1:42:A:ARG:HA  | 1:42:A:ARG:HD3  | 3        | 0.33          |
| (1,1692) | 1:40:A:GLN:HG2 | 1:73:A:LEU:HD23 | 20       | 0.33          |
| (1,551)  | 1:8:A:LEU:HG   | 1:70:A:VAL:HA   | 2        | 0.33          |
| (1,551)  | 1:8:A:LEU:HG   | 1:70:A:VAL:HA   | 4        | 0.33          |
| (1,551)  | 1:8:A:LEU:HG   | 1:70:A:VAL:HA   | 7        | 0.33          |
| (1,551)  | 1:8:A:LEU:HG   | 1:70:A:VAL:HA   | 14       | 0.33          |
| (1,450)  | 1:11:A:LYS:HE3 | 1:13:A:ILE:HD12 | 4        | 0.33          |
| (1,292)  | 1:4:A:PHE:HB3  | 1:66:A:THR:HA   | 7        | 0.33          |
| (1,292)  | 1:4:A:PHE:HB3  | 1:66:A:THR:HA   | 10       | 0.33          |
| (1,1776) | 1:42:A:ARG:HG3 | 1:72:A:ARG:H    | 1        | 0.32          |
| (1,1726) | 1:42:A:ARG:HA  | 1:42:A:ARG:HD3  | 4        | 0.32          |
| (1,1726) | 1:42:A:ARG:HA  | 1:42:A:ARG:HD3  | 9        | 0.32          |
| (1,1726) | 1:42:A:ARG:HA  | 1:42:A:ARG:HD3  | 10       | 0.32          |
| (1,339)  | 1:5:A:VAL:HG23 | 1:13:A:ILE:HG13 | 20       | 0.32          |
| (1,292)  | 1:4:A:PHE:HB3  | 1:66:A:THR:HA   | 2        | 0.32          |
| (1,19)   | 1:1:A:MET:HE2  | 1:3:A:ILE:HD12  | 8        | 0.32          |
| (1,19)   | 1:1:A:MET:HE2  | 1:3:A:ILE:HD13  | 9        | 0.32          |
| (1,19)   | 1:1:A:MET:HE2  | 1:3:A:ILE:HD11  | 10       | 0.32          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,72)   | 1:27:A:LYS:HE3  | 1:69:A:LEU:HD12 | 5        | 0.31          |
| (1,1776) | 1:42:A:ARG:HG3  | 1:72:A:ARG:H    | 15       | 0.31          |
| (1,1726) | 1:42:A:ARG:HA   | 1:42:A:ARG:HD3  | 7        | 0.31          |
| (1,1511) | 1:34:A:GLU:HG3  | 1:69:A:LEU:HD21 | 20       | 0.31          |
| (1,1294) | 1:27:A:LYS:HE2  | 1:52:A:ASP:HB3  | 4        | 0.31          |
| (1,1294) | 1:27:A:LYS:HE3  | 1:52:A:ASP:HB3  | 4        | 0.31          |
| (1,1294) | 1:27:A:LYS:HE2  | 1:52:A:ASP:HB3  | 8        | 0.31          |
| (1,1294) | 1:27:A:LYS:HE3  | 1:52:A:ASP:HB3  | 8        | 0.31          |
| (1,339)  | 1:5:A:VAL:HG22  | 1:13:A:ILE:HG13 | 10       | 0.31          |
| (1,319)  | 1:5:A:VAL:HG11  | 1:7:A:THR:HG21  | 12       | 0.31          |
| (1,318)  | 1:5:A:VAL:HG11  | 1:7:A:THR:HG22  | 8        | 0.31          |
| (1,292)  | 1:4:A:PHE:HB3   | 1:66:A:THR:HA   | 3        | 0.31          |
| (1,292)  | 1:4:A:PHE:HB3   | 1:66:A:THR:HA   | 17       | 0.31          |
| (1,38)   | 1:1:A:MET:HE3   | 1:17:A:VAL:HG21 | 18       | 0.31          |
| (1,19)   | 1:1:A:MET:HE2   | 1:3:A:ILE:HD11  | 20       | 0.31          |
| (2,72)   | 1:27:A:LYS:HE3  | 1:69:A:LEU:HD12 | 15       | 0.3           |
| (1,2591) | 1:74:A:ARG:HA   | 1:75:A:GLY:H    | 12       | 0.3           |
| (1,1776) | 1:42:A:ARG:HG3  | 1:72:A:ARG:H    | 3        | 0.3           |
| (1,634)  | 1:13:A:ILE:HG12 | 1:30:A:ILE:HD11 | 2        | 0.3           |
| (1,634)  | 1:13:A:ILE:HG12 | 1:30:A:ILE:HD12 | 2        | 0.3           |
| (1,634)  | 1:13:A:ILE:HG12 | 1:30:A:ILE:HD13 | 2        | 0.3           |
| (1,634)  | 1:13:A:ILE:HG13 | 1:30:A:ILE:HD11 | 2        | 0.3           |
| (1,634)  | 1:13:A:ILE:HG13 | 1:30:A:ILE:HD12 | 2        | 0.3           |
| (1,634)  | 1:13:A:ILE:HG13 | 1:30:A:ILE:HD13 | 2        | 0.3           |
| (1,634)  | 1:13:A:ILE:HG12 | 1:30:A:ILE:HD11 | 7        | 0.3           |
| (1,634)  | 1:13:A:ILE:HG12 | 1:30:A:ILE:HD12 | 7        | 0.3           |
| (1,634)  | 1:13:A:ILE:HG12 | 1:30:A:ILE:HD13 | 7        | 0.3           |
| (1,634)  | 1:13:A:ILE:HG13 | 1:30:A:ILE:HD11 | 7        | 0.3           |
| (1,634)  | 1:13:A:ILE:HG13 | 1:30:A:ILE:HD12 | 7        | 0.3           |
| (1,634)  | 1:13:A:ILE:HG13 | 1:30:A:ILE:HD13 | 7        | 0.3           |
| (1,439)  | 1:6:A:LYS:HD2   | 1:12:A:THR:HA   | 15       | 0.3           |
| (1,439)  | 1:6:A:LYS:HD3   | 1:12:A:THR:HA   | 15       | 0.3           |
| (1,292)  | 1:4:A:PHE:HB3   | 1:66:A:THR:HA   | 13       | 0.3           |
| (1,19)   | 1:1:A:MET:HE2   | 1:3:A:ILE:HD13  | 7        | 0.3           |
| (2,72)   | 1:27:A:LYS:HE3  | 1:69:A:LEU:HD13 | 6        | 0.29          |
| (1,2591) | 1:74:A:ARG:HA   | 1:75:A:GLY:H    | 4        | 0.29          |
| (1,634)  | 1:13:A:ILE:HG12 | 1:30:A:ILE:HD11 | 3        | 0.29          |
| (1,634)  | 1:13:A:ILE:HG12 | 1:30:A:ILE:HD12 | 3        | 0.29          |
| (1,634)  | 1:13:A:ILE:HG12 | 1:30:A:ILE:HD13 | 3        | 0.29          |
| (1,634)  | 1:13:A:ILE:HG13 | 1:30:A:ILE:HD11 | 3        | 0.29          |
| (1,634)  | 1:13:A:ILE:HG13 | 1:30:A:ILE:HD12 | 3        | 0.29          |
| (1,634)  | 1:13:A:ILE:HG13 | 1:30:A:ILE:HD13 | 3        | 0.29          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,634)  | 1:13:A:ILE:HG12 | 1:30:A:ILE:HD11 | 10       | 0.29          |
| (1,634)  | 1:13:A:ILE:HG12 | 1:30:A:ILE:HD12 | 10       | 0.29          |
| (1,634)  | 1:13:A:ILE:HG12 | 1:30:A:ILE:HD13 | 10       | 0.29          |
| (1,634)  | 1:13:A:ILE:HG13 | 1:30:A:ILE:HD11 | 10       | 0.29          |
| (1,634)  | 1:13:A:ILE:HG13 | 1:30:A:ILE:HD12 | 10       | 0.29          |
| (1,634)  | 1:13:A:ILE:HG13 | 1:30:A:ILE:HD13 | 10       | 0.29          |
| (1,634)  | 1:13:A:ILE:HG12 | 1:30:A:ILE:HD11 | 13       | 0.29          |
| (1,634)  | 1:13:A:ILE:HG12 | 1:30:A:ILE:HD12 | 13       | 0.29          |
| (1,634)  | 1:13:A:ILE:HG12 | 1:30:A:ILE:HD13 | 13       | 0.29          |
| (1,634)  | 1:13:A:ILE:HG13 | 1:30:A:ILE:HD11 | 13       | 0.29          |
| (1,634)  | 1:13:A:ILE:HG13 | 1:30:A:ILE:HD12 | 13       | 0.29          |
| (1,634)  | 1:13:A:ILE:HG13 | 1:30:A:ILE:HD13 | 13       | 0.29          |
| (1,439)  | 1:6:A:LYS:HD2   | 1:12:A:THR:HA   | 1        | 0.29          |
| (1,439)  | 1:6:A:LYS:HD3   | 1:12:A:THR:HA   | 1        | 0.29          |
| (1,439)  | 1:6:A:LYS:HD2   | 1:12:A:THR:HA   | 5        | 0.29          |
| (1,439)  | 1:6:A:LYS:HD3   | 1:12:A:THR:HA   | 5        | 0.29          |
| (1,387)  | 1:5:A:VAL:HG11  | 1:69:A:LEU:HG   | 9        | 0.29          |
| (1,387)  | 1:5:A:VAL:HG12  | 1:69:A:LEU:HG   | 9        | 0.29          |
| (1,387)  | 1:5:A:VAL:HG13  | 1:69:A:LEU:HG   | 9        | 0.29          |
| (1,339)  | 1:5:A:VAL:HG21  | 1:13:A:ILE:HG13 | 3        | 0.29          |
| (1,318)  | 1:5:A:VAL:HG12  | 1:7:A:THR:HG21  | 5        | 0.29          |
| (1,292)  | 1:4:A:PHE:HB3   | 1:66:A:THR:HA   | 1        | 0.29          |
| (1,292)  | 1:4:A:PHE:HB3   | 1:66:A:THR:HA   | 4        | 0.29          |
| (1,292)  | 1:4:A:PHE:HB3   | 1:66:A:THR:HA   | 5        | 0.29          |
| (1,292)  | 1:4:A:PHE:HB3   | 1:66:A:THR:HA   | 8        | 0.29          |
| (1,292)  | 1:4:A:PHE:HB3   | 1:66:A:THR:HA   | 15       | 0.29          |
| (1,292)  | 1:4:A:PHE:HB3   | 1:66:A:THR:HA   | 19       | 0.29          |
| (1,292)  | 1:4:A:PHE:HB3   | 1:66:A:THR:HA   | 20       | 0.29          |
| (1,264)  | 1:4:A:PHE:HA    | 1:14:A:THR:HG22 | 20       | 0.29          |
| (1,19)   | 1:1:A:MET:HE2   | 1:3:A:ILE:HD13  | 4        | 0.29          |
| (2,72)   | 1:27:A:LYS:HE3  | 1:69:A:LEU:HD12 | 1        | 0.28          |
| (2,72)   | 1:27:A:LYS:HE3  | 1:69:A:LEU:HD13 | 10       | 0.28          |
| (1,1776) | 1:42:A:ARG:HG3  | 1:72:A:ARG:H    | 5        | 0.28          |
| (1,1744) | 1:42:A:ARG:HG2  | 1:44:A:ILE:HD11 | 3        | 0.28          |
| (1,634)  | 1:13:A:ILE:HG12 | 1:30:A:ILE:HD11 | 17       | 0.28          |
| (1,634)  | 1:13:A:ILE:HG12 | 1:30:A:ILE:HD12 | 17       | 0.28          |
| (1,634)  | 1:13:A:ILE:HG12 | 1:30:A:ILE:HD13 | 17       | 0.28          |
| (1,634)  | 1:13:A:ILE:HG13 | 1:30:A:ILE:HD11 | 17       | 0.28          |
| (1,634)  | 1:13:A:ILE:HG13 | 1:30:A:ILE:HD12 | 17       | 0.28          |
| (1,634)  | 1:13:A:ILE:HG13 | 1:30:A:ILE:HD13 | 17       | 0.28          |
| (1,439)  | 1:6:A:LYS:HD2   | 1:12:A:THR:HA   | 8        | 0.28          |
| (1,439)  | 1:6:A:LYS:HD3   | 1:12:A:THR:HA   | 8        | 0.28          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,439)  | 1:6:A:LYS:HD2   | 1:12:A:THR:HA   | 19       | 0.28          |
| (1,439)  | 1:6:A:LYS:HD3   | 1:12:A:THR:HA   | 19       | 0.28          |
| (1,387)  | 1:5:A:VAL:HG11  | 1:69:A:LEU:HG   | 4        | 0.28          |
| (1,387)  | 1:5:A:VAL:HG12  | 1:69:A:LEU:HG   | 4        | 0.28          |
| (1,387)  | 1:5:A:VAL:HG13  | 1:69:A:LEU:HG   | 4        | 0.28          |
| (1,387)  | 1:5:A:VAL:HG11  | 1:69:A:LEU:HG   | 13       | 0.28          |
| (1,387)  | 1:5:A:VAL:HG12  | 1:69:A:LEU:HG   | 13       | 0.28          |
| (1,387)  | 1:5:A:VAL:HG13  | 1:69:A:LEU:HG   | 13       | 0.28          |
| (1,387)  | 1:5:A:VAL:HG11  | 1:69:A:LEU:HG   | 17       | 0.28          |
| (1,387)  | 1:5:A:VAL:HG12  | 1:69:A:LEU:HG   | 17       | 0.28          |
| (1,387)  | 1:5:A:VAL:HG13  | 1:69:A:LEU:HG   | 17       | 0.28          |
| (1,378)  | 1:5:A:VAL:HG21  | 1:67:A:LEU:HG   | 2        | 0.28          |
| (1,378)  | 1:5:A:VAL:HG22  | 1:67:A:LEU:HG   | 2        | 0.28          |
| (1,378)  | 1:5:A:VAL:HG23  | 1:67:A:LEU:HG   | 2        | 0.28          |
| (1,378)  | 1:5:A:VAL:HG21  | 1:67:A:LEU:HG   | 3        | 0.28          |
| (1,378)  | 1:5:A:VAL:HG22  | 1:67:A:LEU:HG   | 3        | 0.28          |
| (1,378)  | 1:5:A:VAL:HG23  | 1:67:A:LEU:HG   | 3        | 0.28          |
| (1,378)  | 1:5:A:VAL:HG21  | 1:67:A:LEU:HG   | 7        | 0.28          |
| (1,378)  | 1:5:A:VAL:HG22  | 1:67:A:LEU:HG   | 7        | 0.28          |
| (1,378)  | 1:5:A:VAL:HG23  | 1:67:A:LEU:HG   | 7        | 0.28          |
| (1,378)  | 1:5:A:VAL:HG21  | 1:67:A:LEU:HG   | 10       | 0.28          |
| (1,378)  | 1:5:A:VAL:HG22  | 1:67:A:LEU:HG   | 10       | 0.28          |
| (1,378)  | 1:5:A:VAL:HG23  | 1:67:A:LEU:HG   | 10       | 0.28          |
| (1,355)  | 1:17:A:VAL:HG11 | 1:29:A:LYS:HE2  | 16       | 0.28          |
| (1,319)  | 1:5:A:VAL:HG11  | 1:7:A:THR:HG21  | 11       | 0.28          |
| (1,292)  | 1:4:A:PHE:HB3   | 1:66:A:THR:HA   | 9        | 0.28          |
| (1,292)  | 1:4:A:PHE:HB3   | 1:66:A:THR:HA   | 16       | 0.28          |
| (1,292)  | 1:4:A:PHE:HB3   | 1:66:A:THR:HA   | 18       | 0.28          |
| (1,264)  | 1:4:A:PHE:HA    | 1:14:A:THR:HG22 | 9        | 0.28          |
| (1,37)   | 1:1:A:MET:HE3   | 1:17:A:VAL:HG23 | 3        | 0.28          |
| (1,1560) | 1:36:A:ILE:HG21 | 1:40:A:GLN:HG2  | 9        | 0.27          |
| (1,1560) | 1:36:A:ILE:HG21 | 1:40:A:GLN:HG3  | 9        | 0.27          |
| (1,1560) | 1:36:A:ILE:HG22 | 1:40:A:GLN:HG2  | 9        | 0.27          |
| (1,1560) | 1:36:A:ILE:HG22 | 1:40:A:GLN:HG3  | 9        | 0.27          |
| (1,1560) | 1:36:A:ILE:HG23 | 1:40:A:GLN:HG2  | 9        | 0.27          |
| (1,1560) | 1:36:A:ILE:HG23 | 1:40:A:GLN:HG3  | 9        | 0.27          |
| (1,1560) | 1:36:A:ILE:HG21 | 1:40:A:GLN:HG2  | 20       | 0.27          |
| (1,1560) | 1:36:A:ILE:HG21 | 1:40:A:GLN:HG3  | 20       | 0.27          |
| (1,1560) | 1:36:A:ILE:HG22 | 1:40:A:GLN:HG2  | 20       | 0.27          |
| (1,1560) | 1:36:A:ILE:HG22 | 1:40:A:GLN:HG3  | 20       | 0.27          |
| (1,1560) | 1:36:A:ILE:HG23 | 1:40:A:GLN:HG2  | 20       | 0.27          |
| (1,1560) | 1:36:A:ILE:HG23 | 1:40:A:GLN:HG3  | 20       | 0.27          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1511) | 1:34:A:GLU:HG3  | 1:69:A:LEU:HD23 | 9        | 0.27          |
| (1,1370) | 1:30:A:ILE:HA   | 1:33:A:LYS:HB3  | 4        | 0.27          |
| (1,1370) | 1:30:A:ILE:HA   | 1:33:A:LYS:HB3  | 5        | 0.27          |
| (1,634)  | 1:13:A:ILE:HG12 | 1:30:A:ILE:HD11 | 9        | 0.27          |
| (1,634)  | 1:13:A:ILE:HG12 | 1:30:A:ILE:HD12 | 9        | 0.27          |
| (1,634)  | 1:13:A:ILE:HG12 | 1:30:A:ILE:HD13 | 9        | 0.27          |
| (1,634)  | 1:13:A:ILE:HG13 | 1:30:A:ILE:HD11 | 9        | 0.27          |
| (1,634)  | 1:13:A:ILE:HG13 | 1:30:A:ILE:HD12 | 9        | 0.27          |
| (1,634)  | 1:13:A:ILE:HG13 | 1:30:A:ILE:HD13 | 9        | 0.27          |
| (1,634)  | 1:13:A:ILE:HG12 | 1:30:A:ILE:HD11 | 18       | 0.27          |
| (1,634)  | 1:13:A:ILE:HG12 | 1:30:A:ILE:HD12 | 18       | 0.27          |
| (1,634)  | 1:13:A:ILE:HG12 | 1:30:A:ILE:HD13 | 18       | 0.27          |
| (1,634)  | 1:13:A:ILE:HG13 | 1:30:A:ILE:HD11 | 18       | 0.27          |
| (1,634)  | 1:13:A:ILE:HG13 | 1:30:A:ILE:HD12 | 18       | 0.27          |
| (1,634)  | 1:13:A:ILE:HG13 | 1:30:A:ILE:HD13 | 18       | 0.27          |
| (1,634)  | 1:13:A:ILE:HG12 | 1:30:A:ILE:HD11 | 20       | 0.27          |
| (1,634)  | 1:13:A:ILE:HG12 | 1:30:A:ILE:HD12 | 20       | 0.27          |
| (1,634)  | 1:13:A:ILE:HG12 | 1:30:A:ILE:HD13 | 20       | 0.27          |
| (1,634)  | 1:13:A:ILE:HG13 | 1:30:A:ILE:HD11 | 20       | 0.27          |
| (1,634)  | 1:13:A:ILE:HG13 | 1:30:A:ILE:HD12 | 20       | 0.27          |
| (1,634)  | 1:13:A:ILE:HG13 | 1:30:A:ILE:HD13 | 20       | 0.27          |
| (1,458)  | 1:6:A:LYS:HD2   | 1:66:A:THR:HG21 | 2        | 0.27          |
| (1,387)  | 1:5:A:VAL:HG11  | 1:69:A:LEU:HG   | 2        | 0.27          |
| (1,387)  | 1:5:A:VAL:HG12  | 1:69:A:LEU:HG   | 2        | 0.27          |
| (1,387)  | 1:5:A:VAL:HG13  | 1:69:A:LEU:HG   | 2        | 0.27          |
| (1,387)  | 1:5:A:VAL:HG11  | 1:69:A:LEU:HG   | 3        | 0.27          |
| (1,387)  | 1:5:A:VAL:HG12  | 1:69:A:LEU:HG   | 3        | 0.27          |
| (1,387)  | 1:5:A:VAL:HG13  | 1:69:A:LEU:HG   | 3        | 0.27          |
| (1,387)  | 1:5:A:VAL:HG11  | 1:69:A:LEU:HG   | 7        | 0.27          |
| (1,387)  | 1:5:A:VAL:HG12  | 1:69:A:LEU:HG   | 7        | 0.27          |
| (1,387)  | 1:5:A:VAL:HG13  | 1:69:A:LEU:HG   | 7        | 0.27          |
| (1,387)  | 1:5:A:VAL:HG11  | 1:69:A:LEU:HG   | 8        | 0.27          |
| (1,387)  | 1:5:A:VAL:HG12  | 1:69:A:LEU:HG   | 8        | 0.27          |
| (1,387)  | 1:5:A:VAL:HG13  | 1:69:A:LEU:HG   | 8        | 0.27          |
| (1,387)  | 1:5:A:VAL:HG11  | 1:69:A:LEU:HG   | 15       | 0.27          |
| (1,387)  | 1:5:A:VAL:HG12  | 1:69:A:LEU:HG   | 15       | 0.27          |
| (1,387)  | 1:5:A:VAL:HG13  | 1:69:A:LEU:HG   | 15       | 0.27          |
| (1,378)  | 1:5:A:VAL:HG21  | 1:67:A:LEU:HG   | 1        | 0.27          |
| (1,378)  | 1:5:A:VAL:HG22  | 1:67:A:LEU:HG   | 1        | 0.27          |
| (1,378)  | 1:5:A:VAL:HG23  | 1:67:A:LEU:HG   | 1        | 0.27          |
| (1,378)  | 1:5:A:VAL:HG21  | 1:67:A:LEU:HG   | 5        | 0.27          |
| (1,378)  | 1:5:A:VAL:HG22  | 1:67:A:LEU:HG   | 5        | 0.27          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,378)  | 1:5:A:VAL:HG23 | 1:67:A:LEU:HG   | 5        | 0.27          |
| (1,378)  | 1:5:A:VAL:HG21 | 1:67:A:LEU:HG   | 6        | 0.27          |
| (1,378)  | 1:5:A:VAL:HG22 | 1:67:A:LEU:HG   | 6        | 0.27          |
| (1,378)  | 1:5:A:VAL:HG23 | 1:67:A:LEU:HG   | 6        | 0.27          |
| (1,378)  | 1:5:A:VAL:HG21 | 1:67:A:LEU:HG   | 9        | 0.27          |
| (1,378)  | 1:5:A:VAL:HG22 | 1:67:A:LEU:HG   | 9        | 0.27          |
| (1,378)  | 1:5:A:VAL:HG23 | 1:67:A:LEU:HG   | 9        | 0.27          |
| (1,378)  | 1:5:A:VAL:HG21 | 1:67:A:LEU:HG   | 13       | 0.27          |
| (1,378)  | 1:5:A:VAL:HG22 | 1:67:A:LEU:HG   | 13       | 0.27          |
| (1,378)  | 1:5:A:VAL:HG23 | 1:67:A:LEU:HG   | 13       | 0.27          |
| (1,378)  | 1:5:A:VAL:HG21 | 1:67:A:LEU:HG   | 16       | 0.27          |
| (1,378)  | 1:5:A:VAL:HG22 | 1:67:A:LEU:HG   | 16       | 0.27          |
| (1,378)  | 1:5:A:VAL:HG23 | 1:67:A:LEU:HG   | 16       | 0.27          |
| (1,378)  | 1:5:A:VAL:HG21 | 1:67:A:LEU:HG   | 17       | 0.27          |
| (1,378)  | 1:5:A:VAL:HG22 | 1:67:A:LEU:HG   | 17       | 0.27          |
| (1,378)  | 1:5:A:VAL:HG23 | 1:67:A:LEU:HG   | 17       | 0.27          |
| (1,378)  | 1:5:A:VAL:HG21 | 1:67:A:LEU:HG   | 18       | 0.27          |
| (1,378)  | 1:5:A:VAL:HG22 | 1:67:A:LEU:HG   | 18       | 0.27          |
| (1,378)  | 1:5:A:VAL:HG23 | 1:67:A:LEU:HG   | 18       | 0.27          |
| (1,378)  | 1:5:A:VAL:HG21 | 1:67:A:LEU:HG   | 20       | 0.27          |
| (1,378)  | 1:5:A:VAL:HG22 | 1:67:A:LEU:HG   | 20       | 0.27          |
| (1,378)  | 1:5:A:VAL:HG23 | 1:67:A:LEU:HG   | 20       | 0.27          |
| (1,339)  | 1:5:A:VAL:HG21 | 1:13:A:ILE:HG13 | 2        | 0.27          |
| (1,339)  | 1:5:A:VAL:HG21 | 1:13:A:ILE:HG13 | 7        | 0.27          |
| (1,318)  | 1:5:A:VAL:HG11 | 1:7:A:THR:HG22  | 1        | 0.27          |
| (1,292)  | 1:4:A:PHE:HB3  | 1:66:A:THR:HA   | 6        | 0.27          |
| (1,292)  | 1:4:A:PHE:HB3  | 1:66:A:THR:HA   | 11       | 0.27          |
| (1,292)  | 1:4:A:PHE:HB3  | 1:66:A:THR:HA   | 12       | 0.27          |
| (1,292)  | 1:4:A:PHE:HB3  | 1:66:A:THR:HA   | 14       | 0.27          |
| (1,264)  | 1:4:A:PHE:HA   | 1:12:A:THR:HG21 | 14       | 0.27          |
| (1,177)  | 1:29:A:LYS:HA  | 1:15:A:LEU:HD22 | 13       | 0.27          |
| (1,19)   | 1:1:A:MET:HE1  | 1:3:A:ILE:HD12  | 17       | 0.27          |
| (1,1744) | 1:42:A:ARG:HG2 | 1:44:A:ILE:HD12 | 13       | 0.26          |
| (1,1675) | 1:40:A:GLN:HA  | 1:72:A:ARG:HD3  | 18       | 0.26          |
| (1,1511) | 1:34:A:GLU:HG3 | 1:69:A:LEU:HD23 | 13       | 0.26          |
| (1,1370) | 1:30:A:ILE:HA  | 1:33:A:LYS:HB3  | 1        | 0.26          |
| (1,1370) | 1:30:A:ILE:HA  | 1:33:A:LYS:HB3  | 2        | 0.26          |
| (1,1370) | 1:30:A:ILE:HA  | 1:33:A:LYS:HB3  | 3        | 0.26          |
| (1,1370) | 1:30:A:ILE:HA  | 1:33:A:LYS:HB3  | 6        | 0.26          |
| (1,1370) | 1:30:A:ILE:HA  | 1:33:A:LYS:HB3  | 7        | 0.26          |
| (1,1370) | 1:30:A:ILE:HA  | 1:33:A:LYS:HB3  | 8        | 0.26          |
| (1,1370) | 1:30:A:ILE:HA  | 1:33:A:LYS:HB3  | 10       | 0.26          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1370) | 1:30:A:ILE:HA   | 1:33:A:LYS:HB3  | 12       | 0.26          |
| (1,1370) | 1:30:A:ILE:HA   | 1:33:A:LYS:HB3  | 14       | 0.26          |
| (1,1370) | 1:30:A:ILE:HA   | 1:33:A:LYS:HB3  | 15       | 0.26          |
| (1,1370) | 1:30:A:ILE:HA   | 1:33:A:LYS:HB3  | 16       | 0.26          |
| (1,1370) | 1:30:A:ILE:HA   | 1:33:A:LYS:HB3  | 18       | 0.26          |
| (1,1370) | 1:30:A:ILE:HA   | 1:33:A:LYS:HB3  | 19       | 0.26          |
| (1,634)  | 1:13:A:ILE:HG12 | 1:30:A:ILE:HD11 | 1        | 0.26          |
| (1,634)  | 1:13:A:ILE:HG12 | 1:30:A:ILE:HD12 | 1        | 0.26          |
| (1,634)  | 1:13:A:ILE:HG12 | 1:30:A:ILE:HD13 | 1        | 0.26          |
| (1,634)  | 1:13:A:ILE:HG13 | 1:30:A:ILE:HD11 | 1        | 0.26          |
| (1,634)  | 1:13:A:ILE:HG13 | 1:30:A:ILE:HD12 | 1        | 0.26          |
| (1,634)  | 1:13:A:ILE:HG13 | 1:30:A:ILE:HD13 | 1        | 0.26          |
| (1,634)  | 1:13:A:ILE:HG12 | 1:30:A:ILE:HD11 | 6        | 0.26          |
| (1,634)  | 1:13:A:ILE:HG12 | 1:30:A:ILE:HD12 | 6        | 0.26          |
| (1,634)  | 1:13:A:ILE:HG12 | 1:30:A:ILE:HD13 | 6        | 0.26          |
| (1,634)  | 1:13:A:ILE:HG13 | 1:30:A:ILE:HD11 | 6        | 0.26          |
| (1,634)  | 1:13:A:ILE:HG13 | 1:30:A:ILE:HD12 | 6        | 0.26          |
| (1,634)  | 1:13:A:ILE:HG13 | 1:30:A:ILE:HD13 | 6        | 0.26          |
| (1,634)  | 1:13:A:ILE:HG12 | 1:30:A:ILE:HD11 | 11       | 0.26          |
| (1,634)  | 1:13:A:ILE:HG12 | 1:30:A:ILE:HD12 | 11       | 0.26          |
| (1,634)  | 1:13:A:ILE:HG12 | 1:30:A:ILE:HD13 | 11       | 0.26          |
| (1,634)  | 1:13:A:ILE:HG13 | 1:30:A:ILE:HD11 | 11       | 0.26          |
| (1,634)  | 1:13:A:ILE:HG13 | 1:30:A:ILE:HD12 | 11       | 0.26          |
| (1,634)  | 1:13:A:ILE:HG13 | 1:30:A:ILE:HD13 | 11       | 0.26          |
| (1,634)  | 1:13:A:ILE:HG12 | 1:30:A:ILE:HD11 | 12       | 0.26          |
| (1,634)  | 1:13:A:ILE:HG12 | 1:30:A:ILE:HD12 | 12       | 0.26          |
| (1,634)  | 1:13:A:ILE:HG12 | 1:30:A:ILE:HD13 | 12       | 0.26          |
| (1,634)  | 1:13:A:ILE:HG13 | 1:30:A:ILE:HD11 | 12       | 0.26          |
| (1,634)  | 1:13:A:ILE:HG13 | 1:30:A:ILE:HD12 | 12       | 0.26          |
| (1,634)  | 1:13:A:ILE:HG13 | 1:30:A:ILE:HD13 | 12       | 0.26          |
| (1,634)  | 1:13:A:ILE:HG12 | 1:30:A:ILE:HD11 | 16       | 0.26          |
| (1,634)  | 1:13:A:ILE:HG12 | 1:30:A:ILE:HD12 | 16       | 0.26          |
| (1,634)  | 1:13:A:ILE:HG12 | 1:30:A:ILE:HD13 | 16       | 0.26          |
| (1,634)  | 1:13:A:ILE:HG13 | 1:30:A:ILE:HD11 | 16       | 0.26          |
| (1,634)  | 1:13:A:ILE:HG13 | 1:30:A:ILE:HD12 | 16       | 0.26          |
| (1,634)  | 1:13:A:ILE:HG13 | 1:30:A:ILE:HD13 | 16       | 0.26          |
| (1,634)  | 1:13:A:ILE:HG12 | 1:30:A:ILE:HD11 | 19       | 0.26          |
| (1,634)  | 1:13:A:ILE:HG12 | 1:30:A:ILE:HD12 | 19       | 0.26          |
| (1,634)  | 1:13:A:ILE:HG12 | 1:30:A:ILE:HD13 | 19       | 0.26          |
| (1,634)  | 1:13:A:ILE:HG13 | 1:30:A:ILE:HD11 | 19       | 0.26          |
| (1,634)  | 1:13:A:ILE:HG13 | 1:30:A:ILE:HD12 | 19       | 0.26          |
| (1,634)  | 1:13:A:ILE:HG13 | 1:30:A:ILE:HD13 | 19       | 0.26          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,387) | 1:5:A:VAL:HG11  | 1:69:A:LEU:HG   | 1        | 0.26          |
| (1,387) | 1:5:A:VAL:HG12  | 1:69:A:LEU:HG   | 1        | 0.26          |
| (1,387) | 1:5:A:VAL:HG13  | 1:69:A:LEU:HG   | 1        | 0.26          |
| (1,387) | 1:5:A:VAL:HG11  | 1:69:A:LEU:HG   | 5        | 0.26          |
| (1,387) | 1:5:A:VAL:HG12  | 1:69:A:LEU:HG   | 5        | 0.26          |
| (1,387) | 1:5:A:VAL:HG13  | 1:69:A:LEU:HG   | 5        | 0.26          |
| (1,387) | 1:5:A:VAL:HG11  | 1:69:A:LEU:HG   | 6        | 0.26          |
| (1,387) | 1:5:A:VAL:HG12  | 1:69:A:LEU:HG   | 6        | 0.26          |
| (1,387) | 1:5:A:VAL:HG13  | 1:69:A:LEU:HG   | 6        | 0.26          |
| (1,387) | 1:5:A:VAL:HG11  | 1:69:A:LEU:HG   | 10       | 0.26          |
| (1,387) | 1:5:A:VAL:HG12  | 1:69:A:LEU:HG   | 10       | 0.26          |
| (1,387) | 1:5:A:VAL:HG13  | 1:69:A:LEU:HG   | 10       | 0.26          |
| (1,387) | 1:5:A:VAL:HG11  | 1:69:A:LEU:HG   | 11       | 0.26          |
| (1,387) | 1:5:A:VAL:HG12  | 1:69:A:LEU:HG   | 11       | 0.26          |
| (1,387) | 1:5:A:VAL:HG13  | 1:69:A:LEU:HG   | 11       | 0.26          |
| (1,387) | 1:5:A:VAL:HG11  | 1:69:A:LEU:HG   | 12       | 0.26          |
| (1,387) | 1:5:A:VAL:HG12  | 1:69:A:LEU:HG   | 12       | 0.26          |
| (1,387) | 1:5:A:VAL:HG13  | 1:69:A:LEU:HG   | 12       | 0.26          |
| (1,387) | 1:5:A:VAL:HG11  | 1:69:A:LEU:HG   | 14       | 0.26          |
| (1,387) | 1:5:A:VAL:HG12  | 1:69:A:LEU:HG   | 14       | 0.26          |
| (1,387) | 1:5:A:VAL:HG13  | 1:69:A:LEU:HG   | 14       | 0.26          |
| (1,387) | 1:5:A:VAL:HG11  | 1:69:A:LEU:HG   | 19       | 0.26          |
| (1,387) | 1:5:A:VAL:HG12  | 1:69:A:LEU:HG   | 19       | 0.26          |
| (1,387) | 1:5:A:VAL:HG13  | 1:69:A:LEU:HG   | 19       | 0.26          |
| (1,387) | 1:5:A:VAL:HG11  | 1:69:A:LEU:HG   | 20       | 0.26          |
| (1,387) | 1:5:A:VAL:HG12  | 1:69:A:LEU:HG   | 20       | 0.26          |
| (1,387) | 1:5:A:VAL:HG13  | 1:69:A:LEU:HG   | 20       | 0.26          |
| (1,378) | 1:5:A:VAL:HG21  | 1:67:A:LEU:HG   | 11       | 0.26          |
| (1,378) | 1:5:A:VAL:HG22  | 1:67:A:LEU:HG   | 11       | 0.26          |
| (1,378) | 1:5:A:VAL:HG23  | 1:67:A:LEU:HG   | 11       | 0.26          |
| (1,378) | 1:5:A:VAL:HG21  | 1:67:A:LEU:HG   | 12       | 0.26          |
| (1,378) | 1:5:A:VAL:HG22  | 1:67:A:LEU:HG   | 12       | 0.26          |
| (1,378) | 1:5:A:VAL:HG23  | 1:67:A:LEU:HG   | 12       | 0.26          |
| (1,378) | 1:5:A:VAL:HG21  | 1:67:A:LEU:HG   | 14       | 0.26          |
| (1,378) | 1:5:A:VAL:HG22  | 1:67:A:LEU:HG   | 14       | 0.26          |
| (1,378) | 1:5:A:VAL:HG23  | 1:67:A:LEU:HG   | 14       | 0.26          |
| (1,378) | 1:5:A:VAL:HG21  | 1:67:A:LEU:HG   | 19       | 0.26          |
| (1,378) | 1:5:A:VAL:HG22  | 1:67:A:LEU:HG   | 19       | 0.26          |
| (1,378) | 1:5:A:VAL:HG23  | 1:67:A:LEU:HG   | 19       | 0.26          |
| (1,357) | 1:17:A:VAL:HG11 | 1:29:A:LYS:HG3  | 16       | 0.26          |
| (1,177) | 1:29:A:LYS:HA   | 1:15:A:LEU:HD22 | 3        | 0.26          |
| (1,37)  | 1:1:A:MET:HE2   | 1:17:A:VAL:HG21 | 15       | 0.26          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1370) | 1:30:A:ILE:HA   | 1:33:A:LYS:HB3  | 9        | 0.25          |
| (1,1370) | 1:30:A:ILE:HA   | 1:33:A:LYS:HB3  | 11       | 0.25          |
| (1,1370) | 1:30:A:ILE:HA   | 1:33:A:LYS:HB3  | 13       | 0.25          |
| (1,1370) | 1:30:A:ILE:HA   | 1:33:A:LYS:HB3  | 17       | 0.25          |
| (1,1370) | 1:30:A:ILE:HA   | 1:33:A:LYS:HB3  | 20       | 0.25          |
| (1,738)  | 1:15:A:LEU:HD11 | 1:33:A:LYS:HD2  | 15       | 0.25          |
| (1,634)  | 1:13:A:ILE:HG12 | 1:30:A:ILE:HD11 | 4        | 0.25          |
| (1,634)  | 1:13:A:ILE:HG12 | 1:30:A:ILE:HD12 | 4        | 0.25          |
| (1,634)  | 1:13:A:ILE:HG12 | 1:30:A:ILE:HD13 | 4        | 0.25          |
| (1,634)  | 1:13:A:ILE:HG13 | 1:30:A:ILE:HD11 | 4        | 0.25          |
| (1,634)  | 1:13:A:ILE:HG13 | 1:30:A:ILE:HD12 | 4        | 0.25          |
| (1,634)  | 1:13:A:ILE:HG13 | 1:30:A:ILE:HD13 | 4        | 0.25          |
| (1,634)  | 1:13:A:ILE:HG12 | 1:30:A:ILE:HD11 | 5        | 0.25          |
| (1,634)  | 1:13:A:ILE:HG12 | 1:30:A:ILE:HD12 | 5        | 0.25          |
| (1,634)  | 1:13:A:ILE:HG12 | 1:30:A:ILE:HD13 | 5        | 0.25          |
| (1,634)  | 1:13:A:ILE:HG13 | 1:30:A:ILE:HD11 | 5        | 0.25          |
| (1,634)  | 1:13:A:ILE:HG13 | 1:30:A:ILE:HD12 | 5        | 0.25          |
| (1,634)  | 1:13:A:ILE:HG13 | 1:30:A:ILE:HD13 | 5        | 0.25          |
| (1,634)  | 1:13:A:ILE:HG12 | 1:30:A:ILE:HD11 | 14       | 0.25          |
| (1,634)  | 1:13:A:ILE:HG12 | 1:30:A:ILE:HD12 | 14       | 0.25          |
| (1,634)  | 1:13:A:ILE:HG12 | 1:30:A:ILE:HD13 | 14       | 0.25          |
| (1,634)  | 1:13:A:ILE:HG13 | 1:30:A:ILE:HD11 | 14       | 0.25          |
| (1,634)  | 1:13:A:ILE:HG13 | 1:30:A:ILE:HD12 | 14       | 0.25          |
| (1,634)  | 1:13:A:ILE:HG13 | 1:30:A:ILE:HD13 | 14       | 0.25          |
| (1,457)  | 1:6:A:LYS:HD3   | 1:66:A:THR:HG22 | 4        | 0.25          |
| (1,457)  | 1:6:A:LYS:HD3   | 1:66:A:THR:HG23 | 9        | 0.25          |
| (1,439)  | 1:6:A:LYS:HD2   | 1:12:A:THR:HA   | 7        | 0.25          |
| (1,439)  | 1:6:A:LYS:HD3   | 1:12:A:THR:HA   | 7        | 0.25          |
| (1,439)  | 1:6:A:LYS:HD2   | 1:12:A:THR:HA   | 10       | 0.25          |
| (1,439)  | 1:6:A:LYS:HD3   | 1:12:A:THR:HA   | 10       | 0.25          |
| (1,387)  | 1:5:A:VAL:HG11  | 1:69:A:LEU:HG   | 16       | 0.25          |
| (1,387)  | 1:5:A:VAL:HG12  | 1:69:A:LEU:HG   | 16       | 0.25          |
| (1,387)  | 1:5:A:VAL:HG13  | 1:69:A:LEU:HG   | 16       | 0.25          |
| (1,387)  | 1:5:A:VAL:HG11  | 1:69:A:LEU:HG   | 18       | 0.25          |
| (1,387)  | 1:5:A:VAL:HG12  | 1:69:A:LEU:HG   | 18       | 0.25          |
| (1,387)  | 1:5:A:VAL:HG13  | 1:69:A:LEU:HG   | 18       | 0.25          |
| (1,264)  | 1:4:A:PHE:HA    | 1:14:A:THR:HG22 | 1        | 0.25          |
| (1,177)  | 1:29:A:LYS:HA   | 1:15:A:LEU:HD22 | 6        | 0.25          |
| (1,177)  | 1:29:A:LYS:HA   | 1:15:A:LEU:HD22 | 7        | 0.25          |
| (1,177)  | 1:29:A:LYS:HA   | 1:15:A:LEU:HD22 | 10       | 0.25          |
| (1,177)  | 1:29:A:LYS:HA   | 1:15:A:LEU:HD23 | 17       | 0.25          |
| (1,45)   | 1:1:A:MET:HE3   | 1:18:A:GLU:HA   | 11       | 0.25          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,38)   | 1:1:A:MET:HE2   | 1:17:A:VAL:HG22 | 1        | 0.25          |
| (1,38)   | 1:1:A:MET:HE2   | 1:17:A:VAL:HG21 | 17       | 0.25          |
| (2,72)   | 1:27:A:LYS:HE3  | 1:69:A:LEU:HD13 | 2        | 0.24          |
| (2,72)   | 1:27:A:LYS:HE3  | 1:69:A:LEU:HD11 | 3        | 0.24          |
| (2,72)   | 1:27:A:LYS:HE3  | 1:69:A:LEU:HD11 | 16       | 0.24          |
| (2,72)   | 1:27:A:LYS:HE3  | 1:69:A:LEU:HD12 | 19       | 0.24          |
| (1,1817) | 1:43:A:LEU:HD23 | 1:67:A:LEU:HB3  | 4        | 0.24          |
| (1,1817) | 1:43:A:LEU:HD22 | 1:67:A:LEU:HB3  | 8        | 0.24          |
| (1,1776) | 1:42:A:ARG:HG3  | 1:72:A:ARG:H    | 8        | 0.24          |
| (1,1560) | 1:36:A:ILE:HG21 | 1:40:A:GLN:HG2  | 18       | 0.24          |
| (1,1560) | 1:36:A:ILE:HG21 | 1:40:A:GLN:HG3  | 18       | 0.24          |
| (1,1560) | 1:36:A:ILE:HG22 | 1:40:A:GLN:HG2  | 18       | 0.24          |
| (1,1560) | 1:36:A:ILE:HG22 | 1:40:A:GLN:HG3  | 18       | 0.24          |
| (1,1560) | 1:36:A:ILE:HG23 | 1:40:A:GLN:HG2  | 18       | 0.24          |
| (1,1560) | 1:36:A:ILE:HG23 | 1:40:A:GLN:HG3  | 18       | 0.24          |
| (1,1511) | 1:34:A:GLU:HG3  | 1:69:A:LEU:HD22 | 14       | 0.24          |
| (1,1294) | 1:27:A:LYS:HE2  | 1:52:A:ASP:HB3  | 14       | 0.24          |
| (1,1294) | 1:27:A:LYS:HE3  | 1:52:A:ASP:HB3  | 14       | 0.24          |
| (1,1294) | 1:27:A:LYS:HE2  | 1:52:A:ASP:HB3  | 15       | 0.24          |
| (1,1294) | 1:27:A:LYS:HE3  | 1:52:A:ASP:HB3  | 15       | 0.24          |
| (1,1294) | 1:27:A:LYS:HE2  | 1:52:A:ASP:HB3  | 19       | 0.24          |
| (1,1294) | 1:27:A:LYS:HE3  | 1:52:A:ASP:HB3  | 19       | 0.24          |
| (1,319)  | 1:5:A:VAL:HG11  | 1:7:A:THR:HG22  | 8        | 0.24          |
| (1,318)  | 1:5:A:VAL:HG11  | 1:7:A:THR:HG22  | 6        | 0.24          |
| (1,264)  | 1:4:A:PHE:HA    | 1:12:A:THR:HG21 | 11       | 0.24          |
| (1,264)  | 1:4:A:PHE:HA    | 1:12:A:THR:HG21 | 12       | 0.24          |
| (1,177)  | 1:29:A:LYS:HA   | 1:15:A:LEU:HD21 | 8        | 0.24          |
| (1,177)  | 1:29:A:LYS:HA   | 1:15:A:LEU:HD21 | 9        | 0.24          |
| (1,38)   | 1:1:A:MET:HE3   | 1:17:A:VAL:HG21 | 6        | 0.24          |
| (1,37)   | 1:1:A:MET:HE2   | 1:17:A:VAL:HG21 | 19       | 0.24          |
| (2,72)   | 1:27:A:LYS:HE3  | 1:69:A:LEU:HD13 | 9        | 0.23          |
| (2,7)    | 1:2:A:GLN:HG2   | 1:3:A:ILE:HA    | 6        | 0.23          |
| (1,1776) | 1:42:A:ARG:HG3  | 1:72:A:ARG:H    | 6        | 0.23          |
| (1,1511) | 1:34:A:GLU:HG3  | 1:69:A:LEU:HD23 | 3        | 0.23          |
| (1,1294) | 1:27:A:LYS:HE2  | 1:52:A:ASP:HB3  | 1        | 0.23          |
| (1,1294) | 1:27:A:LYS:HE3  | 1:52:A:ASP:HB3  | 1        | 0.23          |
| (1,1294) | 1:27:A:LYS:HE2  | 1:52:A:ASP:HB3  | 5        | 0.23          |
| (1,1294) | 1:27:A:LYS:HE3  | 1:52:A:ASP:HB3  | 5        | 0.23          |
| (1,1294) | 1:27:A:LYS:HE2  | 1:52:A:ASP:HB3  | 11       | 0.23          |
| (1,1294) | 1:27:A:LYS:HE3  | 1:52:A:ASP:HB3  | 11       | 0.23          |
| (1,1294) | 1:27:A:LYS:HE2  | 1:52:A:ASP:HB3  | 12       | 0.23          |
| (1,1294) | 1:27:A:LYS:HE3  | 1:52:A:ASP:HB3  | 12       | 0.23          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1294) | 1:27:A:LYS:HE2  | 1:52:A:ASP:HB3  | 13       | 0.23          |
| (1,1294) | 1:27:A:LYS:HE3  | 1:52:A:ASP:HB3  | 13       | 0.23          |
| (1,1294) | 1:27:A:LYS:HE2  | 1:52:A:ASP:HB3  | 16       | 0.23          |
| (1,1294) | 1:27:A:LYS:HE3  | 1:52:A:ASP:HB3  | 16       | 0.23          |
| (1,1294) | 1:27:A:LYS:HE2  | 1:52:A:ASP:HB3  | 17       | 0.23          |
| (1,1294) | 1:27:A:LYS:HE3  | 1:52:A:ASP:HB3  | 17       | 0.23          |
| (1,1294) | 1:27:A:LYS:HE2  | 1:52:A:ASP:HB3  | 18       | 0.23          |
| (1,1294) | 1:27:A:LYS:HE3  | 1:52:A:ASP:HB3  | 18       | 0.23          |
| (1,1294) | 1:27:A:LYS:HE2  | 1:52:A:ASP:HB3  | 20       | 0.23          |
| (1,1294) | 1:27:A:LYS:HE3  | 1:52:A:ASP:HB3  | 20       | 0.23          |
| (1,914)  | 1:52:A:ASP:HB2  | 1:24:A:GLU:HB3  | 3        | 0.23          |
| (1,458)  | 1:6:A:LYS:HD2   | 1:66:A:THR:HG21 | 1        | 0.23          |
| (1,457)  | 1:6:A:LYS:HD3   | 1:66:A:THR:HG21 | 13       | 0.23          |
| (1,439)  | 1:6:A:LYS:HD2   | 1:12:A:THR:HA   | 2        | 0.23          |
| (1,439)  | 1:6:A:LYS:HD3   | 1:12:A:THR:HA   | 2        | 0.23          |
| (1,339)  | 1:5:A:VAL:HG22  | 1:13:A:ILE:HG13 | 17       | 0.23          |
| (1,264)  | 1:4:A:PHE:HA    | 1:12:A:THR:HG22 | 6        | 0.23          |
| (1,177)  | 1:29:A:LYS:HA   | 1:15:A:LEU:HD21 | 14       | 0.23          |
| (2,7)    | 1:2:A:GLN:HG2   | 1:3:A:ILE:HA    | 1        | 0.22          |
| (2,7)    | 1:2:A:GLN:HG2   | 1:3:A:ILE:HA    | 8        | 0.22          |
| (2,7)    | 1:2:A:GLN:HG2   | 1:3:A:ILE:HA    | 9        | 0.22          |
| (2,7)    | 1:2:A:GLN:HG2   | 1:3:A:ILE:HA    | 11       | 0.22          |
| (2,7)    | 1:2:A:GLN:HG2   | 1:3:A:ILE:HA    | 12       | 0.22          |
| (2,7)    | 1:2:A:GLN:HG2   | 1:3:A:ILE:HA    | 14       | 0.22          |
| (2,7)    | 1:2:A:GLN:HG2   | 1:3:A:ILE:HA    | 16       | 0.22          |
| (2,7)    | 1:2:A:GLN:HG2   | 1:3:A:ILE:HA    | 18       | 0.22          |
| (1,1675) | 1:40:A:GLN:HA   | 1:72:A:ARG:HD2  | 7        | 0.22          |
| (1,1675) | 1:40:A:GLN:HA   | 1:72:A:ARG:HD2  | 9        | 0.22          |
| (1,1560) | 1:36:A:ILE:HG21 | 1:40:A:GLN:HG2  | 2        | 0.22          |
| (1,1560) | 1:36:A:ILE:HG21 | 1:40:A:GLN:HG3  | 2        | 0.22          |
| (1,1560) | 1:36:A:ILE:HG22 | 1:40:A:GLN:HG2  | 2        | 0.22          |
| (1,1560) | 1:36:A:ILE:HG22 | 1:40:A:GLN:HG3  | 2        | 0.22          |
| (1,1560) | 1:36:A:ILE:HG23 | 1:40:A:GLN:HG2  | 2        | 0.22          |
| (1,1560) | 1:36:A:ILE:HG23 | 1:40:A:GLN:HG3  | 2        | 0.22          |
| (1,1560) | 1:36:A:ILE:HG21 | 1:40:A:GLN:HG2  | 6        | 0.22          |
| (1,1560) | 1:36:A:ILE:HG21 | 1:40:A:GLN:HG3  | 6        | 0.22          |
| (1,1560) | 1:36:A:ILE:HG22 | 1:40:A:GLN:HG2  | 6        | 0.22          |
| (1,1560) | 1:36:A:ILE:HG22 | 1:40:A:GLN:HG3  | 6        | 0.22          |
| (1,1560) | 1:36:A:ILE:HG23 | 1:40:A:GLN:HG2  | 6        | 0.22          |
| (1,1560) | 1:36:A:ILE:HG23 | 1:40:A:GLN:HG3  | 6        | 0.22          |
| (1,1560) | 1:36:A:ILE:HG21 | 1:40:A:GLN:HG2  | 12       | 0.22          |
| (1,1560) | 1:36:A:ILE:HG21 | 1:40:A:GLN:HG3  | 12       | 0.22          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1560) | 1:36:A:ILE:HG22 | 1:40:A:GLN:HG2  | 12       | 0.22          |
| (1,1560) | 1:36:A:ILE:HG22 | 1:40:A:GLN:HG3  | 12       | 0.22          |
| (1,1560) | 1:36:A:ILE:HG23 | 1:40:A:GLN:HG2  | 12       | 0.22          |
| (1,1560) | 1:36:A:ILE:HG23 | 1:40:A:GLN:HG3  | 12       | 0.22          |
| (1,1560) | 1:36:A:ILE:HG21 | 1:40:A:GLN:HG2  | 15       | 0.22          |
| (1,1560) | 1:36:A:ILE:HG21 | 1:40:A:GLN:HG3  | 15       | 0.22          |
| (1,1560) | 1:36:A:ILE:HG22 | 1:40:A:GLN:HG2  | 15       | 0.22          |
| (1,1560) | 1:36:A:ILE:HG22 | 1:40:A:GLN:HG3  | 15       | 0.22          |
| (1,1560) | 1:36:A:ILE:HG23 | 1:40:A:GLN:HG2  | 15       | 0.22          |
| (1,1560) | 1:36:A:ILE:HG23 | 1:40:A:GLN:HG3  | 15       | 0.22          |
| (1,1560) | 1:36:A:ILE:HG21 | 1:40:A:GLN:HG2  | 16       | 0.22          |
| (1,1560) | 1:36:A:ILE:HG21 | 1:40:A:GLN:HG3  | 16       | 0.22          |
| (1,1560) | 1:36:A:ILE:HG22 | 1:40:A:GLN:HG2  | 16       | 0.22          |
| (1,1560) | 1:36:A:ILE:HG22 | 1:40:A:GLN:HG3  | 16       | 0.22          |
| (1,1560) | 1:36:A:ILE:HG23 | 1:40:A:GLN:HG2  | 16       | 0.22          |
| (1,1560) | 1:36:A:ILE:HG23 | 1:40:A:GLN:HG3  | 16       | 0.22          |
| (1,1560) | 1:36:A:ILE:HG21 | 1:40:A:GLN:HG2  | 19       | 0.22          |
| (1,1560) | 1:36:A:ILE:HG21 | 1:40:A:GLN:HG3  | 19       | 0.22          |
| (1,1560) | 1:36:A:ILE:HG22 | 1:40:A:GLN:HG2  | 19       | 0.22          |
| (1,1560) | 1:36:A:ILE:HG22 | 1:40:A:GLN:HG3  | 19       | 0.22          |
| (1,1560) | 1:36:A:ILE:HG23 | 1:40:A:GLN:HG2  | 19       | 0.22          |
| (1,1560) | 1:36:A:ILE:HG23 | 1:40:A:GLN:HG3  | 19       | 0.22          |
| (1,1511) | 1:34:A:GLU:HG3  | 1:69:A:LEU:HD21 | 10       | 0.22          |
| (1,1511) | 1:34:A:GLU:HG3  | 1:69:A:LEU:HD23 | 17       | 0.22          |
| (1,1294) | 1:27:A:LYS:HE2  | 1:52:A:ASP:HB3  | 2        | 0.22          |
| (1,1294) | 1:27:A:LYS:HE3  | 1:52:A:ASP:HB3  | 2        | 0.22          |
| (1,1294) | 1:27:A:LYS:HE2  | 1:52:A:ASP:HB3  | 3        | 0.22          |
| (1,1294) | 1:27:A:LYS:HE3  | 1:52:A:ASP:HB3  | 3        | 0.22          |
| (1,1294) | 1:27:A:LYS:HE2  | 1:52:A:ASP:HB3  | 6        | 0.22          |
| (1,1294) | 1:27:A:LYS:HE3  | 1:52:A:ASP:HB3  | 6        | 0.22          |
| (1,1294) | 1:27:A:LYS:HE2  | 1:52:A:ASP:HB3  | 9        | 0.22          |
| (1,1294) | 1:27:A:LYS:HE3  | 1:52:A:ASP:HB3  | 9        | 0.22          |
| (1,634)  | 1:13:A:ILE:HG12 | 1:30:A:ILE:HD11 | 8        | 0.22          |
| (1,634)  | 1:13:A:ILE:HG12 | 1:30:A:ILE:HD12 | 8        | 0.22          |
| (1,634)  | 1:13:A:ILE:HG12 | 1:30:A:ILE:HD13 | 8        | 0.22          |
| (1,634)  | 1:13:A:ILE:HG13 | 1:30:A:ILE:HD11 | 8        | 0.22          |
| (1,634)  | 1:13:A:ILE:HG13 | 1:30:A:ILE:HD12 | 8        | 0.22          |
| (1,634)  | 1:13:A:ILE:HG13 | 1:30:A:ILE:HD13 | 8        | 0.22          |
| (1,319)  | 1:5:A:VAL:HG12  | 1:7:A:THR:HG21  | 5        | 0.22          |
| (1,318)  | 1:5:A:VAL:HG12  | 1:7:A:THR:HG23  | 16       | 0.22          |
| (1,177)  | 1:29:A:LYS:HA   | 1:15:A:LEU:HD21 | 5        | 0.22          |
| (1,177)  | 1:29:A:LYS:HA   | 1:15:A:LEU:HD21 | 12       | 0.22          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,177)  | 1:29:A:LYS:HA   | 1:15:A:LEU:HD22 | 18       | 0.22          |
| (1,177)  | 1:29:A:LYS:HA   | 1:15:A:LEU:HD22 | 20       | 0.22          |
| (1,37)   | 1:1:A:MET:HE3   | 1:17:A:VAL:HG21 | 12       | 0.22          |
| (1,37)   | 1:1:A:MET:HE2   | 1:17:A:VAL:HG21 | 16       | 0.22          |
| (1,15)   | 1:1:A:MET:HB3   | 1:3:A:ILE:HG21  | 15       | 0.22          |
| (1,15)   | 1:1:A:MET:HB3   | 1:3:A:ILE:HG22  | 15       | 0.22          |
| (1,15)   | 1:1:A:MET:HB3   | 1:3:A:ILE:HG23  | 15       | 0.22          |
| (2,72)   | 1:27:A:LYS:HE3  | 1:69:A:LEU:HD13 | 12       | 0.21          |
| (2,72)   | 1:27:A:LYS:HE3  | 1:69:A:LEU:HD11 | 14       | 0.21          |
| (2,72)   | 1:27:A:LYS:HE3  | 1:69:A:LEU:HD13 | 18       | 0.21          |
| (2,7)    | 1:2:A:GLN:HG2   | 1:3:A:ILE:HA    | 4        | 0.21          |
| (2,7)    | 1:2:A:GLN:HG2   | 1:3:A:ILE:HA    | 5        | 0.21          |
| (2,7)    | 1:2:A:GLN:HG2   | 1:3:A:ILE:HA    | 13       | 0.21          |
| (2,7)    | 1:2:A:GLN:HG2   | 1:3:A:ILE:HA    | 15       | 0.21          |
| (2,7)    | 1:2:A:GLN:HG2   | 1:3:A:ILE:HA    | 19       | 0.21          |
| (1,1817) | 1:43:A:LEU:HD21 | 1:67:A:LEU:HB3  | 6        | 0.21          |
| (1,1692) | 1:40:A:GLN:HG2  | 1:73:A:LEU:HD12 | 16       | 0.21          |
| (1,1675) | 1:40:A:GLN:HA   | 1:72:A:ARG:HD3  | 10       | 0.21          |
| (1,1560) | 1:36:A:ILE:HG21 | 1:40:A:GLN:HG2  | 5        | 0.21          |
| (1,1560) | 1:36:A:ILE:HG21 | 1:40:A:GLN:HG3  | 5        | 0.21          |
| (1,1560) | 1:36:A:ILE:HG22 | 1:40:A:GLN:HG2  | 5        | 0.21          |
| (1,1560) | 1:36:A:ILE:HG22 | 1:40:A:GLN:HG3  | 5        | 0.21          |
| (1,1560) | 1:36:A:ILE:HG23 | 1:40:A:GLN:HG2  | 5        | 0.21          |
| (1,1560) | 1:36:A:ILE:HG23 | 1:40:A:GLN:HG3  | 5        | 0.21          |
| (1,1560) | 1:36:A:ILE:HG21 | 1:40:A:GLN:HG2  | 7        | 0.21          |
| (1,1560) | 1:36:A:ILE:HG21 | 1:40:A:GLN:HG3  | 7        | 0.21          |
| (1,1560) | 1:36:A:ILE:HG22 | 1:40:A:GLN:HG2  | 7        | 0.21          |
| (1,1560) | 1:36:A:ILE:HG22 | 1:40:A:GLN:HG3  | 7        | 0.21          |
| (1,1560) | 1:36:A:ILE:HG23 | 1:40:A:GLN:HG2  | 7        | 0.21          |
| (1,1560) | 1:36:A:ILE:HG23 | 1:40:A:GLN:HG3  | 7        | 0.21          |
| (1,1560) | 1:36:A:ILE:HG21 | 1:40:A:GLN:HG2  | 11       | 0.21          |
| (1,1560) | 1:36:A:ILE:HG21 | 1:40:A:GLN:HG3  | 11       | 0.21          |
| (1,1560) | 1:36:A:ILE:HG22 | 1:40:A:GLN:HG2  | 11       | 0.21          |
| (1,1560) | 1:36:A:ILE:HG22 | 1:40:A:GLN:HG3  | 11       | 0.21          |
| (1,1560) | 1:36:A:ILE:HG23 | 1:40:A:GLN:HG2  | 11       | 0.21          |
| (1,1560) | 1:36:A:ILE:HG23 | 1:40:A:GLN:HG3  | 11       | 0.21          |
| (1,1560) | 1:36:A:ILE:HG21 | 1:40:A:GLN:HG2  | 17       | 0.21          |
| (1,1560) | 1:36:A:ILE:HG21 | 1:40:A:GLN:HG3  | 17       | 0.21          |
| (1,1560) | 1:36:A:ILE:HG22 | 1:40:A:GLN:HG2  | 17       | 0.21          |
| (1,1560) | 1:36:A:ILE:HG22 | 1:40:A:GLN:HG3  | 17       | 0.21          |
| (1,1560) | 1:36:A:ILE:HG23 | 1:40:A:GLN:HG2  | 17       | 0.21          |
| (1,1560) | 1:36:A:ILE:HG23 | 1:40:A:GLN:HG3  | 17       | 0.21          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1512) | 1:34:A:GLU:HG3  | 1:69:A:LEU:HD21 | 20       | 0.21          |
| (1,1294) | 1:27:A:LYS:HE2  | 1:52:A:ASP:HB3  | 7        | 0.21          |
| (1,1294) | 1:27:A:LYS:HE3  | 1:52:A:ASP:HB3  | 7        | 0.21          |
| (1,1294) | 1:27:A:LYS:HE2  | 1:52:A:ASP:HB3  | 10       | 0.21          |
| (1,1294) | 1:27:A:LYS:HE3  | 1:52:A:ASP:HB3  | 10       | 0.21          |
| (1,356)  | 1:17:A:VAL:HG11 | 1:29:A:LYS:HG2  | 13       | 0.21          |
| (1,319)  | 1:5:A:VAL:HG11  | 1:7:A:THR:HG22  | 1        | 0.21          |
| (1,318)  | 1:5:A:VAL:HG11  | 1:7:A:THR:HG22  | 2        | 0.21          |
| (1,318)  | 1:5:A:VAL:HG11  | 1:7:A:THR:HG22  | 4        | 0.21          |
| (1,318)  | 1:5:A:VAL:HG11  | 1:7:A:THR:HG22  | 9        | 0.21          |
| (1,318)  | 1:5:A:VAL:HG11  | 1:7:A:THR:HG23  | 19       | 0.21          |
| (1,45)   | 1:1:A:MET:HE3   | 1:18:A:GLU:HA   | 14       | 0.21          |
| (1,15)   | 1:1:A:MET:HB3   | 1:3:A:ILE:HG21  | 1        | 0.21          |
| (1,15)   | 1:1:A:MET:HB3   | 1:3:A:ILE:HG22  | 1        | 0.21          |
| (1,15)   | 1:1:A:MET:HB3   | 1:3:A:ILE:HG23  | 1        | 0.21          |
| (1,15)   | 1:1:A:MET:HB3   | 1:3:A:ILE:HG21  | 5        | 0.21          |
| (1,15)   | 1:1:A:MET:HB3   | 1:3:A:ILE:HG22  | 5        | 0.21          |
| (1,15)   | 1:1:A:MET:HB3   | 1:3:A:ILE:HG23  | 5        | 0.21          |
| (1,15)   | 1:1:A:MET:HB3   | 1:3:A:ILE:HG21  | 6        | 0.21          |
| (1,15)   | 1:1:A:MET:HB3   | 1:3:A:ILE:HG22  | 6        | 0.21          |
| (1,15)   | 1:1:A:MET:HB3   | 1:3:A:ILE:HG23  | 6        | 0.21          |
| (1,15)   | 1:1:A:MET:HB3   | 1:3:A:ILE:HG21  | 8        | 0.21          |
| (1,15)   | 1:1:A:MET:HB3   | 1:3:A:ILE:HG22  | 8        | 0.21          |
| (1,15)   | 1:1:A:MET:HB3   | 1:3:A:ILE:HG23  | 8        | 0.21          |
| (1,15)   | 1:1:A:MET:HB3   | 1:3:A:ILE:HG21  | 9        | 0.21          |
| (1,15)   | 1:1:A:MET:HB3   | 1:3:A:ILE:HG22  | 9        | 0.21          |
| (1,15)   | 1:1:A:MET:HB3   | 1:3:A:ILE:HG23  | 9        | 0.21          |
| (1,15)   | 1:1:A:MET:HB3   | 1:3:A:ILE:HG21  | 11       | 0.21          |
| (1,15)   | 1:1:A:MET:HB3   | 1:3:A:ILE:HG22  | 11       | 0.21          |
| (1,15)   | 1:1:A:MET:HB3   | 1:3:A:ILE:HG23  | 11       | 0.21          |
| (1,15)   | 1:1:A:MET:HB3   | 1:3:A:ILE:HG21  | 12       | 0.21          |
| (1,15)   | 1:1:A:MET:HB3   | 1:3:A:ILE:HG22  | 12       | 0.21          |
| (1,15)   | 1:1:A:MET:HB3   | 1:3:A:ILE:HG23  | 12       | 0.21          |
| (1,15)   | 1:1:A:MET:HB3   | 1:3:A:ILE:HG21  | 13       | 0.21          |
| (1,15)   | 1:1:A:MET:HB3   | 1:3:A:ILE:HG22  | 13       | 0.21          |
| (1,15)   | 1:1:A:MET:HB3   | 1:3:A:ILE:HG23  | 13       | 0.21          |
| (1,15)   | 1:1:A:MET:HB3   | 1:3:A:ILE:HG21  | 14       | 0.21          |
| (1,15)   | 1:1:A:MET:HB3   | 1:3:A:ILE:HG22  | 14       | 0.21          |
| (1,15)   | 1:1:A:MET:HB3   | 1:3:A:ILE:HG23  | 14       | 0.21          |
| (1,15)   | 1:1:A:MET:HB3   | 1:3:A:ILE:HG21  | 17       | 0.21          |
| (1,15)   | 1:1:A:MET:HB3   | 1:3:A:ILE:HG22  | 17       | 0.21          |
| (1,15)   | 1:1:A:MET:HB3   | 1:3:A:ILE:HG23  | 17       | 0.21          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,15)   | 1:1:A:MET:HB3   | 1:3:A:ILE:HG21  | 19       | 0.21          |
| (1,15)   | 1:1:A:MET:HB3   | 1:3:A:ILE:HG22  | 19       | 0.21          |
| (1,15)   | 1:1:A:MET:HB3   | 1:3:A:ILE:HG23  | 19       | 0.21          |
| (2,72)   | 1:27:A:LYS:HE3  | 1:69:A:LEU:HD11 | 20       | 0.2           |
| (2,7)    | 1:2:A:GLN:HG2   | 1:3:A:ILE:HA    | 2        | 0.2           |
| (2,7)    | 1:2:A:GLN:HG2   | 1:3:A:ILE:HA    | 3        | 0.2           |
| (2,7)    | 1:2:A:GLN:HG2   | 1:3:A:ILE:HA    | 17       | 0.2           |
| (2,7)    | 1:2:A:GLN:HG2   | 1:3:A:ILE:HA    | 20       | 0.2           |
| (1,1560) | 1:36:A:ILE:HG21 | 1:40:A:GLN:HG2  | 1        | 0.2           |
| (1,1560) | 1:36:A:ILE:HG21 | 1:40:A:GLN:HG3  | 1        | 0.2           |
| (1,1560) | 1:36:A:ILE:HG22 | 1:40:A:GLN:HG2  | 1        | 0.2           |
| (1,1560) | 1:36:A:ILE:HG22 | 1:40:A:GLN:HG3  | 1        | 0.2           |
| (1,1560) | 1:36:A:ILE:HG23 | 1:40:A:GLN:HG2  | 1        | 0.2           |
| (1,1560) | 1:36:A:ILE:HG23 | 1:40:A:GLN:HG3  | 1        | 0.2           |
| (1,1560) | 1:36:A:ILE:HG21 | 1:40:A:GLN:HG2  | 4        | 0.2           |
| (1,1560) | 1:36:A:ILE:HG21 | 1:40:A:GLN:HG3  | 4        | 0.2           |
| (1,1560) | 1:36:A:ILE:HG22 | 1:40:A:GLN:HG2  | 4        | 0.2           |
| (1,1560) | 1:36:A:ILE:HG22 | 1:40:A:GLN:HG3  | 4        | 0.2           |
| (1,1560) | 1:36:A:ILE:HG23 | 1:40:A:GLN:HG2  | 4        | 0.2           |
| (1,1560) | 1:36:A:ILE:HG23 | 1:40:A:GLN:HG3  | 4        | 0.2           |
| (1,1560) | 1:36:A:ILE:HG21 | 1:40:A:GLN:HG2  | 8        | 0.2           |
| (1,1560) | 1:36:A:ILE:HG21 | 1:40:A:GLN:HG3  | 8        | 0.2           |
| (1,1560) | 1:36:A:ILE:HG22 | 1:40:A:GLN:HG2  | 8        | 0.2           |
| (1,1560) | 1:36:A:ILE:HG22 | 1:40:A:GLN:HG3  | 8        | 0.2           |
| (1,1560) | 1:36:A:ILE:HG23 | 1:40:A:GLN:HG2  | 8        | 0.2           |
| (1,1560) | 1:36:A:ILE:HG23 | 1:40:A:GLN:HG3  | 8        | 0.2           |
| (1,1560) | 1:36:A:ILE:HG21 | 1:40:A:GLN:HG2  | 14       | 0.2           |
| (1,1560) | 1:36:A:ILE:HG21 | 1:40:A:GLN:HG3  | 14       | 0.2           |
| (1,1560) | 1:36:A:ILE:HG22 | 1:40:A:GLN:HG2  | 14       | 0.2           |
| (1,1560) | 1:36:A:ILE:HG22 | 1:40:A:GLN:HG3  | 14       | 0.2           |
| (1,1560) | 1:36:A:ILE:HG23 | 1:40:A:GLN:HG2  | 14       | 0.2           |
| (1,1560) | 1:36:A:ILE:HG23 | 1:40:A:GLN:HG3  | 14       | 0.2           |
| (1,1511) | 1:34:A:GLU:HG3  | 1:69:A:LEU:HD22 | 19       | 0.2           |
| (1,865)  | 1:19:A:PRO:HA   | 1:56:A:LEU:HA   | 11       | 0.2           |
| (1,634)  | 1:13:A:ILE:HG12 | 1:30:A:ILE:HD11 | 15       | 0.2           |
| (1,634)  | 1:13:A:ILE:HG12 | 1:30:A:ILE:HD12 | 15       | 0.2           |
| (1,634)  | 1:13:A:ILE:HG12 | 1:30:A:ILE:HD13 | 15       | 0.2           |
| (1,634)  | 1:13:A:ILE:HG13 | 1:30:A:ILE:HD11 | 15       | 0.2           |
| (1,634)  | 1:13:A:ILE:HG13 | 1:30:A:ILE:HD12 | 15       | 0.2           |
| (1,634)  | 1:13:A:ILE:HG13 | 1:30:A:ILE:HD13 | 15       | 0.2           |
| (1,386)  | 1:5:A:VAL:HG11  | 1:69:A:LEU:HG   | 9        | 0.2           |
| (1,386)  | 1:5:A:VAL:HG12  | 1:69:A:LEU:HG   | 9        | 0.2           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,386)  | 1:5:A:VAL:HG13  | 1:69:A:LEU:HG   | 9        | 0.2           |
| (1,386)  | 1:5:A:VAL:HG11  | 1:69:A:LEU:HG   | 13       | 0.2           |
| (1,386)  | 1:5:A:VAL:HG12  | 1:69:A:LEU:HG   | 13       | 0.2           |
| (1,386)  | 1:5:A:VAL:HG13  | 1:69:A:LEU:HG   | 13       | 0.2           |
| (1,356)  | 1:17:A:VAL:HG13 | 1:29:A:LYS:HG3  | 15       | 0.2           |
| (1,318)  | 1:5:A:VAL:HG11  | 1:7:A:THR:HG22  | 3        | 0.2           |
| (1,269)  | 1:4:A:PHE:HB2   | 1:12:A:THR:HG21 | 20       | 0.2           |
| (1,269)  | 1:4:A:PHE:HB2   | 1:12:A:THR:HG22 | 20       | 0.2           |
| (1,269)  | 1:4:A:PHE:HB2   | 1:12:A:THR:HG23 | 20       | 0.2           |
| (1,264)  | 1:4:A:PHE:HA    | 1:12:A:THR:HG23 | 18       | 0.2           |
| (1,177)  | 1:29:A:LYS:HA   | 1:15:A:LEU:HD22 | 1        | 0.2           |
| (1,177)  | 1:29:A:LYS:HA   | 1:15:A:LEU:HD22 | 2        | 0.2           |
| (1,97)   | 1:1:A:MET:HG3   | 1:63:A:LYS:HA   | 12       | 0.2           |
| (1,38)   | 1:1:A:MET:HE3   | 1:17:A:VAL:HG23 | 20       | 0.2           |
| (1,15)   | 1:1:A:MET:HB3   | 1:3:A:ILE:HG21  | 2        | 0.2           |
| (1,15)   | 1:1:A:MET:HB3   | 1:3:A:ILE:HG22  | 2        | 0.2           |
| (1,15)   | 1:1:A:MET:HB3   | 1:3:A:ILE:HG23  | 2        | 0.2           |
| (1,15)   | 1:1:A:MET:HB3   | 1:3:A:ILE:HG21  | 3        | 0.2           |
| (1,15)   | 1:1:A:MET:HB3   | 1:3:A:ILE:HG22  | 3        | 0.2           |
| (1,15)   | 1:1:A:MET:HB3   | 1:3:A:ILE:HG23  | 3        | 0.2           |
| (1,15)   | 1:1:A:MET:HB3   | 1:3:A:ILE:HG21  | 4        | 0.2           |
| (1,15)   | 1:1:A:MET:HB3   | 1:3:A:ILE:HG22  | 4        | 0.2           |
| (1,15)   | 1:1:A:MET:HB3   | 1:3:A:ILE:HG23  | 4        | 0.2           |
| (1,15)   | 1:1:A:MET:HB3   | 1:3:A:ILE:HG21  | 7        | 0.2           |
| (1,15)   | 1:1:A:MET:HB3   | 1:3:A:ILE:HG22  | 7        | 0.2           |
| (1,15)   | 1:1:A:MET:HB3   | 1:3:A:ILE:HG23  | 7        | 0.2           |
| (1,15)   | 1:1:A:MET:HB3   | 1:3:A:ILE:HG21  | 10       | 0.2           |
| (1,15)   | 1:1:A:MET:HB3   | 1:3:A:ILE:HG22  | 10       | 0.2           |
| (1,15)   | 1:1:A:MET:HB3   | 1:3:A:ILE:HG23  | 10       | 0.2           |
| (1,15)   | 1:1:A:MET:HB3   | 1:3:A:ILE:HG21  | 16       | 0.2           |
| (1,15)   | 1:1:A:MET:HB3   | 1:3:A:ILE:HG22  | 16       | 0.2           |
| (1,15)   | 1:1:A:MET:HB3   | 1:3:A:ILE:HG23  | 16       | 0.2           |
| (1,15)   | 1:1:A:MET:HB3   | 1:3:A:ILE:HG21  | 18       | 0.2           |
| (1,15)   | 1:1:A:MET:HB3   | 1:3:A:ILE:HG22  | 18       | 0.2           |
| (1,15)   | 1:1:A:MET:HB3   | 1:3:A:ILE:HG23  | 18       | 0.2           |
| (2,72)   | 1:27:A:LYS:HE3  | 1:69:A:LEU:HD11 | 13       | 0.19          |
| (2,7)    | 1:2:A:GLN:HG2   | 1:3:A:ILE:HA    | 7        | 0.19          |
| (2,7)    | 1:2:A:GLN:HG2   | 1:3:A:ILE:HA    | 10       | 0.19          |
| (1,1887) | 1:44:A:ILE:HD13 | 1:70:A:VAL:HG13 | 15       | 0.19          |
| (1,1861) | 1:44:A:ILE:HD11 | 1:49:A:GLN:HA   | 1        | 0.19          |
| (1,1861) | 1:44:A:ILE:HD12 | 1:49:A:GLN:HA   | 1        | 0.19          |
| (1,1861) | 1:44:A:ILE:HD13 | 1:49:A:GLN:HA   | 1        | 0.19          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1861) | 1:44:A:ILE:HD11 | 1:49:A:GLN:HA   | 4        | 0.19          |
| (1,1861) | 1:44:A:ILE:HD12 | 1:49:A:GLN:HA   | 4        | 0.19          |
| (1,1861) | 1:44:A:ILE:HD13 | 1:49:A:GLN:HA   | 4        | 0.19          |
| (1,1861) | 1:44:A:ILE:HD11 | 1:49:A:GLN:HA   | 6        | 0.19          |
| (1,1861) | 1:44:A:ILE:HD12 | 1:49:A:GLN:HA   | 6        | 0.19          |
| (1,1861) | 1:44:A:ILE:HD13 | 1:49:A:GLN:HA   | 6        | 0.19          |
| (1,1861) | 1:44:A:ILE:HD11 | 1:49:A:GLN:HA   | 7        | 0.19          |
| (1,1861) | 1:44:A:ILE:HD12 | 1:49:A:GLN:HA   | 7        | 0.19          |
| (1,1861) | 1:44:A:ILE:HD13 | 1:49:A:GLN:HA   | 7        | 0.19          |
| (1,1861) | 1:44:A:ILE:HD11 | 1:49:A:GLN:HA   | 9        | 0.19          |
| (1,1861) | 1:44:A:ILE:HD12 | 1:49:A:GLN:HA   | 9        | 0.19          |
| (1,1861) | 1:44:A:ILE:HD13 | 1:49:A:GLN:HA   | 9        | 0.19          |
| (1,1861) | 1:44:A:ILE:HD11 | 1:49:A:GLN:HA   | 12       | 0.19          |
| (1,1861) | 1:44:A:ILE:HD12 | 1:49:A:GLN:HA   | 12       | 0.19          |
| (1,1861) | 1:44:A:ILE:HD13 | 1:49:A:GLN:HA   | 12       | 0.19          |
| (1,1817) | 1:43:A:LEU:HD23 | 1:67:A:LEU:HB3  | 19       | 0.19          |
| (1,1696) | 1:40:A:GLN:HG2  | 1:74:A:ARG:HG3  | 8        | 0.19          |
| (1,1675) | 1:40:A:GLN:HA   | 1:72:A:ARG:HD2  | 17       | 0.19          |
| (1,1560) | 1:36:A:ILE:HG21 | 1:40:A:GLN:HG2  | 3        | 0.19          |
| (1,1560) | 1:36:A:ILE:HG21 | 1:40:A:GLN:HG3  | 3        | 0.19          |
| (1,1560) | 1:36:A:ILE:HG22 | 1:40:A:GLN:HG2  | 3        | 0.19          |
| (1,1560) | 1:36:A:ILE:HG22 | 1:40:A:GLN:HG3  | 3        | 0.19          |
| (1,1560) | 1:36:A:ILE:HG23 | 1:40:A:GLN:HG2  | 3        | 0.19          |
| (1,1560) | 1:36:A:ILE:HG23 | 1:40:A:GLN:HG3  | 3        | 0.19          |
| (1,1560) | 1:36:A:ILE:HG21 | 1:40:A:GLN:HG2  | 10       | 0.19          |
| (1,1560) | 1:36:A:ILE:HG21 | 1:40:A:GLN:HG3  | 10       | 0.19          |
| (1,1560) | 1:36:A:ILE:HG22 | 1:40:A:GLN:HG2  | 10       | 0.19          |
| (1,1560) | 1:36:A:ILE:HG22 | 1:40:A:GLN:HG3  | 10       | 0.19          |
| (1,1560) | 1:36:A:ILE:HG23 | 1:40:A:GLN:HG2  | 10       | 0.19          |
| (1,1560) | 1:36:A:ILE:HG23 | 1:40:A:GLN:HG3  | 10       | 0.19          |
| (1,1511) | 1:34:A:GLU:HG3  | 1:69:A:LEU:HD23 | 7        | 0.19          |
| (1,865)  | 1:19:A:PRO:HA   | 1:56:A:LEU:HA   | 1        | 0.19          |
| (1,865)  | 1:19:A:PRO:HA   | 1:56:A:LEU:HA   | 6        | 0.19          |
| (1,865)  | 1:19:A:PRO:HA   | 1:56:A:LEU:HA   | 16       | 0.19          |
| (1,865)  | 1:19:A:PRO:HA   | 1:56:A:LEU:HA   | 17       | 0.19          |
| (1,865)  | 1:19:A:PRO:HA   | 1:56:A:LEU:HA   | 18       | 0.19          |
| (1,604)  | 1:14:A:THR:HG22 | 1:14:A:THR:H    | 9        | 0.19          |
| (1,386)  | 1:5:A:VAL:HG11  | 1:69:A:LEU:HG   | 4        | 0.19          |
| (1,386)  | 1:5:A:VAL:HG12  | 1:69:A:LEU:HG   | 4        | 0.19          |
| (1,386)  | 1:5:A:VAL:HG13  | 1:69:A:LEU:HG   | 4        | 0.19          |
| (1,386)  | 1:5:A:VAL:HG11  | 1:69:A:LEU:HG   | 7        | 0.19          |
| (1,386)  | 1:5:A:VAL:HG12  | 1:69:A:LEU:HG   | 7        | 0.19          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,386)  | 1:5:A:VAL:HG13  | 1:69:A:LEU:HG   | 7        | 0.19          |
| (1,386)  | 1:5:A:VAL:HG11  | 1:69:A:LEU:HG   | 15       | 0.19          |
| (1,386)  | 1:5:A:VAL:HG12  | 1:69:A:LEU:HG   | 15       | 0.19          |
| (1,386)  | 1:5:A:VAL:HG13  | 1:69:A:LEU:HG   | 15       | 0.19          |
| (1,386)  | 1:5:A:VAL:HG11  | 1:69:A:LEU:HG   | 17       | 0.19          |
| (1,386)  | 1:5:A:VAL:HG12  | 1:69:A:LEU:HG   | 17       | 0.19          |
| (1,386)  | 1:5:A:VAL:HG13  | 1:69:A:LEU:HG   | 17       | 0.19          |
| (1,318)  | 1:5:A:VAL:HG12  | 1:7:A:THR:HG23  | 17       | 0.19          |
| (1,318)  | 1:5:A:VAL:HG13  | 1:7:A:THR:HG23  | 18       | 0.19          |
| (1,269)  | 1:4:A:PHE:HB2   | 1:12:A:THR:HG21 | 2        | 0.19          |
| (1,269)  | 1:4:A:PHE:HB2   | 1:12:A:THR:HG22 | 2        | 0.19          |
| (1,269)  | 1:4:A:PHE:HB2   | 1:12:A:THR:HG23 | 2        | 0.19          |
| (1,269)  | 1:4:A:PHE:HB2   | 1:12:A:THR:HG21 | 7        | 0.19          |
| (1,269)  | 1:4:A:PHE:HB2   | 1:12:A:THR:HG22 | 7        | 0.19          |
| (1,269)  | 1:4:A:PHE:HB2   | 1:12:A:THR:HG23 | 7        | 0.19          |
| (1,269)  | 1:4:A:PHE:HB2   | 1:12:A:THR:HG21 | 10       | 0.19          |
| (1,269)  | 1:4:A:PHE:HB2   | 1:12:A:THR:HG22 | 10       | 0.19          |
| (1,269)  | 1:4:A:PHE:HB2   | 1:12:A:THR:HG23 | 10       | 0.19          |
| (1,264)  | 1:4:A:PHE:HA    | 1:14:A:THR:HG21 | 4        | 0.19          |
| (1,177)  | 1:29:A:LYS:HA   | 1:15:A:LEU:HD22 | 19       | 0.19          |
| (1,148)  | 1:68:A:HIS:HA   | 1:66:A:THR:HG23 | 13       | 0.19          |
| (1,97)   | 1:1:A:MET:HG3   | 1:63:A:LYS:HA   | 3        | 0.19          |
| (1,97)   | 1:1:A:MET:HG3   | 1:63:A:LYS:HA   | 13       | 0.19          |
| (1,97)   | 1:1:A:MET:HG3   | 1:63:A:LYS:HA   | 16       | 0.19          |
| (1,97)   | 1:1:A:MET:HG3   | 1:63:A:LYS:HA   | 18       | 0.19          |
| (1,45)   | 1:1:A:MET:HE3   | 1:18:A:GLU:HA   | 19       | 0.19          |
| (1,37)   | 1:1:A:MET:HE2   | 1:17:A:VAL:HG21 | 14       | 0.19          |
| (1,15)   | 1:1:A:MET:HB3   | 1:3:A:ILE:HG21  | 20       | 0.19          |
| (1,15)   | 1:1:A:MET:HB3   | 1:3:A:ILE:HG22  | 20       | 0.19          |
| (1,15)   | 1:1:A:MET:HB3   | 1:3:A:ILE:HG23  | 20       | 0.19          |
| (2,72)   | 1:27:A:LYS:HE3  | 1:69:A:LEU:HD13 | 11       | 0.18          |
| (2,35)   | 1:34:A:GLU:HG3  | 1:30:A:ILE:HD13 | 8        | 0.18          |
| (1,2564) | 1:72:A:ARG:HA   | 1:72:A:ARG:HD2  | 2        | 0.18          |
| (1,2564) | 1:72:A:ARG:HA   | 1:72:A:ARG:HD3  | 2        | 0.18          |
| (1,2028) | 1:48:A:LYS:HG2  | 1:48:A:LYS:HA   | 4        | 0.18          |
| (1,2028) | 1:48:A:LYS:HG3  | 1:48:A:LYS:HA   | 4        | 0.18          |
| (1,2028) | 1:48:A:LYS:HG2  | 1:48:A:LYS:HA   | 7        | 0.18          |
| (1,2028) | 1:48:A:LYS:HG3  | 1:48:A:LYS:HA   | 7        | 0.18          |
| (1,2028) | 1:48:A:LYS:HG2  | 1:48:A:LYS:HA   | 9        | 0.18          |
| (1,2028) | 1:48:A:LYS:HG3  | 1:48:A:LYS:HA   | 9        | 0.18          |
| (1,1887) | 1:44:A:ILE:HD13 | 1:70:A:VAL:HG13 | 16       | 0.18          |
| (1,1869) | 1:44:A:ILE:HG12 | 1:49:A:GLN:HA   | 14       | 0.18          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1869) | 1:44:A:ILE:HG13 | 1:49:A:GLN:HA   | 14       | 0.18          |
| (1,1861) | 1:44:A:ILE:HD11 | 1:49:A:GLN:HA   | 2        | 0.18          |
| (1,1861) | 1:44:A:ILE:HD12 | 1:49:A:GLN:HA   | 2        | 0.18          |
| (1,1861) | 1:44:A:ILE:HD13 | 1:49:A:GLN:HA   | 2        | 0.18          |
| (1,1861) | 1:44:A:ILE:HD11 | 1:49:A:GLN:HA   | 17       | 0.18          |
| (1,1861) | 1:44:A:ILE:HD12 | 1:49:A:GLN:HA   | 17       | 0.18          |
| (1,1861) | 1:44:A:ILE:HD13 | 1:49:A:GLN:HA   | 17       | 0.18          |
| (1,1861) | 1:44:A:ILE:HD11 | 1:49:A:GLN:HA   | 20       | 0.18          |
| (1,1861) | 1:44:A:ILE:HD12 | 1:49:A:GLN:HA   | 20       | 0.18          |
| (1,1861) | 1:44:A:ILE:HD13 | 1:49:A:GLN:HA   | 20       | 0.18          |
| (1,1817) | 1:43:A:LEU:HD22 | 1:67:A:LEU:HB3  | 9        | 0.18          |
| (1,1817) | 1:43:A:LEU:HD21 | 1:67:A:LEU:HB3  | 15       | 0.18          |
| (1,1511) | 1:34:A:GLU:HG3  | 1:69:A:LEU:HD23 | 11       | 0.18          |
| (1,1350) | 1:30:A:ILE:HA   | 1:30:A:ILE:HD11 | 8        | 0.18          |
| (1,1350) | 1:30:A:ILE:HA   | 1:30:A:ILE:HD12 | 8        | 0.18          |
| (1,1350) | 1:30:A:ILE:HA   | 1:30:A:ILE:HD13 | 8        | 0.18          |
| (1,865)  | 1:19:A:PRO:HA   | 1:56:A:LEU:HA   | 2        | 0.18          |
| (1,865)  | 1:19:A:PRO:HA   | 1:56:A:LEU:HA   | 5        | 0.18          |
| (1,865)  | 1:19:A:PRO:HA   | 1:56:A:LEU:HA   | 8        | 0.18          |
| (1,865)  | 1:19:A:PRO:HA   | 1:56:A:LEU:HA   | 12       | 0.18          |
| (1,604)  | 1:14:A:THR:HG23 | 1:14:A:THR:H    | 17       | 0.18          |
| (1,604)  | 1:14:A:THR:HG23 | 1:14:A:THR:H    | 20       | 0.18          |
| (1,386)  | 1:5:A:VAL:HG11  | 1:69:A:LEU:HG   | 2        | 0.18          |
| (1,386)  | 1:5:A:VAL:HG12  | 1:69:A:LEU:HG   | 2        | 0.18          |
| (1,386)  | 1:5:A:VAL:HG13  | 1:69:A:LEU:HG   | 2        | 0.18          |
| (1,386)  | 1:5:A:VAL:HG11  | 1:69:A:LEU:HG   | 3        | 0.18          |
| (1,386)  | 1:5:A:VAL:HG12  | 1:69:A:LEU:HG   | 3        | 0.18          |
| (1,386)  | 1:5:A:VAL:HG13  | 1:69:A:LEU:HG   | 3        | 0.18          |
| (1,386)  | 1:5:A:VAL:HG11  | 1:69:A:LEU:HG   | 6        | 0.18          |
| (1,386)  | 1:5:A:VAL:HG12  | 1:69:A:LEU:HG   | 6        | 0.18          |
| (1,386)  | 1:5:A:VAL:HG13  | 1:69:A:LEU:HG   | 6        | 0.18          |
| (1,386)  | 1:5:A:VAL:HG11  | 1:69:A:LEU:HG   | 8        | 0.18          |
| (1,386)  | 1:5:A:VAL:HG12  | 1:69:A:LEU:HG   | 8        | 0.18          |
| (1,386)  | 1:5:A:VAL:HG13  | 1:69:A:LEU:HG   | 8        | 0.18          |
| (1,386)  | 1:5:A:VAL:HG11  | 1:69:A:LEU:HG   | 10       | 0.18          |
| (1,386)  | 1:5:A:VAL:HG12  | 1:69:A:LEU:HG   | 10       | 0.18          |
| (1,386)  | 1:5:A:VAL:HG13  | 1:69:A:LEU:HG   | 10       | 0.18          |
| (1,386)  | 1:5:A:VAL:HG11  | 1:69:A:LEU:HG   | 11       | 0.18          |
| (1,386)  | 1:5:A:VAL:HG12  | 1:69:A:LEU:HG   | 11       | 0.18          |
| (1,386)  | 1:5:A:VAL:HG13  | 1:69:A:LEU:HG   | 11       | 0.18          |
| (1,386)  | 1:5:A:VAL:HG11  | 1:69:A:LEU:HG   | 20       | 0.18          |
| (1,386)  | 1:5:A:VAL:HG12  | 1:69:A:LEU:HG   | 20       | 0.18          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,386)  | 1:5:A:VAL:HG13  | 1:69:A:LEU:HG   | 20       | 0.18          |
| (1,341)  | 1:5:A:VAL:HG23  | 1:13:A:ILE:HG13 | 20       | 0.18          |
| (1,318)  | 1:5:A:VAL:HG13  | 1:7:A:THR:HG23  | 14       | 0.18          |
| (1,264)  | 1:4:A:PHE:HA    | 1:12:A:THR:HG23 | 16       | 0.18          |
| (1,177)  | 1:29:A:LYS:HA   | 1:15:A:LEU:HD22 | 11       | 0.18          |
| (1,148)  | 1:68:A:HIS:HA   | 1:66:A:THR:HG23 | 15       | 0.18          |
| (1,148)  | 1:68:A:HIS:HA   | 1:66:A:THR:HG23 | 17       | 0.18          |
| (1,148)  | 1:68:A:HIS:HA   | 1:66:A:THR:HG23 | 18       | 0.18          |
| (1,97)   | 1:1:A:MET:HG3   | 1:63:A:LYS:HA   | 5        | 0.18          |
| (1,97)   | 1:1:A:MET:HG3   | 1:63:A:LYS:HA   | 6        | 0.18          |
| (1,97)   | 1:1:A:MET:HG3   | 1:63:A:LYS:HA   | 8        | 0.18          |
| (1,97)   | 1:1:A:MET:HG3   | 1:63:A:LYS:HA   | 14       | 0.18          |
| (1,97)   | 1:1:A:MET:HG3   | 1:63:A:LYS:HA   | 15       | 0.18          |
| (1,97)   | 1:1:A:MET:HG3   | 1:63:A:LYS:HA   | 19       | 0.18          |
| (1,97)   | 1:1:A:MET:HG3   | 1:63:A:LYS:HA   | 20       | 0.18          |
| (1,45)   | 1:1:A:MET:HE3   | 1:18:A:GLU:HA   | 1        | 0.18          |
| (2,72)   | 1:27:A:LYS:HE3  | 1:69:A:LEU:HD12 | 17       | 0.17          |
| (1,1916) | 1:44:A:ILE:HD11 | 1:70:A:VAL:HG21 | 3        | 0.17          |
| (1,1916) | 1:44:A:ILE:HD11 | 1:70:A:VAL:HG22 | 3        | 0.17          |
| (1,1916) | 1:44:A:ILE:HD11 | 1:70:A:VAL:HG23 | 3        | 0.17          |
| (1,1916) | 1:44:A:ILE:HD12 | 1:70:A:VAL:HG21 | 3        | 0.17          |
| (1,1916) | 1:44:A:ILE:HD12 | 1:70:A:VAL:HG22 | 3        | 0.17          |
| (1,1916) | 1:44:A:ILE:HD12 | 1:70:A:VAL:HG23 | 3        | 0.17          |
| (1,1916) | 1:44:A:ILE:HD13 | 1:70:A:VAL:HG21 | 3        | 0.17          |
| (1,1916) | 1:44:A:ILE:HD13 | 1:70:A:VAL:HG22 | 3        | 0.17          |
| (1,1916) | 1:44:A:ILE:HD13 | 1:70:A:VAL:HG23 | 3        | 0.17          |
| (1,1916) | 1:44:A:ILE:HD11 | 1:70:A:VAL:HG21 | 13       | 0.17          |
| (1,1916) | 1:44:A:ILE:HD11 | 1:70:A:VAL:HG22 | 13       | 0.17          |
| (1,1916) | 1:44:A:ILE:HD11 | 1:70:A:VAL:HG23 | 13       | 0.17          |
| (1,1916) | 1:44:A:ILE:HD12 | 1:70:A:VAL:HG21 | 13       | 0.17          |
| (1,1916) | 1:44:A:ILE:HD12 | 1:70:A:VAL:HG22 | 13       | 0.17          |
| (1,1916) | 1:44:A:ILE:HD12 | 1:70:A:VAL:HG23 | 13       | 0.17          |
| (1,1916) | 1:44:A:ILE:HD13 | 1:70:A:VAL:HG21 | 13       | 0.17          |
| (1,1916) | 1:44:A:ILE:HD13 | 1:70:A:VAL:HG22 | 13       | 0.17          |
| (1,1916) | 1:44:A:ILE:HD13 | 1:70:A:VAL:HG23 | 13       | 0.17          |
| (1,1916) | 1:44:A:ILE:HD11 | 1:70:A:VAL:HG21 | 14       | 0.17          |
| (1,1916) | 1:44:A:ILE:HD11 | 1:70:A:VAL:HG22 | 14       | 0.17          |
| (1,1916) | 1:44:A:ILE:HD11 | 1:70:A:VAL:HG23 | 14       | 0.17          |
| (1,1916) | 1:44:A:ILE:HD12 | 1:70:A:VAL:HG21 | 14       | 0.17          |
| (1,1916) | 1:44:A:ILE:HD12 | 1:70:A:VAL:HG22 | 14       | 0.17          |
| (1,1916) | 1:44:A:ILE:HD12 | 1:70:A:VAL:HG23 | 14       | 0.17          |
| (1,1916) | 1:44:A:ILE:HD13 | 1:70:A:VAL:HG21 | 14       | 0.17          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1916) | 1:44:A:ILE:HD13 | 1:70:A:VAL:HG22 | 14       | 0.17          |
| (1,1916) | 1:44:A:ILE:HD13 | 1:70:A:VAL:HG23 | 14       | 0.17          |
| (1,1869) | 1:44:A:ILE:HG12 | 1:49:A:GLN:HA   | 10       | 0.17          |
| (1,1869) | 1:44:A:ILE:HG13 | 1:49:A:GLN:HA   | 10       | 0.17          |
| (1,1861) | 1:44:A:ILE:HD11 | 1:49:A:GLN:HA   | 5        | 0.17          |
| (1,1861) | 1:44:A:ILE:HD12 | 1:49:A:GLN:HA   | 5        | 0.17          |
| (1,1861) | 1:44:A:ILE:HD13 | 1:49:A:GLN:HA   | 5        | 0.17          |
| (1,1861) | 1:44:A:ILE:HD11 | 1:49:A:GLN:HA   | 11       | 0.17          |
| (1,1861) | 1:44:A:ILE:HD12 | 1:49:A:GLN:HA   | 11       | 0.17          |
| (1,1861) | 1:44:A:ILE:HD13 | 1:49:A:GLN:HA   | 11       | 0.17          |
| (1,1861) | 1:44:A:ILE:HD11 | 1:49:A:GLN:HA   | 18       | 0.17          |
| (1,1861) | 1:44:A:ILE:HD12 | 1:49:A:GLN:HA   | 18       | 0.17          |
| (1,1861) | 1:44:A:ILE:HD13 | 1:49:A:GLN:HA   | 18       | 0.17          |
| (1,1861) | 1:44:A:ILE:HD11 | 1:49:A:GLN:HA   | 19       | 0.17          |
| (1,1861) | 1:44:A:ILE:HD12 | 1:49:A:GLN:HA   | 19       | 0.17          |
| (1,1861) | 1:44:A:ILE:HD13 | 1:49:A:GLN:HA   | 19       | 0.17          |
| (1,1512) | 1:34:A:GLU:HG3  | 1:69:A:LEU:HD23 | 9        | 0.17          |
| (1,1512) | 1:34:A:GLU:HG3  | 1:69:A:LEU:HD23 | 13       | 0.17          |
| (1,1511) | 1:34:A:GLU:HG3  | 1:69:A:LEU:HD22 | 2        | 0.17          |
| (1,1350) | 1:30:A:ILE:HA   | 1:30:A:ILE:HD11 | 4        | 0.17          |
| (1,1350) | 1:30:A:ILE:HA   | 1:30:A:ILE:HD12 | 4        | 0.17          |
| (1,1350) | 1:30:A:ILE:HA   | 1:30:A:ILE:HD13 | 4        | 0.17          |
| (1,1350) | 1:30:A:ILE:HA   | 1:30:A:ILE:HD11 | 15       | 0.17          |
| (1,1350) | 1:30:A:ILE:HA   | 1:30:A:ILE:HD12 | 15       | 0.17          |
| (1,1350) | 1:30:A:ILE:HA   | 1:30:A:ILE:HD13 | 15       | 0.17          |
| (1,865)  | 1:19:A:PRO:HA   | 1:56:A:LEU:HA   | 3        | 0.17          |
| (1,865)  | 1:19:A:PRO:HA   | 1:56:A:LEU:HA   | 7        | 0.17          |
| (1,865)  | 1:19:A:PRO:HA   | 1:56:A:LEU:HA   | 9        | 0.17          |
| (1,865)  | 1:19:A:PRO:HA   | 1:56:A:LEU:HA   | 10       | 0.17          |
| (1,865)  | 1:19:A:PRO:HA   | 1:56:A:LEU:HA   | 14       | 0.17          |
| (1,865)  | 1:19:A:PRO:HA   | 1:56:A:LEU:HA   | 19       | 0.17          |
| (1,630)  | 1:13:A:ILE:HG21 | 1:15:A:LEU:HD23 | 7        | 0.17          |
| (1,604)  | 1:14:A:THR:HG22 | 1:14:A:THR:H    | 1        | 0.17          |
| (1,604)  | 1:14:A:THR:HG21 | 1:14:A:THR:H    | 3        | 0.17          |
| (1,604)  | 1:14:A:THR:HG21 | 1:14:A:THR:H    | 5        | 0.17          |
| (1,604)  | 1:14:A:THR:HG22 | 1:14:A:THR:H    | 7        | 0.17          |
| (1,604)  | 1:14:A:THR:HG23 | 1:14:A:THR:H    | 19       | 0.17          |
| (1,386)  | 1:5:A:VAL:HG11  | 1:69:A:LEU:HG   | 1        | 0.17          |
| (1,386)  | 1:5:A:VAL:HG12  | 1:69:A:LEU:HG   | 1        | 0.17          |
| (1,386)  | 1:5:A:VAL:HG13  | 1:69:A:LEU:HG   | 1        | 0.17          |
| (1,386)  | 1:5:A:VAL:HG11  | 1:69:A:LEU:HG   | 5        | 0.17          |
| (1,386)  | 1:5:A:VAL:HG12  | 1:69:A:LEU:HG   | 5        | 0.17          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,386)  | 1:5:A:VAL:HG13  | 1:69:A:LEU:HG   | 5        | 0.17          |
| (1,386)  | 1:5:A:VAL:HG11  | 1:69:A:LEU:HG   | 12       | 0.17          |
| (1,386)  | 1:5:A:VAL:HG12  | 1:69:A:LEU:HG   | 12       | 0.17          |
| (1,386)  | 1:5:A:VAL:HG13  | 1:69:A:LEU:HG   | 12       | 0.17          |
| (1,386)  | 1:5:A:VAL:HG11  | 1:69:A:LEU:HG   | 14       | 0.17          |
| (1,386)  | 1:5:A:VAL:HG12  | 1:69:A:LEU:HG   | 14       | 0.17          |
| (1,386)  | 1:5:A:VAL:HG13  | 1:69:A:LEU:HG   | 14       | 0.17          |
| (1,386)  | 1:5:A:VAL:HG11  | 1:69:A:LEU:HG   | 19       | 0.17          |
| (1,386)  | 1:5:A:VAL:HG12  | 1:69:A:LEU:HG   | 19       | 0.17          |
| (1,386)  | 1:5:A:VAL:HG13  | 1:69:A:LEU:HG   | 19       | 0.17          |
| (1,319)  | 1:5:A:VAL:HG11  | 1:7:A:THR:HG22  | 6        | 0.17          |
| (1,318)  | 1:5:A:VAL:HG11  | 1:7:A:THR:HG22  | 7        | 0.17          |
| (1,269)  | 1:4:A:PHE:HB2   | 1:12:A:THR:HG21 | 3        | 0.17          |
| (1,269)  | 1:4:A:PHE:HB2   | 1:12:A:THR:HG22 | 3        | 0.17          |
| (1,269)  | 1:4:A:PHE:HB2   | 1:12:A:THR:HG23 | 3        | 0.17          |
| (1,148)  | 1:68:A:HIS:HA   | 1:66:A:THR:HG21 | 4        | 0.17          |
| (1,148)  | 1:68:A:HIS:HA   | 1:66:A:THR:HG23 | 20       | 0.17          |
| (1,97)   | 1:1:A:MET:HG3   | 1:63:A:LYS:HA   | 1        | 0.17          |
| (1,97)   | 1:1:A:MET:HG3   | 1:63:A:LYS:HA   | 7        | 0.17          |
| (1,97)   | 1:1:A:MET:HG3   | 1:63:A:LYS:HA   | 9        | 0.17          |
| (1,97)   | 1:1:A:MET:HG3   | 1:63:A:LYS:HA   | 10       | 0.17          |
| (1,97)   | 1:1:A:MET:HG3   | 1:63:A:LYS:HA   | 11       | 0.17          |
| (1,97)   | 1:1:A:MET:HG3   | 1:63:A:LYS:HA   | 17       | 0.17          |
| (1,60)   | 1:28:A:ALA:HB1  | 1:25:A:ASN:HA   | 14       | 0.17          |
| (1,60)   | 1:28:A:ALA:HB1  | 1:25:A:ASN:HA   | 16       | 0.17          |
| (1,45)   | 1:1:A:MET:HE3   | 1:18:A:GLU:HA   | 15       | 0.17          |
| (1,38)   | 1:1:A:MET:HE3   | 1:17:A:VAL:HG21 | 4        | 0.17          |
| (1,19)   | 1:1:A:MET:HE2   | 1:3:A:ILE:HD12  | 18       | 0.17          |
| (1,1990) | 1:45:A:PHE:HB3  | 1:67:A:LEU:HD11 | 10       | 0.16          |
| (1,1990) | 1:45:A:PHE:HB3  | 1:67:A:LEU:HD12 | 10       | 0.16          |
| (1,1990) | 1:45:A:PHE:HB3  | 1:67:A:LEU:HD13 | 10       | 0.16          |
| (1,1990) | 1:45:A:PHE:HB3  | 1:67:A:LEU:HD21 | 10       | 0.16          |
| (1,1990) | 1:45:A:PHE:HB3  | 1:67:A:LEU:HD22 | 10       | 0.16          |
| (1,1990) | 1:45:A:PHE:HB3  | 1:67:A:LEU:HD23 | 10       | 0.16          |
| (1,1990) | 1:45:A:PHE:HB3  | 1:67:A:LEU:HD11 | 20       | 0.16          |
| (1,1990) | 1:45:A:PHE:HB3  | 1:67:A:LEU:HD12 | 20       | 0.16          |
| (1,1990) | 1:45:A:PHE:HB3  | 1:67:A:LEU:HD13 | 20       | 0.16          |
| (1,1990) | 1:45:A:PHE:HB3  | 1:67:A:LEU:HD21 | 20       | 0.16          |
| (1,1990) | 1:45:A:PHE:HB3  | 1:67:A:LEU:HD22 | 20       | 0.16          |
| (1,1990) | 1:45:A:PHE:HB3  | 1:67:A:LEU:HD23 | 20       | 0.16          |
| (1,1916) | 1:44:A:ILE:HD11 | 1:70:A:VAL:HG21 | 10       | 0.16          |
| (1,1916) | 1:44:A:ILE:HD11 | 1:70:A:VAL:HG22 | 10       | 0.16          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1916) | 1:44:A:ILE:HD11 | 1:70:A:VAL:HG23 | 10       | 0.16          |
| (1,1916) | 1:44:A:ILE:HD12 | 1:70:A:VAL:HG21 | 10       | 0.16          |
| (1,1916) | 1:44:A:ILE:HD12 | 1:70:A:VAL:HG22 | 10       | 0.16          |
| (1,1916) | 1:44:A:ILE:HD12 | 1:70:A:VAL:HG23 | 10       | 0.16          |
| (1,1916) | 1:44:A:ILE:HD13 | 1:70:A:VAL:HG21 | 10       | 0.16          |
| (1,1916) | 1:44:A:ILE:HD13 | 1:70:A:VAL:HG22 | 10       | 0.16          |
| (1,1916) | 1:44:A:ILE:HD13 | 1:70:A:VAL:HG23 | 10       | 0.16          |
| (1,1887) | 1:44:A:ILE:HD12 | 1:70:A:VAL:HG11 | 8        | 0.16          |
| (1,1887) | 1:44:A:ILE:HD11 | 1:70:A:VAL:HG11 | 12       | 0.16          |
| (1,1887) | 1:44:A:ILE:HD11 | 1:70:A:VAL:HG11 | 14       | 0.16          |
| (1,1826) | 1:44:A:ILE:HA   | 1:44:A:ILE:HD11 | 8        | 0.16          |
| (1,1826) | 1:44:A:ILE:HA   | 1:44:A:ILE:HD12 | 8        | 0.16          |
| (1,1826) | 1:44:A:ILE:HA   | 1:44:A:ILE:HD13 | 8        | 0.16          |
| (1,1817) | 1:43:A:LEU:HD22 | 1:67:A:LEU:HB3  | 1        | 0.16          |
| (1,1817) | 1:43:A:LEU:HD21 | 1:67:A:LEU:HB3  | 2        | 0.16          |
| (1,1744) | 1:42:A:ARG:HG2  | 1:44:A:ILE:HD11 | 10       | 0.16          |
| (1,1744) | 1:42:A:ARG:HG2  | 1:44:A:ILE:HD11 | 14       | 0.16          |
| (1,1350) | 1:30:A:ILE:HA   | 1:30:A:ILE:HD11 | 1        | 0.16          |
| (1,1350) | 1:30:A:ILE:HA   | 1:30:A:ILE:HD12 | 1        | 0.16          |
| (1,1350) | 1:30:A:ILE:HA   | 1:30:A:ILE:HD13 | 1        | 0.16          |
| (1,1350) | 1:30:A:ILE:HA   | 1:30:A:ILE:HD11 | 5        | 0.16          |
| (1,1350) | 1:30:A:ILE:HA   | 1:30:A:ILE:HD12 | 5        | 0.16          |
| (1,1350) | 1:30:A:ILE:HA   | 1:30:A:ILE:HD13 | 5        | 0.16          |
| (1,1350) | 1:30:A:ILE:HA   | 1:30:A:ILE:HD11 | 6        | 0.16          |
| (1,1350) | 1:30:A:ILE:HA   | 1:30:A:ILE:HD12 | 6        | 0.16          |
| (1,1350) | 1:30:A:ILE:HA   | 1:30:A:ILE:HD13 | 6        | 0.16          |
| (1,1350) | 1:30:A:ILE:HA   | 1:30:A:ILE:HD11 | 11       | 0.16          |
| (1,1350) | 1:30:A:ILE:HA   | 1:30:A:ILE:HD12 | 11       | 0.16          |
| (1,1350) | 1:30:A:ILE:HA   | 1:30:A:ILE:HD13 | 11       | 0.16          |
| (1,1350) | 1:30:A:ILE:HA   | 1:30:A:ILE:HD11 | 12       | 0.16          |
| (1,1350) | 1:30:A:ILE:HA   | 1:30:A:ILE:HD12 | 12       | 0.16          |
| (1,1350) | 1:30:A:ILE:HA   | 1:30:A:ILE:HD13 | 12       | 0.16          |
| (1,1350) | 1:30:A:ILE:HA   | 1:30:A:ILE:HD11 | 14       | 0.16          |
| (1,1350) | 1:30:A:ILE:HA   | 1:30:A:ILE:HD12 | 14       | 0.16          |
| (1,1350) | 1:30:A:ILE:HA   | 1:30:A:ILE:HD13 | 14       | 0.16          |
| (1,1350) | 1:30:A:ILE:HA   | 1:30:A:ILE:HD11 | 16       | 0.16          |
| (1,1350) | 1:30:A:ILE:HA   | 1:30:A:ILE:HD12 | 16       | 0.16          |
| (1,1350) | 1:30:A:ILE:HA   | 1:30:A:ILE:HD13 | 16       | 0.16          |
| (1,1350) | 1:30:A:ILE:HA   | 1:30:A:ILE:HD11 | 18       | 0.16          |
| (1,1350) | 1:30:A:ILE:HA   | 1:30:A:ILE:HD12 | 18       | 0.16          |
| (1,1350) | 1:30:A:ILE:HA   | 1:30:A:ILE:HD13 | 18       | 0.16          |
| (1,1350) | 1:30:A:ILE:HA   | 1:30:A:ILE:HD11 | 19       | 0.16          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1350) | 1:30:A:ILE:HA   | 1:30:A:ILE:HD12 | 19       | 0.16          |
| (1,1350) | 1:30:A:ILE:HA   | 1:30:A:ILE:HD13 | 19       | 0.16          |
| (1,1134) | 1:24:A:GLU:HA   | 1:27:A:LYS:HD2  | 4        | 0.16          |
| (1,1134) | 1:24:A:GLU:HA   | 1:27:A:LYS:HD3  | 4        | 0.16          |
| (1,865)  | 1:19:A:PRO:HA   | 1:56:A:LEU:HA   | 4        | 0.16          |
| (1,865)  | 1:19:A:PRO:HA   | 1:56:A:LEU:HA   | 13       | 0.16          |
| (1,865)  | 1:19:A:PRO:HA   | 1:56:A:LEU:HA   | 15       | 0.16          |
| (1,865)  | 1:19:A:PRO:HA   | 1:56:A:LEU:HA   | 20       | 0.16          |
| (1,604)  | 1:14:A:THR:HG21 | 1:14:A:THR:H    | 4        | 0.16          |
| (1,604)  | 1:14:A:THR:HG21 | 1:14:A:THR:H    | 8        | 0.16          |
| (1,604)  | 1:14:A:THR:HG22 | 1:14:A:THR:H    | 13       | 0.16          |
| (1,604)  | 1:14:A:THR:HG23 | 1:14:A:THR:H    | 16       | 0.16          |
| (1,439)  | 1:6:A:LYS:HD2   | 1:12:A:THR:HA   | 3        | 0.16          |
| (1,439)  | 1:6:A:LYS:HD3   | 1:12:A:THR:HA   | 3        | 0.16          |
| (1,439)  | 1:6:A:LYS:HD2   | 1:12:A:THR:HA   | 18       | 0.16          |
| (1,439)  | 1:6:A:LYS:HD3   | 1:12:A:THR:HA   | 18       | 0.16          |
| (1,386)  | 1:5:A:VAL:HG11  | 1:69:A:LEU:HG   | 16       | 0.16          |
| (1,386)  | 1:5:A:VAL:HG12  | 1:69:A:LEU:HG   | 16       | 0.16          |
| (1,386)  | 1:5:A:VAL:HG13  | 1:69:A:LEU:HG   | 16       | 0.16          |
| (1,386)  | 1:5:A:VAL:HG11  | 1:69:A:LEU:HG   | 18       | 0.16          |
| (1,386)  | 1:5:A:VAL:HG12  | 1:69:A:LEU:HG   | 18       | 0.16          |
| (1,386)  | 1:5:A:VAL:HG13  | 1:69:A:LEU:HG   | 18       | 0.16          |
| (1,341)  | 1:5:A:VAL:HG22  | 1:13:A:ILE:HG13 | 10       | 0.16          |
| (1,339)  | 1:5:A:VAL:HG23  | 1:13:A:ILE:HG13 | 9        | 0.16          |
| (1,339)  | 1:5:A:VAL:HG21  | 1:13:A:ILE:HG13 | 13       | 0.16          |
| (1,319)  | 1:5:A:VAL:HG12  | 1:7:A:THR:HG23  | 16       | 0.16          |
| (1,318)  | 1:5:A:VAL:HG11  | 1:7:A:THR:HG22  | 10       | 0.16          |
| (1,318)  | 1:5:A:VAL:HG12  | 1:7:A:THR:HG23  | 13       | 0.16          |
| (1,318)  | 1:5:A:VAL:HG13  | 1:7:A:THR:HG23  | 15       | 0.16          |
| (1,264)  | 1:4:A:PHE:HA    | 1:14:A:THR:HG21 | 3        | 0.16          |
| (1,264)  | 1:4:A:PHE:HA    | 1:12:A:THR:HG23 | 15       | 0.16          |
| (1,148)  | 1:68:A:HIS:HA   | 1:66:A:THR:HG23 | 14       | 0.16          |
| (1,148)  | 1:68:A:HIS:HA   | 1:66:A:THR:HG23 | 16       | 0.16          |
| (1,97)   | 1:1:A:MET:HG3   | 1:63:A:LYS:HA   | 2        | 0.16          |
| (1,97)   | 1:1:A:MET:HG3   | 1:63:A:LYS:HA   | 4        | 0.16          |
| (1,60)   | 1:28:A:ALA:HB1  | 1:25:A:ASN:HA   | 11       | 0.16          |
| (1,60)   | 1:28:A:ALA:HB1  | 1:25:A:ASN:HA   | 12       | 0.16          |
| (1,60)   | 1:28:A:ALA:HB1  | 1:25:A:ASN:HA   | 18       | 0.16          |
| (1,60)   | 1:28:A:ALA:HB1  | 1:25:A:ASN:HA   | 19       | 0.16          |
| (1,60)   | 1:28:A:ALA:HB1  | 1:25:A:ASN:HA   | 20       | 0.16          |
| (1,48)   | 1:1:A:MET:HE3   | 1:19:A:PRO:HA   | 6        | 0.16          |
| (1,37)   | 1:1:A:MET:HE1   | 1:17:A:VAL:HG23 | 5        | 0.16          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2564) | 1:72:A:ARG:HA   | 1:72:A:ARG:HD2  | 6        | 0.15          |
| (1,2564) | 1:72:A:ARG:HA   | 1:72:A:ARG:HD3  | 6        | 0.15          |
| (1,2564) | 1:72:A:ARG:HA   | 1:72:A:ARG:HD2  | 19       | 0.15          |
| (1,2564) | 1:72:A:ARG:HA   | 1:72:A:ARG:HD3  | 19       | 0.15          |
| (1,1990) | 1:45:A:PHE:HB3  | 1:67:A:LEU:HD11 | 3        | 0.15          |
| (1,1990) | 1:45:A:PHE:HB3  | 1:67:A:LEU:HD12 | 3        | 0.15          |
| (1,1990) | 1:45:A:PHE:HB3  | 1:67:A:LEU:HD13 | 3        | 0.15          |
| (1,1990) | 1:45:A:PHE:HB3  | 1:67:A:LEU:HD21 | 3        | 0.15          |
| (1,1990) | 1:45:A:PHE:HB3  | 1:67:A:LEU:HD22 | 3        | 0.15          |
| (1,1990) | 1:45:A:PHE:HB3  | 1:67:A:LEU:HD23 | 3        | 0.15          |
| (1,1990) | 1:45:A:PHE:HB3  | 1:67:A:LEU:HD11 | 4        | 0.15          |
| (1,1990) | 1:45:A:PHE:HB3  | 1:67:A:LEU:HD12 | 4        | 0.15          |
| (1,1990) | 1:45:A:PHE:HB3  | 1:67:A:LEU:HD13 | 4        | 0.15          |
| (1,1990) | 1:45:A:PHE:HB3  | 1:67:A:LEU:HD21 | 4        | 0.15          |
| (1,1990) | 1:45:A:PHE:HB3  | 1:67:A:LEU:HD22 | 4        | 0.15          |
| (1,1990) | 1:45:A:PHE:HB3  | 1:67:A:LEU:HD23 | 4        | 0.15          |
| (1,1990) | 1:45:A:PHE:HB3  | 1:67:A:LEU:HD11 | 13       | 0.15          |
| (1,1990) | 1:45:A:PHE:HB3  | 1:67:A:LEU:HD12 | 13       | 0.15          |
| (1,1990) | 1:45:A:PHE:HB3  | 1:67:A:LEU:HD13 | 13       | 0.15          |
| (1,1990) | 1:45:A:PHE:HB3  | 1:67:A:LEU:HD21 | 13       | 0.15          |
| (1,1990) | 1:45:A:PHE:HB3  | 1:67:A:LEU:HD22 | 13       | 0.15          |
| (1,1990) | 1:45:A:PHE:HB3  | 1:67:A:LEU:HD23 | 13       | 0.15          |
| (1,1990) | 1:45:A:PHE:HB3  | 1:67:A:LEU:HD11 | 14       | 0.15          |
| (1,1990) | 1:45:A:PHE:HB3  | 1:67:A:LEU:HD12 | 14       | 0.15          |
| (1,1990) | 1:45:A:PHE:HB3  | 1:67:A:LEU:HD13 | 14       | 0.15          |
| (1,1990) | 1:45:A:PHE:HB3  | 1:67:A:LEU:HD21 | 14       | 0.15          |
| (1,1990) | 1:45:A:PHE:HB3  | 1:67:A:LEU:HD22 | 14       | 0.15          |
| (1,1990) | 1:45:A:PHE:HB3  | 1:67:A:LEU:HD23 | 14       | 0.15          |
| (1,1990) | 1:45:A:PHE:HB3  | 1:67:A:LEU:HD11 | 15       | 0.15          |
| (1,1990) | 1:45:A:PHE:HB3  | 1:67:A:LEU:HD12 | 15       | 0.15          |
| (1,1990) | 1:45:A:PHE:HB3  | 1:67:A:LEU:HD13 | 15       | 0.15          |
| (1,1990) | 1:45:A:PHE:HB3  | 1:67:A:LEU:HD21 | 15       | 0.15          |
| (1,1990) | 1:45:A:PHE:HB3  | 1:67:A:LEU:HD22 | 15       | 0.15          |
| (1,1990) | 1:45:A:PHE:HB3  | 1:67:A:LEU:HD23 | 15       | 0.15          |
| (1,1990) | 1:45:A:PHE:HB3  | 1:67:A:LEU:HD11 | 16       | 0.15          |
| (1,1990) | 1:45:A:PHE:HB3  | 1:67:A:LEU:HD12 | 16       | 0.15          |
| (1,1990) | 1:45:A:PHE:HB3  | 1:67:A:LEU:HD13 | 16       | 0.15          |
| (1,1990) | 1:45:A:PHE:HB3  | 1:67:A:LEU:HD21 | 16       | 0.15          |
| (1,1990) | 1:45:A:PHE:HB3  | 1:67:A:LEU:HD22 | 16       | 0.15          |
| (1,1990) | 1:45:A:PHE:HB3  | 1:67:A:LEU:HD23 | 16       | 0.15          |
| (1,1887) | 1:44:A:ILE:HD11 | 1:70:A:VAL:HG11 | 3        | 0.15          |
| (1,1887) | 1:44:A:ILE:HD13 | 1:70:A:VAL:HG11 | 4        | 0.15          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1861) | 1:44:A:ILE:HD11 | 1:49:A:GLN:HA   | 15       | 0.15          |
| (1,1861) | 1:44:A:ILE:HD12 | 1:49:A:GLN:HA   | 15       | 0.15          |
| (1,1861) | 1:44:A:ILE:HD13 | 1:49:A:GLN:HA   | 15       | 0.15          |
| (1,1861) | 1:44:A:ILE:HD11 | 1:49:A:GLN:HA   | 16       | 0.15          |
| (1,1861) | 1:44:A:ILE:HD12 | 1:49:A:GLN:HA   | 16       | 0.15          |
| (1,1861) | 1:44:A:ILE:HD13 | 1:49:A:GLN:HA   | 16       | 0.15          |
| (1,1722) | 1:41:A:GLN:H    | 1:71:A:LEU:HD23 | 5        | 0.15          |
| (1,1659) | 1:38:A:PRO:HA   | 1:41:A:GLN:HE21 | 9        | 0.15          |
| (1,1511) | 1:34:A:GLU:HG3  | 1:69:A:LEU:HD21 | 5        | 0.15          |
| (1,1511) | 1:34:A:GLU:HG3  | 1:69:A:LEU:HD21 | 16       | 0.15          |
| (1,1350) | 1:30:A:ILE:HA   | 1:30:A:ILE:HD11 | 2        | 0.15          |
| (1,1350) | 1:30:A:ILE:HA   | 1:30:A:ILE:HD12 | 2        | 0.15          |
| (1,1350) | 1:30:A:ILE:HA   | 1:30:A:ILE:HD13 | 2        | 0.15          |
| (1,1350) | 1:30:A:ILE:HA   | 1:30:A:ILE:HD11 | 3        | 0.15          |
| (1,1350) | 1:30:A:ILE:HA   | 1:30:A:ILE:HD12 | 3        | 0.15          |
| (1,1350) | 1:30:A:ILE:HA   | 1:30:A:ILE:HD13 | 3        | 0.15          |
| (1,1350) | 1:30:A:ILE:HA   | 1:30:A:ILE:HD11 | 7        | 0.15          |
| (1,1350) | 1:30:A:ILE:HA   | 1:30:A:ILE:HD12 | 7        | 0.15          |
| (1,1350) | 1:30:A:ILE:HA   | 1:30:A:ILE:HD13 | 7        | 0.15          |
| (1,1350) | 1:30:A:ILE:HA   | 1:30:A:ILE:HD11 | 9        | 0.15          |
| (1,1350) | 1:30:A:ILE:HA   | 1:30:A:ILE:HD12 | 9        | 0.15          |
| (1,1350) | 1:30:A:ILE:HA   | 1:30:A:ILE:HD13 | 9        | 0.15          |
| (1,1350) | 1:30:A:ILE:HA   | 1:30:A:ILE:HD11 | 10       | 0.15          |
| (1,1350) | 1:30:A:ILE:HA   | 1:30:A:ILE:HD12 | 10       | 0.15          |
| (1,1350) | 1:30:A:ILE:HA   | 1:30:A:ILE:HD13 | 10       | 0.15          |
| (1,1350) | 1:30:A:ILE:HA   | 1:30:A:ILE:HD11 | 13       | 0.15          |
| (1,1350) | 1:30:A:ILE:HA   | 1:30:A:ILE:HD12 | 13       | 0.15          |
| (1,1350) | 1:30:A:ILE:HA   | 1:30:A:ILE:HD13 | 13       | 0.15          |
| (1,1350) | 1:30:A:ILE:HA   | 1:30:A:ILE:HD11 | 17       | 0.15          |
| (1,1350) | 1:30:A:ILE:HA   | 1:30:A:ILE:HD12 | 17       | 0.15          |
| (1,1350) | 1:30:A:ILE:HA   | 1:30:A:ILE:HD13 | 17       | 0.15          |
| (1,1350) | 1:30:A:ILE:HA   | 1:30:A:ILE:HD11 | 20       | 0.15          |
| (1,1350) | 1:30:A:ILE:HA   | 1:30:A:ILE:HD12 | 20       | 0.15          |
| (1,1350) | 1:30:A:ILE:HA   | 1:30:A:ILE:HD13 | 20       | 0.15          |
| (1,1134) | 1:24:A:GLU:HA   | 1:27:A:LYS:HD2  | 8        | 0.15          |
| (1,1134) | 1:24:A:GLU:HA   | 1:27:A:LYS:HD3  | 8        | 0.15          |
| (1,630)  | 1:13:A:ILE:HG22 | 1:15:A:LEU:HD23 | 6        | 0.15          |
| (1,630)  | 1:13:A:ILE:HG21 | 1:15:A:LEU:HD23 | 10       | 0.15          |
| (1,604)  | 1:14:A:THR:HG21 | 1:14:A:THR:H    | 2        | 0.15          |
| (1,604)  | 1:14:A:THR:HG21 | 1:14:A:THR:H    | 10       | 0.15          |
| (1,604)  | 1:14:A:THR:HG23 | 1:14:A:THR:H    | 11       | 0.15          |
| (1,604)  | 1:14:A:THR:HG23 | 1:14:A:THR:H    | 12       | 0.15          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,604)  | 1:14:A:THR:HG22 | 1:14:A:THR:H    | 14       | 0.15          |
| (1,604)  | 1:14:A:THR:HG23 | 1:14:A:THR:H    | 15       | 0.15          |
| (1,604)  | 1:14:A:THR:HG22 | 1:14:A:THR:H    | 18       | 0.15          |
| (1,459)  | 1:6:A:LYS:HE2   | 1:66:A:THR:HG23 | 10       | 0.15          |
| (1,420)  | 1:6:A:LYS:HE2   | 1:10:A:GLY:HA2  | 4        | 0.15          |
| (1,420)  | 1:6:A:LYS:HE2   | 1:10:A:GLY:HA3  | 4        | 0.15          |
| (1,420)  | 1:6:A:LYS:HE3   | 1:10:A:GLY:HA2  | 4        | 0.15          |
| (1,420)  | 1:6:A:LYS:HE3   | 1:10:A:GLY:HA3  | 4        | 0.15          |
| (1,420)  | 1:6:A:LYS:HE2   | 1:10:A:GLY:HA2  | 13       | 0.15          |
| (1,420)  | 1:6:A:LYS:HE2   | 1:10:A:GLY:HA3  | 13       | 0.15          |
| (1,420)  | 1:6:A:LYS:HE3   | 1:10:A:GLY:HA2  | 13       | 0.15          |
| (1,420)  | 1:6:A:LYS:HE3   | 1:10:A:GLY:HA3  | 13       | 0.15          |
| (1,356)  | 1:17:A:VAL:HG11 | 1:29:A:LYS:HG3  | 8        | 0.15          |
| (1,341)  | 1:5:A:VAL:HG21  | 1:13:A:ILE:HG13 | 3        | 0.15          |
| (1,319)  | 1:5:A:VAL:HG11  | 1:7:A:THR:HG22  | 9        | 0.15          |
| (1,269)  | 1:4:A:PHE:HB2   | 1:12:A:THR:HG21 | 17       | 0.15          |
| (1,269)  | 1:4:A:PHE:HB2   | 1:12:A:THR:HG22 | 17       | 0.15          |
| (1,269)  | 1:4:A:PHE:HB2   | 1:12:A:THR:HG23 | 17       | 0.15          |
| (1,264)  | 1:4:A:PHE:HA    | 1:12:A:THR:HG21 | 5        | 0.15          |
| (1,264)  | 1:4:A:PHE:HA    | 1:14:A:THR:HG22 | 7        | 0.15          |
| (1,177)  | 1:29:A:LYS:HA   | 1:15:A:LEU:HD22 | 4        | 0.15          |
| (1,148)  | 1:68:A:HIS:HA   | 1:66:A:THR:HG23 | 11       | 0.15          |
| (1,126)  | 1:2:A:GLN:HA    | 1:14:A:THR:HG23 | 7        | 0.15          |
| (1,60)   | 1:28:A:ALA:HB1  | 1:25:A:ASN:HA   | 13       | 0.15          |
| (1,60)   | 1:28:A:ALA:HB1  | 1:25:A:ASN:HA   | 15       | 0.15          |
| (1,60)   | 1:28:A:ALA:HB1  | 1:25:A:ASN:HA   | 17       | 0.15          |
| (1,45)   | 1:1:A:MET:HE3   | 1:18:A:GLU:HA   | 16       | 0.15          |
| (1,1990) | 1:45:A:PHE:HB3  | 1:67:A:LEU:HD11 | 2        | 0.14          |
| (1,1990) | 1:45:A:PHE:HB3  | 1:67:A:LEU:HD12 | 2        | 0.14          |
| (1,1990) | 1:45:A:PHE:HB3  | 1:67:A:LEU:HD13 | 2        | 0.14          |
| (1,1990) | 1:45:A:PHE:HB3  | 1:67:A:LEU:HD21 | 2        | 0.14          |
| (1,1990) | 1:45:A:PHE:HB3  | 1:67:A:LEU:HD22 | 2        | 0.14          |
| (1,1990) | 1:45:A:PHE:HB3  | 1:67:A:LEU:HD23 | 2        | 0.14          |
| (1,1990) | 1:45:A:PHE:HB3  | 1:67:A:LEU:HD11 | 8        | 0.14          |
| (1,1990) | 1:45:A:PHE:HB3  | 1:67:A:LEU:HD12 | 8        | 0.14          |
| (1,1990) | 1:45:A:PHE:HB3  | 1:67:A:LEU:HD13 | 8        | 0.14          |
| (1,1990) | 1:45:A:PHE:HB3  | 1:67:A:LEU:HD21 | 8        | 0.14          |
| (1,1990) | 1:45:A:PHE:HB3  | 1:67:A:LEU:HD22 | 8        | 0.14          |
| (1,1990) | 1:45:A:PHE:HB3  | 1:67:A:LEU:HD23 | 8        | 0.14          |
| (1,1990) | 1:45:A:PHE:HB3  | 1:67:A:LEU:HD11 | 12       | 0.14          |
| (1,1990) | 1:45:A:PHE:HB3  | 1:67:A:LEU:HD12 | 12       | 0.14          |
| (1,1990) | 1:45:A:PHE:HB3  | 1:67:A:LEU:HD13 | 12       | 0.14          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1990) | 1:45:A:PHE:HB3  | 1:67:A:LEU:HD21 | 12       | 0.14          |
| (1,1990) | 1:45:A:PHE:HB3  | 1:67:A:LEU:HD22 | 12       | 0.14          |
| (1,1990) | 1:45:A:PHE:HB3  | 1:67:A:LEU:HD23 | 12       | 0.14          |
| (1,1990) | 1:45:A:PHE:HB3  | 1:67:A:LEU:HD11 | 17       | 0.14          |
| (1,1990) | 1:45:A:PHE:HB3  | 1:67:A:LEU:HD12 | 17       | 0.14          |
| (1,1990) | 1:45:A:PHE:HB3  | 1:67:A:LEU:HD13 | 17       | 0.14          |
| (1,1990) | 1:45:A:PHE:HB3  | 1:67:A:LEU:HD21 | 17       | 0.14          |
| (1,1990) | 1:45:A:PHE:HB3  | 1:67:A:LEU:HD22 | 17       | 0.14          |
| (1,1990) | 1:45:A:PHE:HB3  | 1:67:A:LEU:HD23 | 17       | 0.14          |
| (1,1990) | 1:45:A:PHE:HB3  | 1:67:A:LEU:HD11 | 18       | 0.14          |
| (1,1990) | 1:45:A:PHE:HB3  | 1:67:A:LEU:HD12 | 18       | 0.14          |
| (1,1990) | 1:45:A:PHE:HB3  | 1:67:A:LEU:HD13 | 18       | 0.14          |
| (1,1990) | 1:45:A:PHE:HB3  | 1:67:A:LEU:HD21 | 18       | 0.14          |
| (1,1990) | 1:45:A:PHE:HB3  | 1:67:A:LEU:HD22 | 18       | 0.14          |
| (1,1990) | 1:45:A:PHE:HB3  | 1:67:A:LEU:HD23 | 18       | 0.14          |
| (1,1990) | 1:45:A:PHE:HB3  | 1:67:A:LEU:HD11 | 19       | 0.14          |
| (1,1990) | 1:45:A:PHE:HB3  | 1:67:A:LEU:HD12 | 19       | 0.14          |
| (1,1990) | 1:45:A:PHE:HB3  | 1:67:A:LEU:HD13 | 19       | 0.14          |
| (1,1990) | 1:45:A:PHE:HB3  | 1:67:A:LEU:HD21 | 19       | 0.14          |
| (1,1990) | 1:45:A:PHE:HB3  | 1:67:A:LEU:HD22 | 19       | 0.14          |
| (1,1990) | 1:45:A:PHE:HB3  | 1:67:A:LEU:HD23 | 19       | 0.14          |
| (1,1887) | 1:44:A:ILE:HD13 | 1:70:A:VAL:HG11 | 1        | 0.14          |
| (1,1887) | 1:44:A:ILE:HD11 | 1:70:A:VAL:HG12 | 10       | 0.14          |
| (1,1887) | 1:44:A:ILE:HD11 | 1:70:A:VAL:HG13 | 11       | 0.14          |
| (1,1887) | 1:44:A:ILE:HD11 | 1:70:A:VAL:HG11 | 17       | 0.14          |
| (1,1869) | 1:44:A:ILE:HG12 | 1:49:A:GLN:HA   | 3        | 0.14          |
| (1,1869) | 1:44:A:ILE:HG13 | 1:49:A:GLN:HA   | 3        | 0.14          |
| (1,1869) | 1:44:A:ILE:HG12 | 1:49:A:GLN:HA   | 13       | 0.14          |
| (1,1869) | 1:44:A:ILE:HG13 | 1:49:A:GLN:HA   | 13       | 0.14          |
| (1,1867) | 1:44:A:ILE:HG12 | 1:49:A:GLN:HA   | 10       | 0.14          |
| (1,1867) | 1:44:A:ILE:HG13 | 1:49:A:GLN:HA   | 10       | 0.14          |
| (1,1867) | 1:44:A:ILE:HG12 | 1:49:A:GLN:HA   | 14       | 0.14          |
| (1,1867) | 1:44:A:ILE:HG13 | 1:49:A:GLN:HA   | 14       | 0.14          |
| (1,1817) | 1:43:A:LEU:HD23 | 1:67:A:LEU:HB3  | 17       | 0.14          |
| (1,1817) | 1:43:A:LEU:HD23 | 1:67:A:LEU:HB3  | 18       | 0.14          |
| (1,1770) | 1:42:A:ARG:HG2  | 1:70:A:VAL:HG21 | 11       | 0.14          |
| (1,1770) | 1:42:A:ARG:HG2  | 1:70:A:VAL:HG22 | 11       | 0.14          |
| (1,1770) | 1:42:A:ARG:HG2  | 1:70:A:VAL:HG23 | 11       | 0.14          |
| (1,1770) | 1:42:A:ARG:HG3  | 1:70:A:VAL:HG21 | 11       | 0.14          |
| (1,1770) | 1:42:A:ARG:HG3  | 1:70:A:VAL:HG22 | 11       | 0.14          |
| (1,1770) | 1:42:A:ARG:HG3  | 1:70:A:VAL:HG23 | 11       | 0.14          |
| (1,1675) | 1:40:A:GLN:HA   | 1:72:A:ARG:HD3  | 14       | 0.14          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1512) | 1:34:A:GLU:HG3  | 1:69:A:LEU:HD22 | 14       | 0.14          |
| (1,1511) | 1:34:A:GLU:HG3  | 1:69:A:LEU:HD23 | 4        | 0.14          |
| (1,1511) | 1:34:A:GLU:HG3  | 1:69:A:LEU:HD23 | 8        | 0.14          |
| (1,1475) | 1:33:A:LYS:HD2  | 1:33:A:LYS:HA   | 6        | 0.14          |
| (1,1475) | 1:33:A:LYS:HD3  | 1:33:A:LYS:HA   | 6        | 0.14          |
| (1,1125) | 1:24:A:GLU:HG2  | 1:24:A:GLU:HA   | 3        | 0.14          |
| (1,738)  | 1:15:A:LEU:HD13 | 1:33:A:LYS:HD2  | 8        | 0.14          |
| (1,604)  | 1:14:A:THR:HG21 | 1:14:A:THR:H    | 6        | 0.14          |
| (1,532)  | 1:8:A:LEU:HG    | 1:8:A:LEU:H     | 4        | 0.14          |
| (1,506)  | 1:7:A:THR:HA    | 1:69:A:LEU:HD22 | 15       | 0.14          |
| (1,506)  | 1:7:A:THR:HA    | 1:69:A:LEU:HD22 | 17       | 0.14          |
| (1,460)  | 1:6:A:LYS:HG3   | 1:66:A:THR:HG22 | 18       | 0.14          |
| (1,459)  | 1:6:A:LYS:HE2   | 1:66:A:THR:HG23 | 7        | 0.14          |
| (1,420)  | 1:6:A:LYS:HE2   | 1:10:A:GLY:HA2  | 9        | 0.14          |
| (1,420)  | 1:6:A:LYS:HE2   | 1:10:A:GLY:HA3  | 9        | 0.14          |
| (1,420)  | 1:6:A:LYS:HE3   | 1:10:A:GLY:HA2  | 9        | 0.14          |
| (1,420)  | 1:6:A:LYS:HE3   | 1:10:A:GLY:HA3  | 9        | 0.14          |
| (1,356)  | 1:17:A:VAL:HG11 | 1:29:A:LYS:HG3  | 5        | 0.14          |
| (1,319)  | 1:5:A:VAL:HG11  | 1:7:A:THR:HG22  | 2        | 0.14          |
| (1,319)  | 1:5:A:VAL:HG11  | 1:7:A:THR:HG22  | 3        | 0.14          |
| (1,319)  | 1:5:A:VAL:HG11  | 1:7:A:THR:HG22  | 4        | 0.14          |
| (1,319)  | 1:5:A:VAL:HG11  | 1:7:A:THR:HG23  | 19       | 0.14          |
| (1,264)  | 1:4:A:PHE:HA    | 1:12:A:THR:HG23 | 19       | 0.14          |
| (1,66)   | 1:28:A:ALA:HB1  | 1:27:A:LYS:HA   | 16       | 0.14          |
| (1,49)   | 1:1:A:MET:HE3   | 1:19:A:PRO:HA   | 6        | 0.14          |
| (1,38)   | 1:1:A:MET:HE3   | 1:17:A:VAL:HG21 | 10       | 0.14          |
| (1,37)   | 1:1:A:MET:HE2   | 1:17:A:VAL:HG22 | 2        | 0.14          |
| (2,72)   | 1:27:A:LYS:HE3  | 1:69:A:LEU:HD12 | 7        | 0.13          |
| (1,2583) | 1:74:A:ARG:HG2  | 1:73:A:LEU:H    | 7        | 0.13          |
| (1,1990) | 1:45:A:PHE:HB3  | 1:67:A:LEU:HD11 | 1        | 0.13          |
| (1,1990) | 1:45:A:PHE:HB3  | 1:67:A:LEU:HD12 | 1        | 0.13          |
| (1,1990) | 1:45:A:PHE:HB3  | 1:67:A:LEU:HD13 | 1        | 0.13          |
| (1,1990) | 1:45:A:PHE:HB3  | 1:67:A:LEU:HD21 | 1        | 0.13          |
| (1,1990) | 1:45:A:PHE:HB3  | 1:67:A:LEU:HD22 | 1        | 0.13          |
| (1,1990) | 1:45:A:PHE:HB3  | 1:67:A:LEU:HD23 | 1        | 0.13          |
| (1,1990) | 1:45:A:PHE:HB3  | 1:67:A:LEU:HD11 | 5        | 0.13          |
| (1,1990) | 1:45:A:PHE:HB3  | 1:67:A:LEU:HD12 | 5        | 0.13          |
| (1,1990) | 1:45:A:PHE:HB3  | 1:67:A:LEU:HD13 | 5        | 0.13          |
| (1,1990) | 1:45:A:PHE:HB3  | 1:67:A:LEU:HD21 | 5        | 0.13          |
| (1,1990) | 1:45:A:PHE:HB3  | 1:67:A:LEU:HD22 | 5        | 0.13          |
| (1,1990) | 1:45:A:PHE:HB3  | 1:67:A:LEU:HD23 | 5        | 0.13          |
| (1,1990) | 1:45:A:PHE:HB3  | 1:67:A:LEU:HD11 | 6        | 0.13          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1990) | 1:45:A:PHE:HB3  | 1:67:A:LEU:HD12 | 6        | 0.13          |
| (1,1990) | 1:45:A:PHE:HB3  | 1:67:A:LEU:HD13 | 6        | 0.13          |
| (1,1990) | 1:45:A:PHE:HB3  | 1:67:A:LEU:HD21 | 6        | 0.13          |
| (1,1990) | 1:45:A:PHE:HB3  | 1:67:A:LEU:HD22 | 6        | 0.13          |
| (1,1990) | 1:45:A:PHE:HB3  | 1:67:A:LEU:HD23 | 6        | 0.13          |
| (1,1990) | 1:45:A:PHE:HB3  | 1:67:A:LEU:HD11 | 9        | 0.13          |
| (1,1990) | 1:45:A:PHE:HB3  | 1:67:A:LEU:HD12 | 9        | 0.13          |
| (1,1990) | 1:45:A:PHE:HB3  | 1:67:A:LEU:HD13 | 9        | 0.13          |
| (1,1990) | 1:45:A:PHE:HB3  | 1:67:A:LEU:HD21 | 9        | 0.13          |
| (1,1990) | 1:45:A:PHE:HB3  | 1:67:A:LEU:HD22 | 9        | 0.13          |
| (1,1990) | 1:45:A:PHE:HB3  | 1:67:A:LEU:HD23 | 9        | 0.13          |
| (1,1990) | 1:45:A:PHE:HB3  | 1:67:A:LEU:HD11 | 11       | 0.13          |
| (1,1990) | 1:45:A:PHE:HB3  | 1:67:A:LEU:HD12 | 11       | 0.13          |
| (1,1990) | 1:45:A:PHE:HB3  | 1:67:A:LEU:HD13 | 11       | 0.13          |
| (1,1990) | 1:45:A:PHE:HB3  | 1:67:A:LEU:HD21 | 11       | 0.13          |
| (1,1990) | 1:45:A:PHE:HB3  | 1:67:A:LEU:HD22 | 11       | 0.13          |
| (1,1990) | 1:45:A:PHE:HB3  | 1:67:A:LEU:HD23 | 11       | 0.13          |
| (1,1903) | 1:44:A:ILE:HG21 | 1:68:A:HIS:HB3  | 13       | 0.13          |
| (1,1903) | 1:44:A:ILE:HG22 | 1:68:A:HIS:HB3  | 13       | 0.13          |
| (1,1903) | 1:44:A:ILE:HG23 | 1:68:A:HIS:HB3  | 13       | 0.13          |
| (1,1903) | 1:44:A:ILE:HG21 | 1:68:A:HIS:HB3  | 14       | 0.13          |
| (1,1903) | 1:44:A:ILE:HG22 | 1:68:A:HIS:HB3  | 14       | 0.13          |
| (1,1903) | 1:44:A:ILE:HG23 | 1:68:A:HIS:HB3  | 14       | 0.13          |
| (1,1887) | 1:44:A:ILE:HD11 | 1:70:A:VAL:HG13 | 9        | 0.13          |
| (1,1887) | 1:44:A:ILE:HD12 | 1:70:A:VAL:HG11 | 13       | 0.13          |
| (1,1887) | 1:44:A:ILE:HD11 | 1:70:A:VAL:HG13 | 18       | 0.13          |
| (1,1887) | 1:44:A:ILE:HD11 | 1:70:A:VAL:HG11 | 19       | 0.13          |
| (1,1860) | 1:44:A:ILE:HD11 | 1:49:A:GLN:HA   | 4        | 0.13          |
| (1,1860) | 1:44:A:ILE:HD12 | 1:49:A:GLN:HA   | 4        | 0.13          |
| (1,1860) | 1:44:A:ILE:HD13 | 1:49:A:GLN:HA   | 4        | 0.13          |
| (1,1860) | 1:44:A:ILE:HD11 | 1:49:A:GLN:HA   | 6        | 0.13          |
| (1,1860) | 1:44:A:ILE:HD12 | 1:49:A:GLN:HA   | 6        | 0.13          |
| (1,1860) | 1:44:A:ILE:HD13 | 1:49:A:GLN:HA   | 6        | 0.13          |
| (1,1860) | 1:44:A:ILE:HD11 | 1:49:A:GLN:HA   | 9        | 0.13          |
| (1,1860) | 1:44:A:ILE:HD12 | 1:49:A:GLN:HA   | 9        | 0.13          |
| (1,1860) | 1:44:A:ILE:HD13 | 1:49:A:GLN:HA   | 9        | 0.13          |
| (1,1770) | 1:42:A:ARG:HG2  | 1:70:A:VAL:HG21 | 2        | 0.13          |
| (1,1770) | 1:42:A:ARG:HG2  | 1:70:A:VAL:HG22 | 2        | 0.13          |
| (1,1770) | 1:42:A:ARG:HG2  | 1:70:A:VAL:HG23 | 2        | 0.13          |
| (1,1770) | 1:42:A:ARG:HG3  | 1:70:A:VAL:HG21 | 2        | 0.13          |
| (1,1770) | 1:42:A:ARG:HG3  | 1:70:A:VAL:HG22 | 2        | 0.13          |
| (1,1770) | 1:42:A:ARG:HG3  | 1:70:A:VAL:HG23 | 2        | 0.13          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,1722) | 1:41:A:GLN:H   | 1:71:A:LEU:HD23 | 4        | 0.13          |
| (1,1659) | 1:38:A:PRO:HA  | 1:41:A:GLN:HE21 | 20       | 0.13          |
| (1,1512) | 1:34:A:GLU:HG3 | 1:69:A:LEU:HD23 | 3        | 0.13          |
| (1,1512) | 1:34:A:GLU:HG3 | 1:69:A:LEU:HD21 | 10       | 0.13          |
| (1,1511) | 1:34:A:GLU:HG3 | 1:69:A:LEU:HD22 | 6        | 0.13          |
| (1,1511) | 1:34:A:GLU:HG3 | 1:69:A:LEU:HD23 | 12       | 0.13          |
| (1,1511) | 1:34:A:GLU:HG3 | 1:69:A:LEU:HD23 | 18       | 0.13          |
| (1,1475) | 1:33:A:LYS:HD2 | 1:33:A:LYS:HA   | 11       | 0.13          |
| (1,1475) | 1:33:A:LYS:HD3 | 1:33:A:LYS:HA   | 11       | 0.13          |
| (1,532)  | 1:8:A:LEU:HG   | 1:8:A:LEU:H     | 2        | 0.13          |
| (1,532)  | 1:8:A:LEU:HG   | 1:8:A:LEU:H     | 7        | 0.13          |
| (1,506)  | 1:7:A:THR:HA   | 1:69:A:LEU:HD21 | 6        | 0.13          |
| (1,506)  | 1:7:A:THR:HA   | 1:69:A:LEU:HD23 | 16       | 0.13          |
| (1,341)  | 1:5:A:VAL:HG21 | 1:13:A:ILE:HG13 | 2        | 0.13          |
| (1,319)  | 1:5:A:VAL:HG12 | 1:7:A:THR:HG23  | 17       | 0.13          |
| (1,319)  | 1:5:A:VAL:HG13 | 1:7:A:THR:HG23  | 18       | 0.13          |
| (1,269)  | 1:4:A:PHE:HB2  | 1:12:A:THR:HG21 | 4        | 0.13          |
| (1,269)  | 1:4:A:PHE:HB2  | 1:12:A:THR:HG22 | 4        | 0.13          |
| (1,269)  | 1:4:A:PHE:HB2  | 1:12:A:THR:HG23 | 4        | 0.13          |
| (1,148)  | 1:68:A:HIS:HA  | 1:66:A:THR:HG22 | 9        | 0.13          |
| (1,148)  | 1:68:A:HIS:HA  | 1:66:A:THR:HG23 | 12       | 0.13          |
| (1,148)  | 1:68:A:HIS:HA  | 1:66:A:THR:HG23 | 19       | 0.13          |
| (1,126)  | 1:2:A:GLN:HA   | 1:14:A:THR:HG22 | 3        | 0.13          |
| (1,126)  | 1:2:A:GLN:HA   | 1:14:A:THR:HG22 | 4        | 0.13          |
| (1,66)   | 1:28:A:ALA:HB1 | 1:27:A:LYS:HA   | 11       | 0.13          |
| (1,66)   | 1:28:A:ALA:HB1 | 1:27:A:LYS:HA   | 12       | 0.13          |
| (1,66)   | 1:28:A:ALA:HB1 | 1:27:A:LYS:HA   | 13       | 0.13          |
| (1,66)   | 1:28:A:ALA:HB1 | 1:27:A:LYS:HA   | 14       | 0.13          |
| (1,66)   | 1:28:A:ALA:HB1 | 1:27:A:LYS:HA   | 15       | 0.13          |
| (1,66)   | 1:28:A:ALA:HB1 | 1:27:A:LYS:HA   | 17       | 0.13          |
| (1,66)   | 1:28:A:ALA:HB1 | 1:27:A:LYS:HA   | 18       | 0.13          |
| (1,66)   | 1:28:A:ALA:HB1 | 1:27:A:LYS:HA   | 19       | 0.13          |
| (1,66)   | 1:28:A:ALA:HB1 | 1:27:A:LYS:HA   | 20       | 0.13          |
| (1,45)   | 1:1:A:MET:HE2  | 1:18:A:GLU:HA   | 5        | 0.13          |
| (1,37)   | 1:1:A:MET:HE2  | 1:17:A:VAL:HG22 | 11       | 0.13          |
| (1,2564) | 1:72:A:ARG:HA  | 1:72:A:ARG:HD2  | 18       | 0.12          |
| (1,2564) | 1:72:A:ARG:HA  | 1:72:A:ARG:HD3  | 18       | 0.12          |
| (1,1990) | 1:45:A:PHE:HB3 | 1:67:A:LEU:HD11 | 7        | 0.12          |
| (1,1990) | 1:45:A:PHE:HB3 | 1:67:A:LEU:HD12 | 7        | 0.12          |
| (1,1990) | 1:45:A:PHE:HB3 | 1:67:A:LEU:HD13 | 7        | 0.12          |
| (1,1990) | 1:45:A:PHE:HB3 | 1:67:A:LEU:HD21 | 7        | 0.12          |
| (1,1990) | 1:45:A:PHE:HB3 | 1:67:A:LEU:HD22 | 7        | 0.12          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1990) | 1:45:A:PHE:HB3  | 1:67:A:LEU:HD23 | 7        | 0.12          |
| (1,1887) | 1:44:A:ILE:HD11 | 1:70:A:VAL:HG12 | 2        | 0.12          |
| (1,1887) | 1:44:A:ILE:HD13 | 1:70:A:VAL:HG13 | 5        | 0.12          |
| (1,1887) | 1:44:A:ILE:HD11 | 1:70:A:VAL:HG12 | 6        | 0.12          |
| (1,1863) | 1:44:A:ILE:HD11 | 1:49:A:GLN:HB2  | 2        | 0.12          |
| (1,1863) | 1:44:A:ILE:HD11 | 1:49:A:GLN:HB3  | 2        | 0.12          |
| (1,1863) | 1:44:A:ILE:HD12 | 1:49:A:GLN:HB2  | 2        | 0.12          |
| (1,1863) | 1:44:A:ILE:HD12 | 1:49:A:GLN:HB3  | 2        | 0.12          |
| (1,1863) | 1:44:A:ILE:HD13 | 1:49:A:GLN:HB2  | 2        | 0.12          |
| (1,1863) | 1:44:A:ILE:HD13 | 1:49:A:GLN:HB3  | 2        | 0.12          |
| (1,1861) | 1:44:A:ILE:HD11 | 1:49:A:GLN:HA   | 8        | 0.12          |
| (1,1861) | 1:44:A:ILE:HD12 | 1:49:A:GLN:HA   | 8        | 0.12          |
| (1,1861) | 1:44:A:ILE:HD13 | 1:49:A:GLN:HA   | 8        | 0.12          |
| (1,1860) | 1:44:A:ILE:HD11 | 1:49:A:GLN:HA   | 1        | 0.12          |
| (1,1860) | 1:44:A:ILE:HD12 | 1:49:A:GLN:HA   | 1        | 0.12          |
| (1,1860) | 1:44:A:ILE:HD13 | 1:49:A:GLN:HA   | 1        | 0.12          |
| (1,1860) | 1:44:A:ILE:HD11 | 1:49:A:GLN:HA   | 2        | 0.12          |
| (1,1860) | 1:44:A:ILE:HD12 | 1:49:A:GLN:HA   | 2        | 0.12          |
| (1,1860) | 1:44:A:ILE:HD13 | 1:49:A:GLN:HA   | 2        | 0.12          |
| (1,1860) | 1:44:A:ILE:HD11 | 1:49:A:GLN:HA   | 7        | 0.12          |
| (1,1860) | 1:44:A:ILE:HD12 | 1:49:A:GLN:HA   | 7        | 0.12          |
| (1,1860) | 1:44:A:ILE:HD13 | 1:49:A:GLN:HA   | 7        | 0.12          |
| (1,1860) | 1:44:A:ILE:HD11 | 1:49:A:GLN:HA   | 12       | 0.12          |
| (1,1860) | 1:44:A:ILE:HD12 | 1:49:A:GLN:HA   | 12       | 0.12          |
| (1,1860) | 1:44:A:ILE:HD13 | 1:49:A:GLN:HA   | 12       | 0.12          |
| (1,1860) | 1:44:A:ILE:HD11 | 1:49:A:GLN:HA   | 17       | 0.12          |
| (1,1860) | 1:44:A:ILE:HD12 | 1:49:A:GLN:HA   | 17       | 0.12          |
| (1,1860) | 1:44:A:ILE:HD13 | 1:49:A:GLN:HA   | 17       | 0.12          |
| (1,1860) | 1:44:A:ILE:HD11 | 1:49:A:GLN:HA   | 20       | 0.12          |
| (1,1860) | 1:44:A:ILE:HD12 | 1:49:A:GLN:HA   | 20       | 0.12          |
| (1,1860) | 1:44:A:ILE:HD13 | 1:49:A:GLN:HA   | 20       | 0.12          |
| (1,1817) | 1:43:A:LEU:HD21 | 1:67:A:LEU:HB3  | 20       | 0.12          |
| (1,1776) | 1:42:A:ARG:HG3  | 1:72:A:ARG:H    | 16       | 0.12          |
| (1,1770) | 1:42:A:ARG:HG2  | 1:70:A:VAL:HG21 | 10       | 0.12          |
| (1,1770) | 1:42:A:ARG:HG2  | 1:70:A:VAL:HG22 | 10       | 0.12          |
| (1,1770) | 1:42:A:ARG:HG2  | 1:70:A:VAL:HG23 | 10       | 0.12          |
| (1,1770) | 1:42:A:ARG:HG3  | 1:70:A:VAL:HG21 | 10       | 0.12          |
| (1,1770) | 1:42:A:ARG:HG3  | 1:70:A:VAL:HG22 | 10       | 0.12          |
| (1,1770) | 1:42:A:ARG:HG3  | 1:70:A:VAL:HG23 | 10       | 0.12          |
| (1,1770) | 1:42:A:ARG:HG2  | 1:70:A:VAL:HG21 | 12       | 0.12          |
| (1,1770) | 1:42:A:ARG:HG2  | 1:70:A:VAL:HG22 | 12       | 0.12          |
| (1,1770) | 1:42:A:ARG:HG2  | 1:70:A:VAL:HG23 | 12       | 0.12          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1770) | 1:42:A:ARG:HG3  | 1:70:A:VAL:HG21 | 12       | 0.12          |
| (1,1770) | 1:42:A:ARG:HG3  | 1:70:A:VAL:HG22 | 12       | 0.12          |
| (1,1770) | 1:42:A:ARG:HG3  | 1:70:A:VAL:HG23 | 12       | 0.12          |
| (1,1770) | 1:42:A:ARG:HG2  | 1:70:A:VAL:HG21 | 14       | 0.12          |
| (1,1770) | 1:42:A:ARG:HG2  | 1:70:A:VAL:HG22 | 14       | 0.12          |
| (1,1770) | 1:42:A:ARG:HG2  | 1:70:A:VAL:HG23 | 14       | 0.12          |
| (1,1770) | 1:42:A:ARG:HG3  | 1:70:A:VAL:HG21 | 14       | 0.12          |
| (1,1770) | 1:42:A:ARG:HG3  | 1:70:A:VAL:HG22 | 14       | 0.12          |
| (1,1770) | 1:42:A:ARG:HG3  | 1:70:A:VAL:HG23 | 14       | 0.12          |
| (1,1770) | 1:42:A:ARG:HG2  | 1:70:A:VAL:HG21 | 18       | 0.12          |
| (1,1770) | 1:42:A:ARG:HG2  | 1:70:A:VAL:HG22 | 18       | 0.12          |
| (1,1770) | 1:42:A:ARG:HG2  | 1:70:A:VAL:HG23 | 18       | 0.12          |
| (1,1770) | 1:42:A:ARG:HG3  | 1:70:A:VAL:HG21 | 18       | 0.12          |
| (1,1770) | 1:42:A:ARG:HG3  | 1:70:A:VAL:HG22 | 18       | 0.12          |
| (1,1770) | 1:42:A:ARG:HG3  | 1:70:A:VAL:HG23 | 18       | 0.12          |
| (1,1722) | 1:41:A:GLN:H    | 1:71:A:LEU:HD23 | 6        | 0.12          |
| (1,1512) | 1:34:A:GLU:HG3  | 1:69:A:LEU:HD23 | 17       | 0.12          |
| (1,1511) | 1:34:A:GLU:HG3  | 1:69:A:LEU:HD21 | 1        | 0.12          |
| (1,1475) | 1:33:A:LYS:HD2  | 1:33:A:LYS:HA   | 20       | 0.12          |
| (1,1475) | 1:33:A:LYS:HD3  | 1:33:A:LYS:HA   | 20       | 0.12          |
| (1,973)  | 1:22:A:THR:HA   | 1:55:A:THR:HB   | 13       | 0.12          |
| (1,914)  | 1:52:A:ASP:HB2  | 1:24:A:GLU:HB2  | 9        | 0.12          |
| (1,790)  | 1:17:A:VAL:HA   | 1:29:A:LYS:HE2  | 16       | 0.12          |
| (1,790)  | 1:17:A:VAL:HA   | 1:29:A:LYS:HE3  | 16       | 0.12          |
| (1,630)  | 1:13:A:ILE:HG22 | 1:15:A:LEU:HD23 | 20       | 0.12          |
| (1,562)  | 1:9:A:THR:HG21  | 1:11:A:LYS:HD2  | 15       | 0.12          |
| (1,562)  | 1:9:A:THR:HG21  | 1:11:A:LYS:HD3  | 15       | 0.12          |
| (1,562)  | 1:9:A:THR:HG22  | 1:11:A:LYS:HD2  | 15       | 0.12          |
| (1,562)  | 1:9:A:THR:HG22  | 1:11:A:LYS:HD3  | 15       | 0.12          |
| (1,562)  | 1:9:A:THR:HG23  | 1:11:A:LYS:HD2  | 15       | 0.12          |
| (1,562)  | 1:9:A:THR:HG23  | 1:11:A:LYS:HD3  | 15       | 0.12          |
| (1,562)  | 1:9:A:THR:HG21  | 1:11:A:LYS:HD2  | 16       | 0.12          |
| (1,562)  | 1:9:A:THR:HG21  | 1:11:A:LYS:HD3  | 16       | 0.12          |
| (1,562)  | 1:9:A:THR:HG22  | 1:11:A:LYS:HD2  | 16       | 0.12          |
| (1,562)  | 1:9:A:THR:HG22  | 1:11:A:LYS:HD3  | 16       | 0.12          |
| (1,562)  | 1:9:A:THR:HG23  | 1:11:A:LYS:HD2  | 16       | 0.12          |
| (1,562)  | 1:9:A:THR:HG23  | 1:11:A:LYS:HD3  | 16       | 0.12          |
| (1,532)  | 1:8:A:LEU:HG    | 1:8:A:LEU:H     | 10       | 0.12          |
| (1,532)  | 1:8:A:LEU:HG    | 1:8:A:LEU:H     | 20       | 0.12          |
| (1,506)  | 1:7:A:THR:HA    | 1:69:A:LEU:HD22 | 11       | 0.12          |
| (1,356)  | 1:17:A:VAL:HG11 | 1:29:A:LYS:HG3  | 1        | 0.12          |
| (1,356)  | 1:17:A:VAL:HG11 | 1:29:A:LYS:HG3  | 6        | 0.12          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,356)  | 1:17:A:VAL:HG12 | 1:29:A:LYS:HG3  | 11       | 0.12          |
| (1,356)  | 1:17:A:VAL:HG12 | 1:29:A:LYS:HG3  | 14       | 0.12          |
| (1,341)  | 1:5:A:VAL:HG21  | 1:13:A:ILE:HG13 | 7        | 0.12          |
| (1,319)  | 1:5:A:VAL:HG13  | 1:7:A:THR:HG23  | 14       | 0.12          |
| (1,264)  | 1:4:A:PHE:HA    | 1:12:A:THR:HG21 | 8        | 0.12          |
| (1,177)  | 1:29:A:LYS:HA   | 1:15:A:LEU:HD22 | 15       | 0.12          |
| (1,79)   | 1:1:A:MET:HE2   | 1:56:A:LEU:HD13 | 5        | 0.12          |
| (1,48)   | 1:1:A:MET:HE3   | 1:19:A:PRO:HA   | 9        | 0.12          |
| (1,19)   | 1:1:A:MET:HE2   | 1:3:A:ILE:HD11  | 12       | 0.12          |
| (1,1903) | 1:44:A:ILE:HG21 | 1:68:A:HIS:HB3  | 3        | 0.11          |
| (1,1903) | 1:44:A:ILE:HG22 | 1:68:A:HIS:HB3  | 3        | 0.11          |
| (1,1903) | 1:44:A:ILE:HG23 | 1:68:A:HIS:HB3  | 3        | 0.11          |
| (1,1903) | 1:44:A:ILE:HG21 | 1:68:A:HIS:HB3  | 10       | 0.11          |
| (1,1903) | 1:44:A:ILE:HG22 | 1:68:A:HIS:HB3  | 10       | 0.11          |
| (1,1903) | 1:44:A:ILE:HG23 | 1:68:A:HIS:HB3  | 10       | 0.11          |
| (1,1892) | 1:44:A:ILE:HB   | 1:68:A:HIS:HB3  | 9        | 0.11          |
| (1,1887) | 1:44:A:ILE:HD11 | 1:70:A:VAL:HG12 | 7        | 0.11          |
| (1,1878) | 1:44:A:ILE:HG21 | 1:49:A:GLN:HB2  | 11       | 0.11          |
| (1,1878) | 1:44:A:ILE:HG21 | 1:49:A:GLN:HB3  | 11       | 0.11          |
| (1,1878) | 1:44:A:ILE:HG22 | 1:49:A:GLN:HB2  | 11       | 0.11          |
| (1,1878) | 1:44:A:ILE:HG22 | 1:49:A:GLN:HB3  | 11       | 0.11          |
| (1,1878) | 1:44:A:ILE:HG23 | 1:49:A:GLN:HB2  | 11       | 0.11          |
| (1,1878) | 1:44:A:ILE:HG23 | 1:49:A:GLN:HB3  | 11       | 0.11          |
| (1,1867) | 1:44:A:ILE:HG12 | 1:49:A:GLN:HA   | 3        | 0.11          |
| (1,1867) | 1:44:A:ILE:HG13 | 1:49:A:GLN:HA   | 3        | 0.11          |
| (1,1867) | 1:44:A:ILE:HG12 | 1:49:A:GLN:HA   | 13       | 0.11          |
| (1,1867) | 1:44:A:ILE:HG13 | 1:49:A:GLN:HA   | 13       | 0.11          |
| (1,1863) | 1:44:A:ILE:HD11 | 1:49:A:GLN:HB2  | 7        | 0.11          |
| (1,1863) | 1:44:A:ILE:HD11 | 1:49:A:GLN:HB3  | 7        | 0.11          |
| (1,1863) | 1:44:A:ILE:HD12 | 1:49:A:GLN:HB2  | 7        | 0.11          |
| (1,1863) | 1:44:A:ILE:HD12 | 1:49:A:GLN:HB3  | 7        | 0.11          |
| (1,1863) | 1:44:A:ILE:HD13 | 1:49:A:GLN:HB2  | 7        | 0.11          |
| (1,1863) | 1:44:A:ILE:HD13 | 1:49:A:GLN:HB3  | 7        | 0.11          |
| (1,1863) | 1:44:A:ILE:HD11 | 1:49:A:GLN:HB2  | 9        | 0.11          |
| (1,1863) | 1:44:A:ILE:HD11 | 1:49:A:GLN:HB3  | 9        | 0.11          |
| (1,1863) | 1:44:A:ILE:HD12 | 1:49:A:GLN:HB2  | 9        | 0.11          |
| (1,1863) | 1:44:A:ILE:HD12 | 1:49:A:GLN:HB3  | 9        | 0.11          |
| (1,1863) | 1:44:A:ILE:HD13 | 1:49:A:GLN:HB2  | 9        | 0.11          |
| (1,1863) | 1:44:A:ILE:HD13 | 1:49:A:GLN:HB3  | 9        | 0.11          |
| (1,1863) | 1:44:A:ILE:HD11 | 1:49:A:GLN:HB2  | 11       | 0.11          |
| (1,1863) | 1:44:A:ILE:HD11 | 1:49:A:GLN:HB3  | 11       | 0.11          |
| (1,1863) | 1:44:A:ILE:HD12 | 1:49:A:GLN:HB2  | 11       | 0.11          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1863) | 1:44:A:ILE:HD12 | 1:49:A:GLN:HB3  | 11       | 0.11          |
| (1,1863) | 1:44:A:ILE:HD13 | 1:49:A:GLN:HB2  | 11       | 0.11          |
| (1,1863) | 1:44:A:ILE:HD13 | 1:49:A:GLN:HB3  | 11       | 0.11          |
| (1,1863) | 1:44:A:ILE:HD11 | 1:49:A:GLN:HB2  | 18       | 0.11          |
| (1,1863) | 1:44:A:ILE:HD11 | 1:49:A:GLN:HB3  | 18       | 0.11          |
| (1,1863) | 1:44:A:ILE:HD12 | 1:49:A:GLN:HB2  | 18       | 0.11          |
| (1,1863) | 1:44:A:ILE:HD12 | 1:49:A:GLN:HB3  | 18       | 0.11          |
| (1,1863) | 1:44:A:ILE:HD13 | 1:49:A:GLN:HB2  | 18       | 0.11          |
| (1,1863) | 1:44:A:ILE:HD13 | 1:49:A:GLN:HB3  | 18       | 0.11          |
| (1,1863) | 1:44:A:ILE:HD11 | 1:49:A:GLN:HB2  | 19       | 0.11          |
| (1,1863) | 1:44:A:ILE:HD11 | 1:49:A:GLN:HB3  | 19       | 0.11          |
| (1,1863) | 1:44:A:ILE:HD12 | 1:49:A:GLN:HB2  | 19       | 0.11          |
| (1,1863) | 1:44:A:ILE:HD12 | 1:49:A:GLN:HB3  | 19       | 0.11          |
| (1,1863) | 1:44:A:ILE:HD13 | 1:49:A:GLN:HB2  | 19       | 0.11          |
| (1,1863) | 1:44:A:ILE:HD13 | 1:49:A:GLN:HB3  | 19       | 0.11          |
| (1,1860) | 1:44:A:ILE:HD11 | 1:49:A:GLN:HA   | 5        | 0.11          |
| (1,1860) | 1:44:A:ILE:HD12 | 1:49:A:GLN:HA   | 5        | 0.11          |
| (1,1860) | 1:44:A:ILE:HD13 | 1:49:A:GLN:HA   | 5        | 0.11          |
| (1,1860) | 1:44:A:ILE:HD11 | 1:49:A:GLN:HA   | 11       | 0.11          |
| (1,1860) | 1:44:A:ILE:HD12 | 1:49:A:GLN:HA   | 11       | 0.11          |
| (1,1860) | 1:44:A:ILE:HD13 | 1:49:A:GLN:HA   | 11       | 0.11          |
| (1,1860) | 1:44:A:ILE:HD11 | 1:49:A:GLN:HA   | 18       | 0.11          |
| (1,1860) | 1:44:A:ILE:HD12 | 1:49:A:GLN:HA   | 18       | 0.11          |
| (1,1860) | 1:44:A:ILE:HD13 | 1:49:A:GLN:HA   | 18       | 0.11          |
| (1,1860) | 1:44:A:ILE:HD11 | 1:49:A:GLN:HA   | 19       | 0.11          |
| (1,1860) | 1:44:A:ILE:HD12 | 1:49:A:GLN:HA   | 19       | 0.11          |
| (1,1860) | 1:44:A:ILE:HD13 | 1:49:A:GLN:HA   | 19       | 0.11          |
| (1,1817) | 1:43:A:LEU:HD23 | 1:67:A:LEU:HB3  | 5        | 0.11          |
| (1,1817) | 1:43:A:LEU:HD23 | 1:67:A:LEU:HB3  | 7        | 0.11          |
| (1,1817) | 1:43:A:LEU:HD21 | 1:67:A:LEU:HB3  | 12       | 0.11          |
| (1,1770) | 1:42:A:ARG:HG2  | 1:70:A:VAL:HG21 | 7        | 0.11          |
| (1,1770) | 1:42:A:ARG:HG2  | 1:70:A:VAL:HG22 | 7        | 0.11          |
| (1,1770) | 1:42:A:ARG:HG2  | 1:70:A:VAL:HG23 | 7        | 0.11          |
| (1,1770) | 1:42:A:ARG:HG3  | 1:70:A:VAL:HG21 | 7        | 0.11          |
| (1,1770) | 1:42:A:ARG:HG3  | 1:70:A:VAL:HG22 | 7        | 0.11          |
| (1,1770) | 1:42:A:ARG:HG3  | 1:70:A:VAL:HG23 | 7        | 0.11          |
| (1,1770) | 1:42:A:ARG:HG2  | 1:70:A:VAL:HG21 | 19       | 0.11          |
| (1,1770) | 1:42:A:ARG:HG2  | 1:70:A:VAL:HG22 | 19       | 0.11          |
| (1,1770) | 1:42:A:ARG:HG2  | 1:70:A:VAL:HG23 | 19       | 0.11          |
| (1,1770) | 1:42:A:ARG:HG3  | 1:70:A:VAL:HG21 | 19       | 0.11          |
| (1,1770) | 1:42:A:ARG:HG3  | 1:70:A:VAL:HG22 | 19       | 0.11          |
| (1,1770) | 1:42:A:ARG:HG3  | 1:70:A:VAL:HG23 | 19       | 0.11          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,1713) | 1:41:A:GLN:HA  | 1:71:A:LEU:HD23 | 18       | 0.11          |
| (1,1511) | 1:34:A:GLU:HG3 | 1:69:A:LEU:HD23 | 15       | 0.11          |
| (1,1149) | 1:24:A:GLU:HA  | 1:52:A:ASP:HB3  | 6        | 0.11          |
| (1,1149) | 1:24:A:GLU:HA  | 1:52:A:ASP:HB3  | 9        | 0.11          |
| (1,973)  | 1:22:A:THR:HA  | 1:55:A:THR:HB   | 4        | 0.11          |
| (1,973)  | 1:22:A:THR:HA  | 1:55:A:THR:HB   | 15       | 0.11          |
| (1,973)  | 1:22:A:THR:HA  | 1:55:A:THR:HB   | 19       | 0.11          |
| (1,973)  | 1:22:A:THR:HA  | 1:55:A:THR:HB   | 20       | 0.11          |
| (1,914)  | 1:52:A:ASP:HB2 | 1:24:A:GLU:HB2  | 5        | 0.11          |
| (1,914)  | 1:52:A:ASP:HB2 | 1:24:A:GLU:HB2  | 6        | 0.11          |
| (1,914)  | 1:52:A:ASP:HB2 | 1:24:A:GLU:HB2  | 7        | 0.11          |
| (1,562)  | 1:9:A:THR:HG21 | 1:11:A:LYS:HD2  | 1        | 0.11          |
| (1,562)  | 1:9:A:THR:HG21 | 1:11:A:LYS:HD3  | 1        | 0.11          |
| (1,562)  | 1:9:A:THR:HG22 | 1:11:A:LYS:HD2  | 1        | 0.11          |
| (1,562)  | 1:9:A:THR:HG22 | 1:11:A:LYS:HD3  | 1        | 0.11          |
| (1,562)  | 1:9:A:THR:HG23 | 1:11:A:LYS:HD2  | 1        | 0.11          |
| (1,562)  | 1:9:A:THR:HG23 | 1:11:A:LYS:HD3  | 1        | 0.11          |
| (1,562)  | 1:9:A:THR:HG21 | 1:11:A:LYS:HD2  | 5        | 0.11          |
| (1,562)  | 1:9:A:THR:HG21 | 1:11:A:LYS:HD3  | 5        | 0.11          |
| (1,562)  | 1:9:A:THR:HG22 | 1:11:A:LYS:HD2  | 5        | 0.11          |
| (1,562)  | 1:9:A:THR:HG22 | 1:11:A:LYS:HD3  | 5        | 0.11          |
| (1,562)  | 1:9:A:THR:HG23 | 1:11:A:LYS:HD2  | 5        | 0.11          |
| (1,562)  | 1:9:A:THR:HG23 | 1:11:A:LYS:HD3  | 5        | 0.11          |
| (1,562)  | 1:9:A:THR:HG21 | 1:11:A:LYS:HD2  | 6        | 0.11          |
| (1,562)  | 1:9:A:THR:HG21 | 1:11:A:LYS:HD3  | 6        | 0.11          |
| (1,562)  | 1:9:A:THR:HG22 | 1:11:A:LYS:HD2  | 6        | 0.11          |
| (1,562)  | 1:9:A:THR:HG22 | 1:11:A:LYS:HD3  | 6        | 0.11          |
| (1,562)  | 1:9:A:THR:HG23 | 1:11:A:LYS:HD2  | 6        | 0.11          |
| (1,562)  | 1:9:A:THR:HG23 | 1:11:A:LYS:HD3  | 6        | 0.11          |
| (1,562)  | 1:9:A:THR:HG21 | 1:11:A:LYS:HD2  | 8        | 0.11          |
| (1,562)  | 1:9:A:THR:HG21 | 1:11:A:LYS:HD3  | 8        | 0.11          |
| (1,562)  | 1:9:A:THR:HG22 | 1:11:A:LYS:HD2  | 8        | 0.11          |
| (1,562)  | 1:9:A:THR:HG22 | 1:11:A:LYS:HD3  | 8        | 0.11          |
| (1,562)  | 1:9:A:THR:HG23 | 1:11:A:LYS:HD2  | 8        | 0.11          |
| (1,562)  | 1:9:A:THR:HG23 | 1:11:A:LYS:HD3  | 8        | 0.11          |
| (1,562)  | 1:9:A:THR:HG21 | 1:11:A:LYS:HD2  | 14       | 0.11          |
| (1,562)  | 1:9:A:THR:HG21 | 1:11:A:LYS:HD3  | 14       | 0.11          |
| (1,562)  | 1:9:A:THR:HG22 | 1:11:A:LYS:HD2  | 14       | 0.11          |
| (1,562)  | 1:9:A:THR:HG22 | 1:11:A:LYS:HD3  | 14       | 0.11          |
| (1,562)  | 1:9:A:THR:HG23 | 1:11:A:LYS:HD2  | 14       | 0.11          |
| (1,562)  | 1:9:A:THR:HG23 | 1:11:A:LYS:HD3  | 14       | 0.11          |
| (1,532)  | 1:8:A:LEU:HG   | 1:8:A:LEU:H     | 3        | 0.11          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,517)  | 1:7:A:THR:HG23  | 1:69:A:LEU:HD22 | 15       | 0.11          |
| (1,506)  | 1:7:A:THR:HA    | 1:69:A:LEU:HD22 | 12       | 0.11          |
| (1,506)  | 1:7:A:THR:HA    | 1:69:A:LEU:HD22 | 18       | 0.11          |
| (1,463)  | 1:6:A:LYS:HG3   | 1:66:A:THR:HG21 | 3        | 0.11          |
| (1,459)  | 1:6:A:LYS:HE3   | 1:66:A:THR:HG23 | 5        | 0.11          |
| (1,420)  | 1:6:A:LYS:HE2   | 1:10:A:GLY:HA2  | 11       | 0.11          |
| (1,420)  | 1:6:A:LYS:HE2   | 1:10:A:GLY:HA3  | 11       | 0.11          |
| (1,420)  | 1:6:A:LYS:HE3   | 1:10:A:GLY:HA2  | 11       | 0.11          |
| (1,420)  | 1:6:A:LYS:HE3   | 1:10:A:GLY:HA3  | 11       | 0.11          |
| (1,420)  | 1:6:A:LYS:HE2   | 1:10:A:GLY:HA2  | 12       | 0.11          |
| (1,420)  | 1:6:A:LYS:HE2   | 1:10:A:GLY:HA3  | 12       | 0.11          |
| (1,420)  | 1:6:A:LYS:HE3   | 1:10:A:GLY:HA2  | 12       | 0.11          |
| (1,420)  | 1:6:A:LYS:HE3   | 1:10:A:GLY:HA3  | 12       | 0.11          |
| (1,356)  | 1:17:A:VAL:HG11 | 1:29:A:LYS:HG3  | 12       | 0.11          |
| (1,356)  | 1:17:A:VAL:HG12 | 1:29:A:LYS:HG3  | 19       | 0.11          |
| (1,319)  | 1:5:A:VAL:HG11  | 1:7:A:THR:HG22  | 7        | 0.11          |
| (1,318)  | 1:5:A:VAL:HG11  | 1:7:A:THR:HG23  | 20       | 0.11          |
| (1,269)  | 1:4:A:PHE:HB2   | 1:12:A:THR:HG21 | 13       | 0.11          |
| (1,269)  | 1:4:A:PHE:HB2   | 1:12:A:THR:HG22 | 13       | 0.11          |
| (1,269)  | 1:4:A:PHE:HB2   | 1:12:A:THR:HG23 | 13       | 0.11          |
| (1,177)  | 1:29:A:LYS:HA   | 1:15:A:LEU:HD22 | 16       | 0.11          |
| (1,48)   | 1:1:A:MET:HE3   | 1:19:A:PRO:HA   | 8        | 0.11          |
| (1,38)   | 1:1:A:MET:HE3   | 1:17:A:VAL:HG22 | 7        | 0.11          |
| (1,38)   | 1:1:A:MET:HE3   | 1:17:A:VAL:HG22 | 8        | 0.11          |
| (1,1887) | 1:44:A:ILE:HD11 | 1:70:A:VAL:HG11 | 20       | 0.1           |
| (1,1878) | 1:44:A:ILE:HG21 | 1:49:A:GLN:HB2  | 18       | 0.1           |
| (1,1878) | 1:44:A:ILE:HG21 | 1:49:A:GLN:HB3  | 18       | 0.1           |
| (1,1878) | 1:44:A:ILE:HG22 | 1:49:A:GLN:HB2  | 18       | 0.1           |
| (1,1878) | 1:44:A:ILE:HG22 | 1:49:A:GLN:HB3  | 18       | 0.1           |
| (1,1878) | 1:44:A:ILE:HG23 | 1:49:A:GLN:HB2  | 18       | 0.1           |
| (1,1878) | 1:44:A:ILE:HG23 | 1:49:A:GLN:HB3  | 18       | 0.1           |
| (1,1770) | 1:42:A:ARG:HG2  | 1:70:A:VAL:HG21 | 9        | 0.1           |
| (1,1770) | 1:42:A:ARG:HG2  | 1:70:A:VAL:HG22 | 9        | 0.1           |
| (1,1770) | 1:42:A:ARG:HG2  | 1:70:A:VAL:HG23 | 9        | 0.1           |
| (1,1770) | 1:42:A:ARG:HG3  | 1:70:A:VAL:HG21 | 9        | 0.1           |
| (1,1770) | 1:42:A:ARG:HG3  | 1:70:A:VAL:HG22 | 9        | 0.1           |
| (1,1770) | 1:42:A:ARG:HG3  | 1:70:A:VAL:HG23 | 9        | 0.1           |
| (1,1722) | 1:41:A:GLN:H    | 1:71:A:LEU:HD23 | 10       | 0.1           |
| (1,1695) | 1:40:A:GLN:HG2  | 1:73:A:LEU:HA   | 20       | 0.1           |
| (1,1695) | 1:40:A:GLN:HG3  | 1:73:A:LEU:HA   | 20       | 0.1           |
| (1,1475) | 1:33:A:LYS:HD2  | 1:33:A:LYS:HA   | 9        | 0.1           |
| (1,1475) | 1:33:A:LYS:HD3  | 1:33:A:LYS:HA   | 9        | 0.1           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1285) | 1:27:A:LYS:HE2  | 1:43:A:LEU:HB3  | 15       | 0.1           |
| (1,1285) | 1:27:A:LYS:HE3  | 1:43:A:LEU:HB3  | 15       | 0.1           |
| (1,1149) | 1:24:A:GLU:HA   | 1:52:A:ASP:HB3  | 1        | 0.1           |
| (1,1149) | 1:24:A:GLU:HA   | 1:52:A:ASP:HB3  | 7        | 0.1           |
| (1,1149) | 1:24:A:GLU:HA   | 1:52:A:ASP:HB3  | 10       | 0.1           |
| (1,1149) | 1:24:A:GLU:HA   | 1:52:A:ASP:HB3  | 14       | 0.1           |
| (1,1149) | 1:24:A:GLU:HA   | 1:52:A:ASP:HB3  | 15       | 0.1           |
| (1,973)  | 1:22:A:THR:HA   | 1:55:A:THR:HB   | 2        | 0.1           |
| (1,973)  | 1:22:A:THR:HA   | 1:55:A:THR:HB   | 3        | 0.1           |
| (1,973)  | 1:22:A:THR:HA   | 1:55:A:THR:HB   | 5        | 0.1           |
| (1,973)  | 1:22:A:THR:HA   | 1:55:A:THR:HB   | 9        | 0.1           |
| (1,973)  | 1:22:A:THR:HA   | 1:55:A:THR:HB   | 10       | 0.1           |
| (1,973)  | 1:22:A:THR:HA   | 1:55:A:THR:HB   | 14       | 0.1           |
| (1,914)  | 1:52:A:ASP:HB2  | 1:24:A:GLU:HB2  | 1        | 0.1           |
| (1,914)  | 1:52:A:ASP:HB2  | 1:24:A:GLU:HB2  | 16       | 0.1           |
| (1,914)  | 1:52:A:ASP:HB2  | 1:24:A:GLU:HB2  | 20       | 0.1           |
| (1,788)  | 1:17:A:VAL:HA   | 1:29:A:LYS:HE2  | 16       | 0.1           |
| (1,788)  | 1:17:A:VAL:HA   | 1:29:A:LYS:HE3  | 16       | 0.1           |
| (1,598)  | 1:12:A:THR:HA   | 1:13:A:ILE:HG21 | 1        | 0.1           |
| (1,598)  | 1:12:A:THR:HA   | 1:13:A:ILE:HG22 | 1        | 0.1           |
| (1,598)  | 1:12:A:THR:HA   | 1:13:A:ILE:HG23 | 1        | 0.1           |
| (1,598)  | 1:12:A:THR:HA   | 1:13:A:ILE:HG21 | 5        | 0.1           |
| (1,598)  | 1:12:A:THR:HA   | 1:13:A:ILE:HG22 | 5        | 0.1           |
| (1,598)  | 1:12:A:THR:HA   | 1:13:A:ILE:HG23 | 5        | 0.1           |
| (1,598)  | 1:12:A:THR:HA   | 1:13:A:ILE:HG21 | 19       | 0.1           |
| (1,598)  | 1:12:A:THR:HA   | 1:13:A:ILE:HG22 | 19       | 0.1           |
| (1,598)  | 1:12:A:THR:HA   | 1:13:A:ILE:HG23 | 19       | 0.1           |
| (1,562)  | 1:9:A:THR:HG21  | 1:11:A:LYS:HD2  | 19       | 0.1           |
| (1,562)  | 1:9:A:THR:HG21  | 1:11:A:LYS:HD3  | 19       | 0.1           |
| (1,562)  | 1:9:A:THR:HG22  | 1:11:A:LYS:HD2  | 19       | 0.1           |
| (1,562)  | 1:9:A:THR:HG22  | 1:11:A:LYS:HD3  | 19       | 0.1           |
| (1,562)  | 1:9:A:THR:HG23  | 1:11:A:LYS:HD2  | 19       | 0.1           |
| (1,562)  | 1:9:A:THR:HG23  | 1:11:A:LYS:HD3  | 19       | 0.1           |
| (1,364)  | 1:5:A:VAL:HA    | 1:66:A:THR:HG21 | 3        | 0.1           |
| (1,356)  | 1:17:A:VAL:HG11 | 1:29:A:LYS:HG3  | 2        | 0.1           |
| (1,339)  | 1:5:A:VAL:HG23  | 1:13:A:ILE:HG13 | 19       | 0.1           |
| (1,48)   | 1:1:A:MET:HE3   | 1:19:A:PRO:HA   | 10       | 0.1           |

## 10 Dihedral-angle violation analysis ⓘ

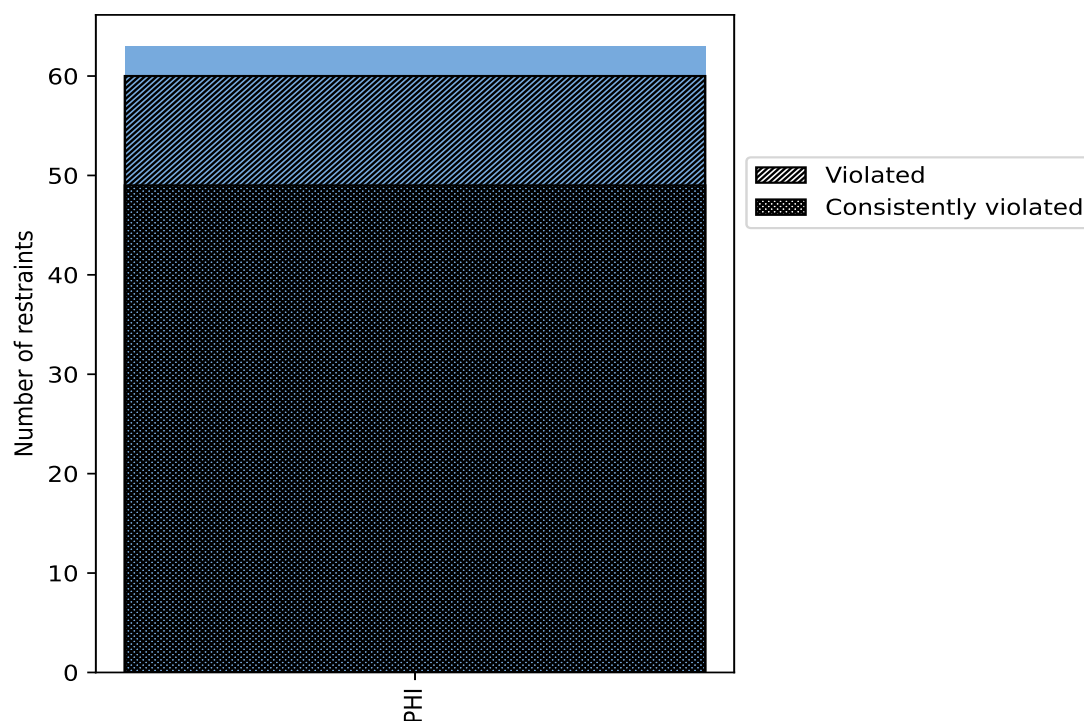
### 10.1 Summary of dihedral-angle violations ⓘ

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

| Angle type | Count | % <sup>1</sup> | Violated <sup>3</sup> |                |                | Consistently Violated <sup>4</sup> |                |                |
|------------|-------|----------------|-----------------------|----------------|----------------|------------------------------------|----------------|----------------|
|            |       |                | Count                 | % <sup>2</sup> | % <sup>1</sup> | Count                              | % <sup>2</sup> | % <sup>1</sup> |
| PHI        | 63    | 100.0          | 60                    | 95.2           | 95.2           | 49                                 | 77.8           | 77.8           |
| Total      | 63    | 100.0          | 60                    | 95.2           | 95.2           | 49                                 | 77.8           | 77.8           |

<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 ⓘ



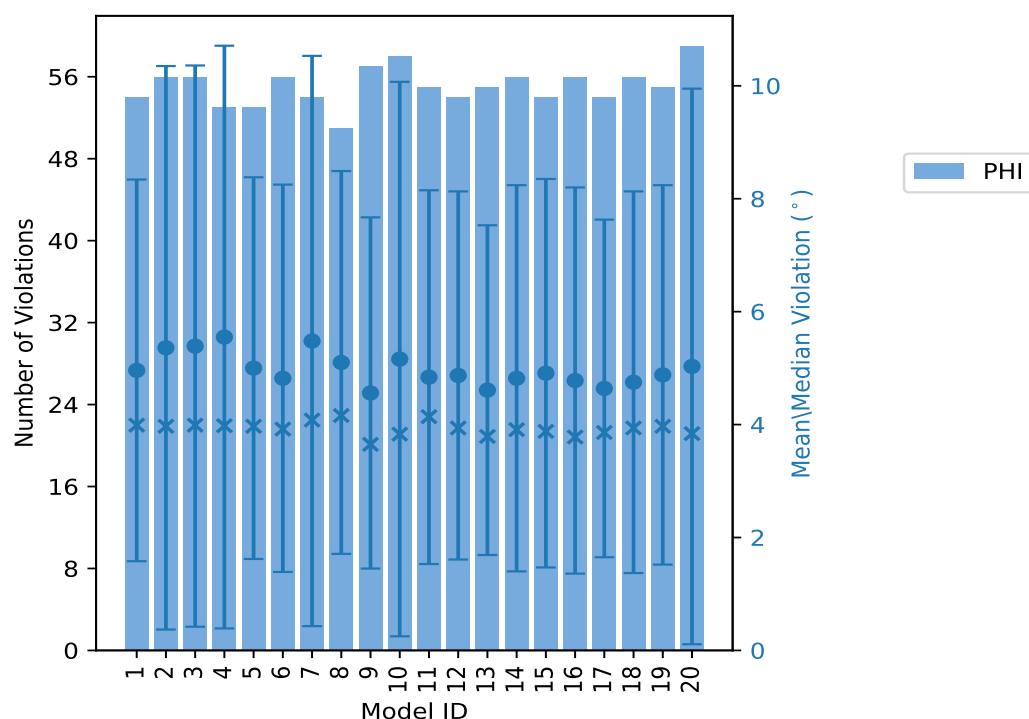
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

## 10.2 Dihedral-angle violation statistics for each model

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

| Model ID | Number of violations |       | Mean (°) | Max (°) | SD (°) | Median (°) |
|----------|----------------------|-------|----------|---------|--------|------------|
|          | PHI                  | Total |          |         |        |            |
| 1        | 54                   | 54    | 4.96     | 17.15   | 3.38   | 3.99       |
| 2        | 56                   | 56    | 5.36     | 34.09   | 4.99   | 3.97       |
| 3        | 56                   | 56    | 5.39     | 33.91   | 4.97   | 3.99       |
| 4        | 53                   | 53    | 5.55     | 34.33   | 5.16   | 3.98       |
| 5        | 53                   | 53    | 5.0      | 16.99   | 3.38   | 3.97       |
| 6        | 56                   | 56    | 4.82     | 17.67   | 3.43   | 3.92       |
| 7        | 54                   | 54    | 5.48     | 34.16   | 5.05   | 4.08       |
| 8        | 51                   | 51    | 5.1      | 16.99   | 3.39   | 4.16       |
| 9        | 57                   | 57    | 4.56     | 14.61   | 3.11   | 3.65       |
| 10       | 58                   | 58    | 5.16     | 33.92   | 4.91   | 3.83       |
| 11       | 55                   | 55    | 4.84     | 15.3    | 3.31   | 4.14       |
| 12       | 54                   | 54    | 4.87     | 15.41   | 3.26   | 3.94       |
| 13       | 55                   | 55    | 4.61     | 14.43   | 2.92   | 3.79       |
| 14       | 56                   | 56    | 4.82     | 17.53   | 3.42   | 3.91       |
| 15       | 54                   | 54    | 4.91     | 17.53   | 3.44   | 3.88       |
| 16       | 56                   | 56    | 4.78     | 17.61   | 3.42   | 3.78       |
| 17       | 54                   | 54    | 4.64     | 14.3    | 2.99   | 3.86       |
| 18       | 56                   | 56    | 4.75     | 17.05   | 3.38   | 3.94       |
| 19       | 55                   | 55    | 4.88     | 16.59   | 3.36   | 3.97       |
| 20       | 59                   | 59    | 5.03     | 33.7    | 4.92   | 3.84       |

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

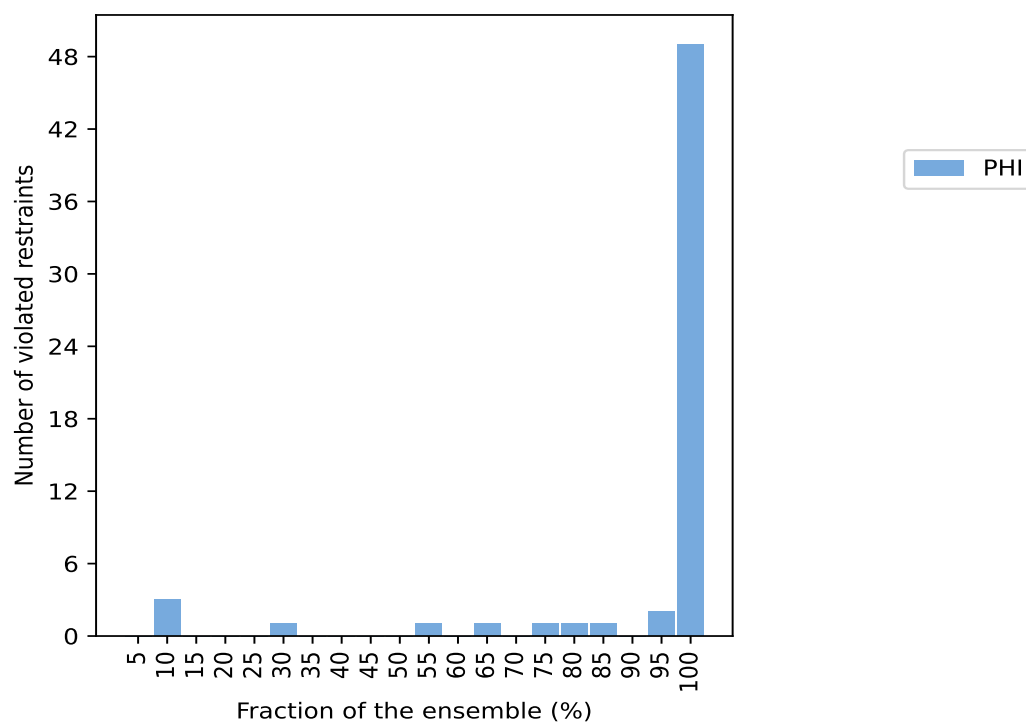
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| Number of violated restraints |       | Fraction of the ensemble |       |
|-------------------------------|-------|--------------------------|-------|
| PHI                           | Total | Count <sup>1</sup>       | %     |
| 0                             | 0     | 12                       | 60.0  |
| 1                             | 1     | 13                       | 65.0  |
| 0                             | 0     | 14                       | 70.0  |
| 1                             | 1     | 15                       | 75.0  |
| 1                             | 1     | 16                       | 80.0  |
| 1                             | 1     | 17                       | 85.0  |
| 0                             | 0     | 18                       | 90.0  |
| 2                             | 2     | 19                       | 95.0  |
| 49                            | 49    | 20                       | 100.0 |

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

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

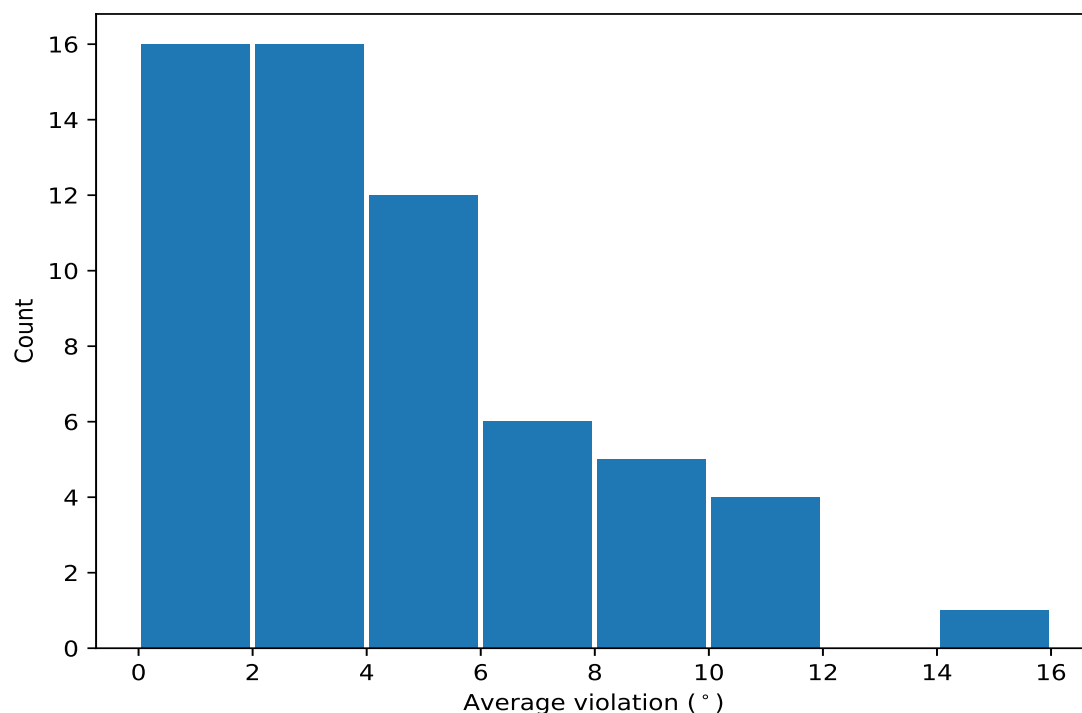


## 10.4 Most violated dihedral-angle restraints in the ensemble ⓘ

### 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 |
|--------|--------------|--------------|---------------|--------------|---------------------|-------|-----------------|--------|
| (1,44) | 1:51:A:GLU:C | 1:52:A:ASP:N | 1:52:A:ASP:CA | 1:52:A:ASP:C | 20                  | 14.48 | 0.14            | 14.49  |
| (1,7)  | 1:8:A:LEU:C  | 1:9:A:THR:N  | 1:9:A:THR:CA  | 1:9:A:THR:C  | 20                  | 11.92 | 14.47           | 2.68   |
| (1,2)  | 1:3:A:ILE:C  | 1:4:A:PHE:N  | 1:4:A:PHE:CA  | 1:4:A:PHE:C  | 20                  | 11.76 | 0.33            | 11.84  |
| (1,8)  | 1:10:A:GLY:C | 1:11:A:LYS:N | 1:11:A:LYS:CA | 1:11:A:LYS:C | 20                  | 11.17 | 6.42            | 15.36  |
| (1,49) | 1:56:A:LEU:C | 1:57:A:SER:N | 1:57:A:SER:CA | 1:57:A:SER:C | 20                  | 10.76 | 0.43            | 10.86  |
| (1,34) | 1:40:A:GLN:C | 1:41:A:GLN:N | 1:41:A:GLN:CA | 1:41:A:GLN:C | 20                  | 9.5   | 0.49            | 9.31   |
| (1,13) | 1:15:A:LEU:C | 1:16:A:GLU:N | 1:16:A:GLU:CA | 1:16:A:GLU:C | 20                  | 8.84  | 0.38            | 8.82   |
| (1,21) | 1:25:A:ASN:C | 1:26:A:VAL:N | 1:26:A:VAL:CA | 1:26:A:VAL:C | 20                  | 8.68  | 0.32            | 8.59   |
| (1,54) | 1:61:A:ILE:C | 1:62:A:GLN:N | 1:62:A:GLN:CA | 1:62:A:GLN:C | 20                  | 8.5   | 0.2             | 8.48   |
| (1,29) | 1:33:A:LYS:C | 1:34:A:GLU:N | 1:34:A:GLU:CA | 1:34:A:GLU:C | 20                  | 8.02  | 0.27            | 7.94   |
| (1,3)  | 1:4:A:PHE:C  | 1:5:A:VAL:N  | 1:5:A:VAL:CA  | 1:5:A:VAL:C  | 20                  | 7.97  | 0.39            | 7.82   |
| (1,63) | 1:70:A:VAL:C | 1:71:A:LEU:N | 1:71:A:LEU:CA | 1:71:A:LEU:C | 20                  | 7.67  | 1.5             | 7.92   |
| (1,35) | 1:41:A:GLN:C | 1:42:A:ARG:N | 1:42:A:ARG:CA | 1:42:A:ARG:C | 20                  | 7.4   | 0.21            | 7.44   |
| (1,55) | 1:62:A:GLN:C | 1:63:A:LYS:N | 1:63:A:LYS:CA | 1:63:A:LYS:C | 20                  | 7.07  | 0.14            | 7.07   |
| (1,48) | 1:55:A:THR:C | 1:56:A:LEU:N | 1:56:A:LEU:CA | 1:56:A:LEU:C | 20                  | 6.43  | 0.12            | 6.43   |
| (1,27) | 1:31:A:GLN:C | 1:32:A:ASP:N | 1:32:A:ASP:CA | 1:32:A:ASP:C | 20                  | 5.98  | 0.23            | 6.04   |
| (1,52) | 1:59:A:TYR:C | 1:60:A:ASN:N | 1:60:A:ASN:CA | 1:60:A:ASN:C | 20                  | 5.78  | 0.2             | 5.73   |
| (1,30) | 1:35:A:GLY:C | 1:36:A:ILE:N | 1:36:A:ILE:CA | 1:36:A:ILE:C | 20                  | 5.74  | 0.17            | 5.72   |
| (1,57) | 1:64:A:GLU:C | 1:65:A:SER:N | 1:65:A:SER:CA | 1:65:A:SER:C | 20                  | 5.64  | 0.15            | 5.63   |
| (1,5)  | 1:6:A:LYS:C  | 1:7:A:THR:N  | 1:7:A:THR:CA  | 1:7:A:THR:C  | 20                  | 5.45  | 1.07            | 6.1    |

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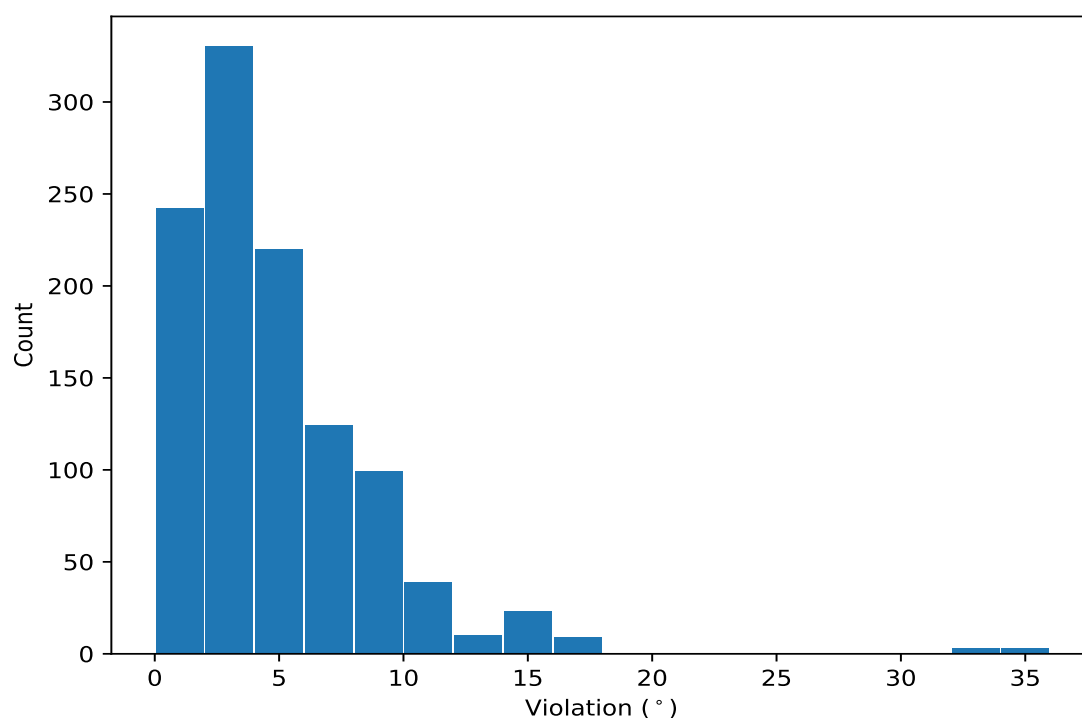
| Key    | Atom-1       | Atom-2       | Atom-3        | Atom-4       | Models <sup>1</sup> | Mean | SD <sup>2</sup> | Median |
|--------|--------------|--------------|---------------|--------------|---------------------|------|-----------------|--------|
| (1,39) | 1:45:A:PHE:C | 1:46:A:ALA:N | 1:46:A:ALA:CA | 1:46:A:ALA:C | 20                  | 5.19 | 0.29            | 5.3    |
| (1,62) | 1:69:A:LEU:C | 1:70:A:VAL:N | 1:70:A:VAL:CA | 1:70:A:VAL:C | 20                  | 4.92 | 0.36            | 4.94   |
| (1,38) | 1:44:A:ILE:C | 1:45:A:PHE:N | 1:45:A:PHE:CA | 1:45:A:PHE:C | 20                  | 4.85 | 0.65            | 4.94   |
| (1,36) | 1:42:A:ARG:C | 1:43:A:LEU:N | 1:43:A:LEU:CA | 1:43:A:LEU:C | 20                  | 4.8  | 0.41            | 4.93   |
| (1,58) | 1:65:A:SER:C | 1:66:A:THR:N | 1:66:A:THR:CA | 1:66:A:THR:C | 20                  | 4.55 | 0.2             | 4.49   |
| (1,28) | 1:32:A:ASP:C | 1:33:A:LYS:N | 1:33:A:LYS:CA | 1:33:A:LYS:C | 20                  | 4.12 | 0.09            | 4.14   |
| (1,37) | 1:43:A:LEU:C | 1:44:A:ILE:N | 1:44:A:ILE:CA | 1:44:A:ILE:C | 20                  | 4.03 | 0.88            | 3.91   |
| (1,43) | 1:50:A:LEU:C | 1:51:A:GLU:N | 1:51:A:GLU:CA | 1:51:A:GLU:C | 20                  | 3.97 | 0.15            | 3.96   |
| (1,15) | 1:17:A:VAL:C | 1:18:A:GLU:N | 1:18:A:GLU:CA | 1:18:A:GLU:C | 20                  | 3.86 | 0.27            | 3.86   |
| (1,1)  | 1:2:A:GLN:C  | 1:3:A:ILE:N  | 1:3:A:ILE:CA  | 1:3:A:ILE:C  | 20                  | 3.86 | 0.65            | 3.9    |
| (1,18) | 1:21:A:ASP:C | 1:22:A:THR:N | 1:22:A:THR:CA | 1:22:A:THR:C | 20                  | 3.75 | 0.16            | 3.78   |
| (1,59) | 1:66:A:THR:C | 1:67:A:LEU:N | 1:67:A:LEU:CA | 1:67:A:LEU:C | 20                  | 3.68 | 0.18            | 3.68   |
| (1,47) | 1:54:A:ARG:C | 1:55:A:THR:N | 1:55:A:THR:CA | 1:55:A:THR:C | 20                  | 3.63 | 0.15            | 3.63   |
| (1,60) | 1:67:A:LEU:C | 1:68:A:HIS:N | 1:68:A:HIS:CA | 1:68:A:HIS:C | 20                  | 3.62 | 0.23            | 3.62   |
| (1,46) | 1:53:A:GLY:C | 1:54:A:ARG:N | 1:54:A:ARG:CA | 1:54:A:ARG:C | 20                  | 3.62 | 0.23            | 3.64   |
| (1,24) | 1:28:A:ALA:C | 1:29:A:LYS:N | 1:29:A:LYS:CA | 1:29:A:LYS:C | 20                  | 3.43 | 0.15            | 3.48   |
| (1,12) | 1:14:A:THR:C | 1:15:A:LEU:N | 1:15:A:LEU:CA | 1:15:A:LEU:C | 20                  | 3.27 | 0.75            | 3.56   |
| (1,4)  | 1:5:A:VAL:C  | 1:6:A:LYS:N  | 1:6:A:LYS:CA  | 1:6:A:LYS:C  | 20                  | 2.68 | 0.29            | 2.71   |
| (1,51) | 1:58:A:ASP:C | 1:59:A:TYR:N | 1:59:A:TYR:CA | 1:59:A:TYR:C | 20                  | 2.22 | 0.25            | 2.25   |
| (1,42) | 1:49:A:GLN:C | 1:50:A:LEU:N | 1:50:A:LEU:CA | 1:50:A:LEU:C | 20                  | 2.19 | 0.16            | 2.16   |
| (1,26) | 1:30:A:ILE:C | 1:31:A:GLN:N | 1:31:A:GLN:CA | 1:31:A:GLN:C | 20                  | 2.04 | 0.1             | 2.08   |
| (1,56) | 1:63:A:LYS:C | 1:64:A:GLU:N | 1:64:A:GLU:CA | 1:64:A:GLU:C | 20                  | 2.04 | 0.08            | 2.03   |
| (1,16) | 1:19:A:PRO:C | 1:20:A:SER:N | 1:20:A:SER:CA | 1:20:A:SER:C | 20                  | 1.85 | 0.14            | 1.88   |
| (1,22) | 1:26:A:VAL:C | 1:27:A:LYS:N | 1:27:A:LYS:CA | 1:27:A:LYS:C | 20                  | 1.8  | 0.16            | 1.83   |
| (1,20) | 1:24:A:GLU:C | 1:25:A:ASN:N | 1:25:A:ASN:CA | 1:25:A:ASN:C | 20                  | 1.6  | 0.22            | 1.62   |
| (1,17) | 1:20:A:SER:C | 1:21:A:ASP:N | 1:21:A:ASP:CA | 1:21:A:ASP:C | 20                  | 1.46 | 0.13            | 1.51   |
| (1,50) | 1:57:A:SER:C | 1:58:A:ASP:N | 1:58:A:ASP:CA | 1:58:A:ASP:C | 20                  | 1.45 | 0.12            | 1.48   |
| (1,25) | 1:29:A:LYS:C | 1:30:A:ILE:N | 1:30:A:ILE:CA | 1:30:A:ILE:C | 20                  | 1.32 | 0.13            | 1.31   |
| (1,23) | 1:27:A:LYS:C | 1:28:A:ALA:N | 1:28:A:ALA:CA | 1:28:A:ALA:C | 20                  | 1.24 | 0.08            | 1.25   |
| (1,6)  | 1:7:A:THR:C  | 1:8:A:LEU:N  | 1:8:A:LEU:CA  | 1:8:A:LEU:C  | 19                  | 6.19 | 4.86            | 3.35   |
| (1,9)  | 1:11:A:LYS:C | 1:12:A:THR:N | 1:12:A:THR:CA | 1:12:A:THR:C | 19                  | 2.2  | 0.91            | 1.65   |
| (1,11) | 1:13:A:ILE:C | 1:14:A:THR:N | 1:14:A:THR:CA | 1:14:A:THR:C | 17                  | 1.77 | 0.34            | 1.64   |
| (1,31) | 1:37:A:PRO:C | 1:38:A:PRO:N | 1:38:A:PRO:CA | 1:38:A:PRO:C | 16                  | 1.43 | 0.44            | 1.27   |
| (1,45) | 1:52:A:ASP:C | 1:53:A:GLY:N | 1:53:A:GLY:CA | 1:53:A:GLY:C | 15                  | 1.92 | 0.62            | 1.77   |
| (1,40) | 1:47:A:GLY:C | 1:48:A:LYS:N | 1:48:A:LYS:CA | 1:48:A:LYS:C | 13                  | 1.16 | 0.13            | 1.13   |
| (1,10) | 1:12:A:THR:C | 1:13:A:ILE:N | 1:13:A:ILE:CA | 1:13:A:ILE:C | 11                  | 1.4  | 0.31            | 1.4    |
| (1,14) | 1:16:A:GLU:C | 1:17:A:VAL:N | 1:17:A:VAL:CA | 1:17:A:VAL:C | 6                   | 1.09 | 0.11            | 1.04   |
| (1,33) | 1:39:A:ASP:C | 1:40:A:GLN:N | 1:40:A:GLN:CA | 1:40:A:GLN:C | 2                   | 1.23 | 0.03            | 1.23   |
| (1,61) | 1:68:A:HIS:C | 1:69:A:LEU:N | 1:69:A:LEU:CA | 1:69:A:LEU:C | 2                   | 1.08 | 0.01            | 1.08   |
| (1,41) | 1:48:A:LYS:C | 1:49:A:GLN:N | 1:49:A:GLN:CA | 1:49:A:GLN:C | 2                   | 1.04 | 0.02            | 1.04   |

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

## 10.5 All violated dihedral-angle restraints ⓘ

### 10.5.1 Histogram : Distribution of violations ⓘ

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



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

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

| Key    | Atom-1       | Atom-2       | Atom-3        | Atom-4       | Model ID | Violation (°) |
|--------|--------------|--------------|---------------|--------------|----------|---------------|
| (1,7)  | 1:8:A:LEU:C  | 1:9:A:THR:N  | 1:9:A:THR:CA  | 1:9:A:THR:C  | 4        | 34.33         |
| (1,7)  | 1:8:A:LEU:C  | 1:9:A:THR:N  | 1:9:A:THR:CA  | 1:9:A:THR:C  | 7        | 34.16         |
| (1,7)  | 1:8:A:LEU:C  | 1:9:A:THR:N  | 1:9:A:THR:CA  | 1:9:A:THR:C  | 2        | 34.09         |
| (1,7)  | 1:8:A:LEU:C  | 1:9:A:THR:N  | 1:9:A:THR:CA  | 1:9:A:THR:C  | 10       | 33.92         |
| (1,7)  | 1:8:A:LEU:C  | 1:9:A:THR:N  | 1:9:A:THR:CA  | 1:9:A:THR:C  | 3        | 33.91         |
| (1,7)  | 1:8:A:LEU:C  | 1:9:A:THR:N  | 1:9:A:THR:CA  | 1:9:A:THR:C  | 20       | 33.7          |
| (1,8)  | 1:10:A:GLY:C | 1:11:A:LYS:N | 1:11:A:LYS:CA | 1:11:A:LYS:C | 6        | 17.67         |
| (1,8)  | 1:10:A:GLY:C | 1:11:A:LYS:N | 1:11:A:LYS:CA | 1:11:A:LYS:C | 16       | 17.61         |
| (1,8)  | 1:10:A:GLY:C | 1:11:A:LYS:N | 1:11:A:LYS:CA | 1:11:A:LYS:C | 14       | 17.53         |
| (1,8)  | 1:10:A:GLY:C | 1:11:A:LYS:N | 1:11:A:LYS:CA | 1:11:A:LYS:C | 15       | 17.53         |
| (1,8)  | 1:10:A:GLY:C | 1:11:A:LYS:N | 1:11:A:LYS:CA | 1:11:A:LYS:C | 1        | 17.15         |
| (1,8)  | 1:10:A:GLY:C | 1:11:A:LYS:N | 1:11:A:LYS:CA | 1:11:A:LYS:C | 18       | 17.05         |
| (1,8)  | 1:10:A:GLY:C | 1:11:A:LYS:N | 1:11:A:LYS:CA | 1:11:A:LYS:C | 5        | 16.99         |
| (1,8)  | 1:10:A:GLY:C | 1:11:A:LYS:N | 1:11:A:LYS:CA | 1:11:A:LYS:C | 8        | 16.99         |
| (1,8)  | 1:10:A:GLY:C | 1:11:A:LYS:N | 1:11:A:LYS:CA | 1:11:A:LYS:C | 19       | 16.59         |
| (1,8)  | 1:10:A:GLY:C | 1:11:A:LYS:N | 1:11:A:LYS:CA | 1:11:A:LYS:C | 12       | 15.41         |
| (1,8)  | 1:10:A:GLY:C | 1:11:A:LYS:N | 1:11:A:LYS:CA | 1:11:A:LYS:C | 11       | 15.3          |
| (1,44) | 1:51:A:GLU:C | 1:52:A:ASP:N | 1:52:A:ASP:CA | 1:52:A:ASP:C | 20       | 14.77         |
| (1,44) | 1:51:A:GLU:C | 1:52:A:ASP:N | 1:52:A:ASP:CA | 1:52:A:ASP:C | 18       | 14.69         |
| (1,44) | 1:51:A:GLU:C | 1:52:A:ASP:N | 1:52:A:ASP:CA | 1:52:A:ASP:C | 1        | 14.62         |
| (1,44) | 1:51:A:GLU:C | 1:52:A:ASP:N | 1:52:A:ASP:CA | 1:52:A:ASP:C | 19       | 14.62         |

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| Key    | Atom-1       | Atom-2       | Atom-3        | Atom-4       | Model ID | Violation (°) |
|--------|--------------|--------------|---------------|--------------|----------|---------------|
| (1,6)  | 1:7:A:THR:C  | 1:8:A:LEU:N  | 1:8:A:LEU:CA  | 1:8:A:LEU:C  | 4        | 14.62         |
| (1,44) | 1:51:A:GLU:C | 1:52:A:ASP:N | 1:52:A:ASP:CA | 1:52:A:ASP:C | 9        | 14.61         |
| (1,44) | 1:51:A:GLU:C | 1:52:A:ASP:N | 1:52:A:ASP:CA | 1:52:A:ASP:C | 2        | 14.59         |
| (1,44) | 1:51:A:GLU:C | 1:52:A:ASP:N | 1:52:A:ASP:CA | 1:52:A:ASP:C | 6        | 14.57         |
| (1,44) | 1:51:A:GLU:C | 1:52:A:ASP:N | 1:52:A:ASP:CA | 1:52:A:ASP:C | 7        | 14.56         |
| (1,44) | 1:51:A:GLU:C | 1:52:A:ASP:N | 1:52:A:ASP:CA | 1:52:A:ASP:C | 10       | 14.49         |
| (1,44) | 1:51:A:GLU:C | 1:52:A:ASP:N | 1:52:A:ASP:CA | 1:52:A:ASP:C | 11       | 14.49         |
| (1,44) | 1:51:A:GLU:C | 1:52:A:ASP:N | 1:52:A:ASP:CA | 1:52:A:ASP:C | 12       | 14.49         |
| (1,44) | 1:51:A:GLU:C | 1:52:A:ASP:N | 1:52:A:ASP:CA | 1:52:A:ASP:C | 13       | 14.43         |
| (1,44) | 1:51:A:GLU:C | 1:52:A:ASP:N | 1:52:A:ASP:CA | 1:52:A:ASP:C | 3        | 14.41         |
| (1,44) | 1:51:A:GLU:C | 1:52:A:ASP:N | 1:52:A:ASP:CA | 1:52:A:ASP:C | 5        | 14.41         |
| (1,44) | 1:51:A:GLU:C | 1:52:A:ASP:N | 1:52:A:ASP:CA | 1:52:A:ASP:C | 16       | 14.4          |
| (1,44) | 1:51:A:GLU:C | 1:52:A:ASP:N | 1:52:A:ASP:CA | 1:52:A:ASP:C | 8        | 14.34         |
| (1,44) | 1:51:A:GLU:C | 1:52:A:ASP:N | 1:52:A:ASP:CA | 1:52:A:ASP:C | 15       | 14.31         |
| (1,44) | 1:51:A:GLU:C | 1:52:A:ASP:N | 1:52:A:ASP:CA | 1:52:A:ASP:C | 4        | 14.3          |
| (1,44) | 1:51:A:GLU:C | 1:52:A:ASP:N | 1:52:A:ASP:CA | 1:52:A:ASP:C | 17       | 14.3          |
| (1,44) | 1:51:A:GLU:C | 1:52:A:ASP:N | 1:52:A:ASP:CA | 1:52:A:ASP:C | 14       | 14.28         |
| (1,6)  | 1:7:A:THR:C  | 1:8:A:LEU:N  | 1:8:A:LEU:CA  | 1:8:A:LEU:C  | 7        | 13.56         |
| (1,6)  | 1:7:A:THR:C  | 1:8:A:LEU:N  | 1:8:A:LEU:CA  | 1:8:A:LEU:C  | 2        | 13.29         |
| (1,6)  | 1:7:A:THR:C  | 1:8:A:LEU:N  | 1:8:A:LEU:CA  | 1:8:A:LEU:C  | 3        | 13.14         |
| (1,6)  | 1:7:A:THR:C  | 1:8:A:LEU:N  | 1:8:A:LEU:CA  | 1:8:A:LEU:C  | 10       | 13.1          |
| (1,2)  | 1:3:A:ILE:C  | 1:4:A:PHE:N  | 1:4:A:PHE:CA  | 1:4:A:PHE:C  | 11       | 12.15         |
| (1,2)  | 1:3:A:ILE:C  | 1:4:A:PHE:N  | 1:4:A:PHE:CA  | 1:4:A:PHE:C  | 16       | 12.15         |
| (1,2)  | 1:3:A:ILE:C  | 1:4:A:PHE:N  | 1:4:A:PHE:CA  | 1:4:A:PHE:C  | 14       | 12.11         |
| (1,2)  | 1:3:A:ILE:C  | 1:4:A:PHE:N  | 1:4:A:PHE:CA  | 1:4:A:PHE:C  | 6        | 12.1          |
| (1,2)  | 1:3:A:ILE:C  | 1:4:A:PHE:N  | 1:4:A:PHE:CA  | 1:4:A:PHE:C  | 12       | 12.03         |
| (1,2)  | 1:3:A:ILE:C  | 1:4:A:PHE:N  | 1:4:A:PHE:CA  | 1:4:A:PHE:C  | 18       | 12.03         |
| (1,2)  | 1:3:A:ILE:C  | 1:4:A:PHE:N  | 1:4:A:PHE:CA  | 1:4:A:PHE:C  | 5        | 11.95         |
| (1,2)  | 1:3:A:ILE:C  | 1:4:A:PHE:N  | 1:4:A:PHE:CA  | 1:4:A:PHE:C  | 9        | 11.92         |
| (1,2)  | 1:3:A:ILE:C  | 1:4:A:PHE:N  | 1:4:A:PHE:CA  | 1:4:A:PHE:C  | 19       | 11.92         |
| (1,6)  | 1:7:A:THR:C  | 1:8:A:LEU:N  | 1:8:A:LEU:CA  | 1:8:A:LEU:C  | 20       | 11.9          |
| (1,2)  | 1:3:A:ILE:C  | 1:4:A:PHE:N  | 1:4:A:PHE:CA  | 1:4:A:PHE:C  | 1        | 11.86         |
| (1,2)  | 1:3:A:ILE:C  | 1:4:A:PHE:N  | 1:4:A:PHE:CA  | 1:4:A:PHE:C  | 13       | 11.83         |
| (1,49) | 1:56:A:LEU:C | 1:57:A:SER:N | 1:57:A:SER:CA | 1:57:A:SER:C | 3        | 11.79         |
| (1,2)  | 1:3:A:ILE:C  | 1:4:A:PHE:N  | 1:4:A:PHE:CA  | 1:4:A:PHE:C  | 17       | 11.78         |
| (1,2)  | 1:3:A:ILE:C  | 1:4:A:PHE:N  | 1:4:A:PHE:CA  | 1:4:A:PHE:C  | 20       | 11.73         |
| (1,2)  | 1:3:A:ILE:C  | 1:4:A:PHE:N  | 1:4:A:PHE:CA  | 1:4:A:PHE:C  | 15       | 11.7          |
| (1,2)  | 1:3:A:ILE:C  | 1:4:A:PHE:N  | 1:4:A:PHE:CA  | 1:4:A:PHE:C  | 8        | 11.57         |
| (1,2)  | 1:3:A:ILE:C  | 1:4:A:PHE:N  | 1:4:A:PHE:CA  | 1:4:A:PHE:C  | 3        | 11.52         |
| (1,2)  | 1:3:A:ILE:C  | 1:4:A:PHE:N  | 1:4:A:PHE:CA  | 1:4:A:PHE:C  | 7        | 11.33         |
| (1,49) | 1:56:A:LEU:C | 1:57:A:SER:N | 1:57:A:SER:CA | 1:57:A:SER:C | 9        | 11.27         |
| (1,2)  | 1:3:A:ILE:C  | 1:4:A:PHE:N  | 1:4:A:PHE:CA  | 1:4:A:PHE:C  | 2        | 11.25         |
| (1,49) | 1:56:A:LEU:C | 1:57:A:SER:N | 1:57:A:SER:CA | 1:57:A:SER:C | 6        | 11.16         |
| (1,2)  | 1:3:A:ILE:C  | 1:4:A:PHE:N  | 1:4:A:PHE:CA  | 1:4:A:PHE:C  | 10       | 11.16         |
| (1,2)  | 1:3:A:ILE:C  | 1:4:A:PHE:N  | 1:4:A:PHE:CA  | 1:4:A:PHE:C  | 4        | 11.1          |
| (1,49) | 1:56:A:LEU:C | 1:57:A:SER:N | 1:57:A:SER:CA | 1:57:A:SER:C | 8        | 11.07         |
| (1,49) | 1:56:A:LEU:C | 1:57:A:SER:N | 1:57:A:SER:CA | 1:57:A:SER:C | 20       | 11.01         |
| (1,49) | 1:56:A:LEU:C | 1:57:A:SER:N | 1:57:A:SER:CA | 1:57:A:SER:C | 7        | 11.0          |
| (1,49) | 1:56:A:LEU:C | 1:57:A:SER:N | 1:57:A:SER:CA | 1:57:A:SER:C | 19       | 10.99         |
| (1,49) | 1:56:A:LEU:C | 1:57:A:SER:N | 1:57:A:SER:CA | 1:57:A:SER:C | 4        | 10.98         |
| (1,49) | 1:56:A:LEU:C | 1:57:A:SER:N | 1:57:A:SER:CA | 1:57:A:SER:C | 14       | 10.94         |

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| Key    | Atom-1       | Atom-2       | Atom-3        | Atom-4       | Model ID | Violation (°) |
|--------|--------------|--------------|---------------|--------------|----------|---------------|
| (1,49) | 1:56:A:LEU:C | 1:57:A:SER:N | 1:57:A:SER:CA | 1:57:A:SER:C | 10       | 10.87         |
| (1,49) | 1:56:A:LEU:C | 1:57:A:SER:N | 1:57:A:SER:CA | 1:57:A:SER:C | 2        | 10.85         |
| (1,49) | 1:56:A:LEU:C | 1:57:A:SER:N | 1:57:A:SER:CA | 1:57:A:SER:C | 13       | 10.82         |
| (1,34) | 1:40:A:GLN:C | 1:41:A:GLN:N | 1:41:A:GLN:CA | 1:41:A:GLN:C | 20       | 10.77         |
| (1,49) | 1:56:A:LEU:C | 1:57:A:SER:N | 1:57:A:SER:CA | 1:57:A:SER:C | 11       | 10.69         |
| (1,49) | 1:56:A:LEU:C | 1:57:A:SER:N | 1:57:A:SER:CA | 1:57:A:SER:C | 15       | 10.41         |
| (1,34) | 1:40:A:GLN:C | 1:41:A:GLN:N | 1:41:A:GLN:CA | 1:41:A:GLN:C | 9        | 10.39         |
| (1,49) | 1:56:A:LEU:C | 1:57:A:SER:N | 1:57:A:SER:CA | 1:57:A:SER:C | 18       | 10.35         |
| (1,49) | 1:56:A:LEU:C | 1:57:A:SER:N | 1:57:A:SER:CA | 1:57:A:SER:C | 5        | 10.34         |
| (1,49) | 1:56:A:LEU:C | 1:57:A:SER:N | 1:57:A:SER:CA | 1:57:A:SER:C | 1        | 10.31         |
| (1,49) | 1:56:A:LEU:C | 1:57:A:SER:N | 1:57:A:SER:CA | 1:57:A:SER:C | 12       | 10.27         |
| (1,34) | 1:40:A:GLN:C | 1:41:A:GLN:N | 1:41:A:GLN:CA | 1:41:A:GLN:C | 3        | 10.18         |
| (1,63) | 1:70:A:VAL:C | 1:71:A:LEU:N | 1:71:A:LEU:CA | 1:71:A:LEU:C | 9        | 10.15         |
| (1,49) | 1:56:A:LEU:C | 1:57:A:SER:N | 1:57:A:SER:CA | 1:57:A:SER:C | 17       | 10.08         |
| (1,49) | 1:56:A:LEU:C | 1:57:A:SER:N | 1:57:A:SER:CA | 1:57:A:SER:C | 16       | 10.05         |
| (1,34) | 1:40:A:GLN:C | 1:41:A:GLN:N | 1:41:A:GLN:CA | 1:41:A:GLN:C | 10       | 9.99          |
| (1,63) | 1:70:A:VAL:C | 1:71:A:LEU:N | 1:71:A:LEU:CA | 1:71:A:LEU:C | 17       | 9.93          |
| (1,13) | 1:15:A:LEU:C | 1:16:A:GLU:N | 1:16:A:GLU:CA | 1:16:A:GLU:C | 4        | 9.8           |
| (1,34) | 1:40:A:GLN:C | 1:41:A:GLN:N | 1:41:A:GLN:CA | 1:41:A:GLN:C | 2        | 9.75          |
| (1,34) | 1:40:A:GLN:C | 1:41:A:GLN:N | 1:41:A:GLN:CA | 1:41:A:GLN:C | 4        | 9.73          |
| (1,34) | 1:40:A:GLN:C | 1:41:A:GLN:N | 1:41:A:GLN:CA | 1:41:A:GLN:C | 7        | 9.7           |
| (1,13) | 1:15:A:LEU:C | 1:16:A:GLU:N | 1:16:A:GLU:CA | 1:16:A:GLU:C | 8        | 9.58          |
| (1,34) | 1:40:A:GLN:C | 1:41:A:GLN:N | 1:41:A:GLN:CA | 1:41:A:GLN:C | 13       | 9.57          |
| (1,21) | 1:25:A:ASN:C | 1:26:A:VAL:N | 1:26:A:VAL:CA | 1:26:A:VAL:C | 3        | 9.56          |
| (1,34) | 1:40:A:GLN:C | 1:41:A:GLN:N | 1:41:A:GLN:CA | 1:41:A:GLN:C | 17       | 9.41          |
| (1,34) | 1:40:A:GLN:C | 1:41:A:GLN:N | 1:41:A:GLN:CA | 1:41:A:GLN:C | 8        | 9.34          |
| (1,34) | 1:40:A:GLN:C | 1:41:A:GLN:N | 1:41:A:GLN:CA | 1:41:A:GLN:C | 6        | 9.28          |
| (1,34) | 1:40:A:GLN:C | 1:41:A:GLN:N | 1:41:A:GLN:CA | 1:41:A:GLN:C | 5        | 9.25          |
| (1,21) | 1:25:A:ASN:C | 1:26:A:VAL:N | 1:26:A:VAL:CA | 1:26:A:VAL:C | 9        | 9.22          |
| (1,13) | 1:15:A:LEU:C | 1:16:A:GLU:N | 1:16:A:GLU:CA | 1:16:A:GLU:C | 15       | 9.22          |
| (1,34) | 1:40:A:GLN:C | 1:41:A:GLN:N | 1:41:A:GLN:CA | 1:41:A:GLN:C | 14       | 9.19          |
| (1,34) | 1:40:A:GLN:C | 1:41:A:GLN:N | 1:41:A:GLN:CA | 1:41:A:GLN:C | 1        | 9.13          |
| (1,34) | 1:40:A:GLN:C | 1:41:A:GLN:N | 1:41:A:GLN:CA | 1:41:A:GLN:C | 11       | 9.11          |
| (1,21) | 1:25:A:ASN:C | 1:26:A:VAL:N | 1:26:A:VAL:CA | 1:26:A:VAL:C | 5        | 9.11          |
| (1,54) | 1:61:A:ILE:C | 1:62:A:GLN:N | 1:62:A:GLN:CA | 1:62:A:GLN:C | 4        | 9.07          |
| (1,34) | 1:40:A:GLN:C | 1:41:A:GLN:N | 1:41:A:GLN:CA | 1:41:A:GLN:C | 16       | 9.07          |
| (1,34) | 1:40:A:GLN:C | 1:41:A:GLN:N | 1:41:A:GLN:CA | 1:41:A:GLN:C | 19       | 9.07          |
| (1,13) | 1:15:A:LEU:C | 1:16:A:GLU:N | 1:16:A:GLU:CA | 1:16:A:GLU:C | 11       | 9.03          |
| (1,63) | 1:70:A:VAL:C | 1:71:A:LEU:N | 1:71:A:LEU:CA | 1:71:A:LEU:C | 15       | 9.02          |
| (1,34) | 1:40:A:GLN:C | 1:41:A:GLN:N | 1:41:A:GLN:CA | 1:41:A:GLN:C | 15       | 9.02          |
| (1,34) | 1:40:A:GLN:C | 1:41:A:GLN:N | 1:41:A:GLN:CA | 1:41:A:GLN:C | 18       | 9.02          |
| (1,13) | 1:15:A:LEU:C | 1:16:A:GLU:N | 1:16:A:GLU:CA | 1:16:A:GLU:C | 18       | 9.02          |
| (1,29) | 1:33:A:LYS:C | 1:34:A:GLU:N | 1:34:A:GLU:CA | 1:34:A:GLU:C | 20       | 9.01          |
| (1,63) | 1:70:A:VAL:C | 1:71:A:LEU:N | 1:71:A:LEU:CA | 1:71:A:LEU:C | 11       | 9.0           |
| (1,34) | 1:40:A:GLN:C | 1:41:A:GLN:N | 1:41:A:GLN:CA | 1:41:A:GLN:C | 12       | 9.0           |
| (1,21) | 1:25:A:ASN:C | 1:26:A:VAL:N | 1:26:A:VAL:CA | 1:26:A:VAL:C | 20       | 9.0           |
| (1,13) | 1:15:A:LEU:C | 1:16:A:GLU:N | 1:16:A:GLU:CA | 1:16:A:GLU:C | 16       | 9.0           |
| (1,13) | 1:15:A:LEU:C | 1:16:A:GLU:N | 1:16:A:GLU:CA | 1:16:A:GLU:C | 6        | 8.99          |
| (1,13) | 1:15:A:LEU:C | 1:16:A:GLU:N | 1:16:A:GLU:CA | 1:16:A:GLU:C | 5        | 8.91          |
| (1,21) | 1:25:A:ASN:C | 1:26:A:VAL:N | 1:26:A:VAL:CA | 1:26:A:VAL:C | 14       | 8.89          |
| (1,13) | 1:15:A:LEU:C | 1:16:A:GLU:N | 1:16:A:GLU:CA | 1:16:A:GLU:C | 1        | 8.87          |

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| Key    | Atom-1       | Atom-2       | Atom-3        | Atom-4       | Model ID | Violation (°) |
|--------|--------------|--------------|---------------|--------------|----------|---------------|
| (1,54) | 1:61:A:ILE:C | 1:62:A:GLN:N | 1:62:A:GLN:CA | 1:62:A:GLN:C | 7        | 8.82          |
| (1,13) | 1:15:A:LEU:C | 1:16:A:GLU:N | 1:16:A:GLU:CA | 1:16:A:GLU:C | 9        | 8.82          |
| (1,13) | 1:15:A:LEU:C | 1:16:A:GLU:N | 1:16:A:GLU:CA | 1:16:A:GLU:C | 12       | 8.81          |
| (1,21) | 1:25:A:ASN:C | 1:26:A:VAL:N | 1:26:A:VAL:CA | 1:26:A:VAL:C | 6        | 8.8           |
| (1,54) | 1:61:A:ILE:C | 1:62:A:GLN:N | 1:62:A:GLN:CA | 1:62:A:GLN:C | 3        | 8.74          |
| (1,63) | 1:70:A:VAL:C | 1:71:A:LEU:N | 1:71:A:LEU:CA | 1:71:A:LEU:C | 1        | 8.71          |
| (1,21) | 1:25:A:ASN:C | 1:26:A:VAL:N | 1:26:A:VAL:CA | 1:26:A:VAL:C | 1        | 8.7           |
| (1,13) | 1:15:A:LEU:C | 1:16:A:GLU:N | 1:16:A:GLU:CA | 1:16:A:GLU:C | 14       | 8.7           |
| (1,21) | 1:25:A:ASN:C | 1:26:A:VAL:N | 1:26:A:VAL:CA | 1:26:A:VAL:C | 19       | 8.68          |
| (1,13) | 1:15:A:LEU:C | 1:16:A:GLU:N | 1:16:A:GLU:CA | 1:16:A:GLU:C | 19       | 8.66          |
| (1,3)  | 1:4:A:PHE:C  | 1:5:A:VAL:N  | 1:5:A:VAL:CA  | 1:5:A:VAL:C  | 20       | 8.65          |
| (1,13) | 1:15:A:LEU:C | 1:16:A:GLU:N | 1:16:A:GLU:CA | 1:16:A:GLU:C | 13       | 8.64          |
| (1,21) | 1:25:A:ASN:C | 1:26:A:VAL:N | 1:26:A:VAL:CA | 1:26:A:VAL:C | 15       | 8.62          |
| (1,3)  | 1:4:A:PHE:C  | 1:5:A:VAL:N  | 1:5:A:VAL:CA  | 1:5:A:VAL:C  | 4        | 8.62          |
| (1,54) | 1:61:A:ILE:C | 1:62:A:GLN:N | 1:62:A:GLN:CA | 1:62:A:GLN:C | 9        | 8.6           |
| (1,21) | 1:25:A:ASN:C | 1:26:A:VAL:N | 1:26:A:VAL:CA | 1:26:A:VAL:C | 12       | 8.6           |
| (1,54) | 1:61:A:ILE:C | 1:62:A:GLN:N | 1:62:A:GLN:CA | 1:62:A:GLN:C | 6        | 8.59          |
| (1,21) | 1:25:A:ASN:C | 1:26:A:VAL:N | 1:26:A:VAL:CA | 1:26:A:VAL:C | 18       | 8.59          |
| (1,13) | 1:15:A:LEU:C | 1:16:A:GLU:N | 1:16:A:GLU:CA | 1:16:A:GLU:C | 2        | 8.58          |
| (1,21) | 1:25:A:ASN:C | 1:26:A:VAL:N | 1:26:A:VAL:CA | 1:26:A:VAL:C | 16       | 8.54          |
| (1,13) | 1:15:A:LEU:C | 1:16:A:GLU:N | 1:16:A:GLU:CA | 1:16:A:GLU:C | 3        | 8.54          |
| (1,54) | 1:61:A:ILE:C | 1:62:A:GLN:N | 1:62:A:GLN:CA | 1:62:A:GLN:C | 15       | 8.53          |
| (1,21) | 1:25:A:ASN:C | 1:26:A:VAL:N | 1:26:A:VAL:CA | 1:26:A:VAL:C | 11       | 8.53          |
| (1,3)  | 1:4:A:PHE:C  | 1:5:A:VAL:N  | 1:5:A:VAL:CA  | 1:5:A:VAL:C  | 2        | 8.53          |
| (1,3)  | 1:4:A:PHE:C  | 1:5:A:VAL:N  | 1:5:A:VAL:CA  | 1:5:A:VAL:C  | 3        | 8.53          |
| (1,63) | 1:70:A:VAL:C | 1:71:A:LEU:N | 1:71:A:LEU:CA | 1:71:A:LEU:C | 7        | 8.51          |
| (1,54) | 1:61:A:ILE:C | 1:62:A:GLN:N | 1:62:A:GLN:CA | 1:62:A:GLN:C | 2        | 8.51          |
| (1,29) | 1:33:A:LYS:C | 1:34:A:GLU:N | 1:34:A:GLU:CA | 1:34:A:GLU:C | 9        | 8.51          |
| (1,21) | 1:25:A:ASN:C | 1:26:A:VAL:N | 1:26:A:VAL:CA | 1:26:A:VAL:C | 8        | 8.49          |
| (1,13) | 1:15:A:LEU:C | 1:16:A:GLU:N | 1:16:A:GLU:CA | 1:16:A:GLU:C | 7        | 8.49          |
| (1,54) | 1:61:A:ILE:C | 1:62:A:GLN:N | 1:62:A:GLN:CA | 1:62:A:GLN:C | 8        | 8.48          |
| (1,54) | 1:61:A:ILE:C | 1:62:A:GLN:N | 1:62:A:GLN:CA | 1:62:A:GLN:C | 16       | 8.48          |
| (1,54) | 1:61:A:ILE:C | 1:62:A:GLN:N | 1:62:A:GLN:CA | 1:62:A:GLN:C | 17       | 8.48          |
| (1,54) | 1:61:A:ILE:C | 1:62:A:GLN:N | 1:62:A:GLN:CA | 1:62:A:GLN:C | 13       | 8.47          |
| (1,54) | 1:61:A:ILE:C | 1:62:A:GLN:N | 1:62:A:GLN:CA | 1:62:A:GLN:C | 11       | 8.46          |
| (1,13) | 1:15:A:LEU:C | 1:16:A:GLU:N | 1:16:A:GLU:CA | 1:16:A:GLU:C | 10       | 8.44          |
| (1,21) | 1:25:A:ASN:C | 1:26:A:VAL:N | 1:26:A:VAL:CA | 1:26:A:VAL:C | 2        | 8.43          |
| (1,13) | 1:15:A:LEU:C | 1:16:A:GLU:N | 1:16:A:GLU:CA | 1:16:A:GLU:C | 17       | 8.43          |
| (1,54) | 1:61:A:ILE:C | 1:62:A:GLN:N | 1:62:A:GLN:CA | 1:62:A:GLN:C | 1        | 8.42          |
| (1,54) | 1:61:A:ILE:C | 1:62:A:GLN:N | 1:62:A:GLN:CA | 1:62:A:GLN:C | 12       | 8.42          |
| (1,54) | 1:61:A:ILE:C | 1:62:A:GLN:N | 1:62:A:GLN:CA | 1:62:A:GLN:C | 18       | 8.42          |
| (1,54) | 1:61:A:ILE:C | 1:62:A:GLN:N | 1:62:A:GLN:CA | 1:62:A:GLN:C | 20       | 8.42          |
| (1,21) | 1:25:A:ASN:C | 1:26:A:VAL:N | 1:26:A:VAL:CA | 1:26:A:VAL:C | 7        | 8.42          |
| (1,21) | 1:25:A:ASN:C | 1:26:A:VAL:N | 1:26:A:VAL:CA | 1:26:A:VAL:C | 13       | 8.41          |
| (1,21) | 1:25:A:ASN:C | 1:26:A:VAL:N | 1:26:A:VAL:CA | 1:26:A:VAL:C | 17       | 8.41          |
| (1,54) | 1:61:A:ILE:C | 1:62:A:GLN:N | 1:62:A:GLN:CA | 1:62:A:GLN:C | 14       | 8.39          |
| (1,3)  | 1:4:A:PHE:C  | 1:5:A:VAL:N  | 1:5:A:VAL:CA  | 1:5:A:VAL:C  | 7        | 8.36          |
| (1,21) | 1:25:A:ASN:C | 1:26:A:VAL:N | 1:26:A:VAL:CA | 1:26:A:VAL:C | 4        | 8.34          |
| (1,54) | 1:61:A:ILE:C | 1:62:A:GLN:N | 1:62:A:GLN:CA | 1:62:A:GLN:C | 19       | 8.33          |
| (1,3)  | 1:4:A:PHE:C  | 1:5:A:VAL:N  | 1:5:A:VAL:CA  | 1:5:A:VAL:C  | 17       | 8.33          |
| (1,3)  | 1:4:A:PHE:C  | 1:5:A:VAL:N  | 1:5:A:VAL:CA  | 1:5:A:VAL:C  | 10       | 8.28          |

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| Key    | Atom-1       | Atom-2       | Atom-3        | Atom-4       | Model ID | Violation (°) |
|--------|--------------|--------------|---------------|--------------|----------|---------------|
| (1,21) | 1:25:A:ASN:C | 1:26:A:VAL:N | 1:26:A:VAL:CA | 1:26:A:VAL:C | 10       | 8.23          |
| (1,63) | 1:70:A:VAL:C | 1:71:A:LEU:N | 1:71:A:LEU:CA | 1:71:A:LEU:C | 2        | 8.22          |
| (1,13) | 1:15:A:LEU:C | 1:16:A:GLU:N | 1:16:A:GLU:CA | 1:16:A:GLU:C | 20       | 8.22          |
| (1,54) | 1:61:A:ILE:C | 1:62:A:GLN:N | 1:62:A:GLN:CA | 1:62:A:GLN:C | 5        | 8.21          |
| (1,54) | 1:61:A:ILE:C | 1:62:A:GLN:N | 1:62:A:GLN:CA | 1:62:A:GLN:C | 10       | 8.18          |
| (1,63) | 1:70:A:VAL:C | 1:71:A:LEU:N | 1:71:A:LEU:CA | 1:71:A:LEU:C | 19       | 8.15          |
| (1,29) | 1:33:A:LYS:C | 1:34:A:GLU:N | 1:34:A:GLU:CA | 1:34:A:GLU:C | 17       | 8.11          |
| (1,63) | 1:70:A:VAL:C | 1:71:A:LEU:N | 1:71:A:LEU:CA | 1:71:A:LEU:C | 5        | 8.09          |
| (1,29) | 1:33:A:LYS:C | 1:34:A:GLU:N | 1:34:A:GLU:CA | 1:34:A:GLU:C | 5        | 8.09          |
| (1,29) | 1:33:A:LYS:C | 1:34:A:GLU:N | 1:34:A:GLU:CA | 1:34:A:GLU:C | 18       | 8.09          |
| (1,29) | 1:33:A:LYS:C | 1:34:A:GLU:N | 1:34:A:GLU:CA | 1:34:A:GLU:C | 11       | 8.02          |
| (1,63) | 1:70:A:VAL:C | 1:71:A:LEU:N | 1:71:A:LEU:CA | 1:71:A:LEU:C | 13       | 8.01          |
| (1,29) | 1:33:A:LYS:C | 1:34:A:GLU:N | 1:34:A:GLU:CA | 1:34:A:GLU:C | 19       | 7.99          |
| (1,29) | 1:33:A:LYS:C | 1:34:A:GLU:N | 1:34:A:GLU:CA | 1:34:A:GLU:C | 4        | 7.97          |
| (1,29) | 1:33:A:LYS:C | 1:34:A:GLU:N | 1:34:A:GLU:CA | 1:34:A:GLU:C | 16       | 7.97          |
| (1,29) | 1:33:A:LYS:C | 1:34:A:GLU:N | 1:34:A:GLU:CA | 1:34:A:GLU:C | 3        | 7.95          |
| (1,29) | 1:33:A:LYS:C | 1:34:A:GLU:N | 1:34:A:GLU:CA | 1:34:A:GLU:C | 2        | 7.94          |
| (1,29) | 1:33:A:LYS:C | 1:34:A:GLU:N | 1:34:A:GLU:CA | 1:34:A:GLU:C | 13       | 7.93          |
| (1,29) | 1:33:A:LYS:C | 1:34:A:GLU:N | 1:34:A:GLU:CA | 1:34:A:GLU:C | 7        | 7.92          |
| (1,29) | 1:33:A:LYS:C | 1:34:A:GLU:N | 1:34:A:GLU:CA | 1:34:A:GLU:C | 1        | 7.9           |
| (1,29) | 1:33:A:LYS:C | 1:34:A:GLU:N | 1:34:A:GLU:CA | 1:34:A:GLU:C | 12       | 7.9           |
| (1,29) | 1:33:A:LYS:C | 1:34:A:GLU:N | 1:34:A:GLU:CA | 1:34:A:GLU:C | 14       | 7.9           |
| (1,29) | 1:33:A:LYS:C | 1:34:A:GLU:N | 1:34:A:GLU:CA | 1:34:A:GLU:C | 6        | 7.85          |
| (1,3)  | 1:4:A:PHE:C  | 1:5:A:VAL:N  | 1:5:A:VAL:CA  | 1:5:A:VAL:C  | 13       | 7.84          |
| (1,29) | 1:33:A:LYS:C | 1:34:A:GLU:N | 1:34:A:GLU:CA | 1:34:A:GLU:C | 15       | 7.83          |
| (1,3)  | 1:4:A:PHE:C  | 1:5:A:VAL:N  | 1:5:A:VAL:CA  | 1:5:A:VAL:C  | 8        | 7.83          |
| (1,3)  | 1:4:A:PHE:C  | 1:5:A:VAL:N  | 1:5:A:VAL:CA  | 1:5:A:VAL:C  | 18       | 7.83          |
| (1,63) | 1:70:A:VAL:C | 1:71:A:LEU:N | 1:71:A:LEU:CA | 1:71:A:LEU:C | 8        | 7.82          |
| (1,3)  | 1:4:A:PHE:C  | 1:5:A:VAL:N  | 1:5:A:VAL:CA  | 1:5:A:VAL:C  | 1        | 7.81          |
| (1,29) | 1:33:A:LYS:C | 1:34:A:GLU:N | 1:34:A:GLU:CA | 1:34:A:GLU:C | 10       | 7.8           |
| (1,29) | 1:33:A:LYS:C | 1:34:A:GLU:N | 1:34:A:GLU:CA | 1:34:A:GLU:C | 8        | 7.79          |
| (1,3)  | 1:4:A:PHE:C  | 1:5:A:VAL:N  | 1:5:A:VAL:CA  | 1:5:A:VAL:C  | 9        | 7.79          |
| (1,3)  | 1:4:A:PHE:C  | 1:5:A:VAL:N  | 1:5:A:VAL:CA  | 1:5:A:VAL:C  | 14       | 7.78          |
| (1,3)  | 1:4:A:PHE:C  | 1:5:A:VAL:N  | 1:5:A:VAL:CA  | 1:5:A:VAL:C  | 16       | 7.76          |
| (1,63) | 1:70:A:VAL:C | 1:71:A:LEU:N | 1:71:A:LEU:CA | 1:71:A:LEU:C | 16       | 7.75          |
| (1,35) | 1:41:A:GLN:C | 1:42:A:ARG:N | 1:42:A:ARG:CA | 1:42:A:ARG:C | 7        | 7.71          |
| (1,3)  | 1:4:A:PHE:C  | 1:5:A:VAL:N  | 1:5:A:VAL:CA  | 1:5:A:VAL:C  | 19       | 7.71          |
| (1,63) | 1:70:A:VAL:C | 1:71:A:LEU:N | 1:71:A:LEU:CA | 1:71:A:LEU:C | 14       | 7.7           |
| (1,35) | 1:41:A:GLN:C | 1:42:A:ARG:N | 1:42:A:ARG:CA | 1:42:A:ARG:C | 2        | 7.68          |
| (1,35) | 1:41:A:GLN:C | 1:42:A:ARG:N | 1:42:A:ARG:CA | 1:42:A:ARG:C | 10       | 7.66          |
| (1,3)  | 1:4:A:PHE:C  | 1:5:A:VAL:N  | 1:5:A:VAL:CA  | 1:5:A:VAL:C  | 12       | 7.62          |
| (1,3)  | 1:4:A:PHE:C  | 1:5:A:VAL:N  | 1:5:A:VAL:CA  | 1:5:A:VAL:C  | 15       | 7.62          |
| (1,3)  | 1:4:A:PHE:C  | 1:5:A:VAL:N  | 1:5:A:VAL:CA  | 1:5:A:VAL:C  | 6        | 7.6           |
| (1,3)  | 1:4:A:PHE:C  | 1:5:A:VAL:N  | 1:5:A:VAL:CA  | 1:5:A:VAL:C  | 11       | 7.56          |
| (1,35) | 1:41:A:GLN:C | 1:42:A:ARG:N | 1:42:A:ARG:CA | 1:42:A:ARG:C | 5        | 7.54          |
| (1,35) | 1:41:A:GLN:C | 1:42:A:ARG:N | 1:42:A:ARG:CA | 1:42:A:ARG:C | 6        | 7.54          |
| (1,35) | 1:41:A:GLN:C | 1:42:A:ARG:N | 1:42:A:ARG:CA | 1:42:A:ARG:C | 3        | 7.53          |
| (1,35) | 1:41:A:GLN:C | 1:42:A:ARG:N | 1:42:A:ARG:CA | 1:42:A:ARG:C | 4        | 7.53          |
| (1,35) | 1:41:A:GLN:C | 1:42:A:ARG:N | 1:42:A:ARG:CA | 1:42:A:ARG:C | 12       | 7.51          |
| (1,35) | 1:41:A:GLN:C | 1:42:A:ARG:N | 1:42:A:ARG:CA | 1:42:A:ARG:C | 1        | 7.5           |
| (1,35) | 1:41:A:GLN:C | 1:42:A:ARG:N | 1:42:A:ARG:CA | 1:42:A:ARG:C | 16       | 7.45          |

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| Key    | Atom-1       | Atom-2       | Atom-3        | Atom-4       | Model ID | Violation (°) |
|--------|--------------|--------------|---------------|--------------|----------|---------------|
| (1,35) | 1:41:A:GLN:C | 1:42:A:ARG:N | 1:42:A:ARG:CA | 1:42:A:ARG:C | 11       | 7.44          |
| (1,35) | 1:41:A:GLN:C | 1:42:A:ARG:N | 1:42:A:ARG:CA | 1:42:A:ARG:C | 18       | 7.42          |
| (1,35) | 1:41:A:GLN:C | 1:42:A:ARG:N | 1:42:A:ARG:CA | 1:42:A:ARG:C | 19       | 7.4           |
| (1,3)  | 1:4:A:PHE:C  | 1:5:A:VAL:N  | 1:5:A:VAL:CA  | 1:5:A:VAL:C  | 5        | 7.4           |
| (1,55) | 1:62:A:GLN:C | 1:63:A:LYS:N | 1:63:A:LYS:CA | 1:63:A:LYS:C | 4        | 7.38          |
| (1,35) | 1:41:A:GLN:C | 1:42:A:ARG:N | 1:42:A:ARG:CA | 1:42:A:ARG:C | 9        | 7.35          |
| (1,35) | 1:41:A:GLN:C | 1:42:A:ARG:N | 1:42:A:ARG:CA | 1:42:A:ARG:C | 14       | 7.34          |
| (1,55) | 1:62:A:GLN:C | 1:63:A:LYS:N | 1:63:A:LYS:CA | 1:63:A:LYS:C | 2        | 7.33          |
| (1,63) | 1:70:A:VAL:C | 1:71:A:LEU:N | 1:71:A:LEU:CA | 1:71:A:LEU:C | 4        | 7.3           |
| (1,35) | 1:41:A:GLN:C | 1:42:A:ARG:N | 1:42:A:ARG:CA | 1:42:A:ARG:C | 8        | 7.23          |
| (1,55) | 1:62:A:GLN:C | 1:63:A:LYS:N | 1:63:A:LYS:CA | 1:63:A:LYS:C | 10       | 7.21          |
| (1,55) | 1:62:A:GLN:C | 1:63:A:LYS:N | 1:63:A:LYS:CA | 1:63:A:LYS:C | 3        | 7.18          |
| (1,63) | 1:70:A:VAL:C | 1:71:A:LEU:N | 1:71:A:LEU:CA | 1:71:A:LEU:C | 12       | 7.17          |
| (1,35) | 1:41:A:GLN:C | 1:42:A:ARG:N | 1:42:A:ARG:CA | 1:42:A:ARG:C | 15       | 7.17          |
| (1,55) | 1:62:A:GLN:C | 1:63:A:LYS:N | 1:63:A:LYS:CA | 1:63:A:LYS:C | 9        | 7.16          |
| (1,55) | 1:62:A:GLN:C | 1:63:A:LYS:N | 1:63:A:LYS:CA | 1:63:A:LYS:C | 16       | 7.14          |
| (1,55) | 1:62:A:GLN:C | 1:63:A:LYS:N | 1:63:A:LYS:CA | 1:63:A:LYS:C | 7        | 7.13          |
| (1,55) | 1:62:A:GLN:C | 1:63:A:LYS:N | 1:63:A:LYS:CA | 1:63:A:LYS:C | 14       | 7.12          |
| (1,55) | 1:62:A:GLN:C | 1:63:A:LYS:N | 1:63:A:LYS:CA | 1:63:A:LYS:C | 15       | 7.09          |
| (1,55) | 1:62:A:GLN:C | 1:63:A:LYS:N | 1:63:A:LYS:CA | 1:63:A:LYS:C | 5        | 7.08          |
| (1,55) | 1:62:A:GLN:C | 1:63:A:LYS:N | 1:63:A:LYS:CA | 1:63:A:LYS:C | 6        | 7.06          |
| (1,35) | 1:41:A:GLN:C | 1:42:A:ARG:N | 1:42:A:ARG:CA | 1:42:A:ARG:C | 17       | 7.04          |
| (1,55) | 1:62:A:GLN:C | 1:63:A:LYS:N | 1:63:A:LYS:CA | 1:63:A:LYS:C | 11       | 7.03          |
| (1,55) | 1:62:A:GLN:C | 1:63:A:LYS:N | 1:63:A:LYS:CA | 1:63:A:LYS:C | 8        | 7.01          |
| (1,35) | 1:41:A:GLN:C | 1:42:A:ARG:N | 1:42:A:ARG:CA | 1:42:A:ARG:C | 20       | 7.01          |
| (1,55) | 1:62:A:GLN:C | 1:63:A:LYS:N | 1:63:A:LYS:CA | 1:63:A:LYS:C | 19       | 7.0           |
| (1,35) | 1:41:A:GLN:C | 1:42:A:ARG:N | 1:42:A:ARG:CA | 1:42:A:ARG:C | 13       | 6.99          |
| (1,55) | 1:62:A:GLN:C | 1:63:A:LYS:N | 1:63:A:LYS:CA | 1:63:A:LYS:C | 12       | 6.97          |
| (1,55) | 1:62:A:GLN:C | 1:63:A:LYS:N | 1:63:A:LYS:CA | 1:63:A:LYS:C | 17       | 6.95          |
| (1,55) | 1:62:A:GLN:C | 1:63:A:LYS:N | 1:63:A:LYS:CA | 1:63:A:LYS:C | 20       | 6.95          |
| (1,55) | 1:62:A:GLN:C | 1:63:A:LYS:N | 1:63:A:LYS:CA | 1:63:A:LYS:C | 13       | 6.93          |
| (1,55) | 1:62:A:GLN:C | 1:63:A:LYS:N | 1:63:A:LYS:CA | 1:63:A:LYS:C | 1        | 6.9           |
| (1,55) | 1:62:A:GLN:C | 1:63:A:LYS:N | 1:63:A:LYS:CA | 1:63:A:LYS:C | 18       | 6.84          |
| (1,63) | 1:70:A:VAL:C | 1:71:A:LEU:N | 1:71:A:LEU:CA | 1:71:A:LEU:C | 10       | 6.63          |
| (1,48) | 1:55:A:THR:C | 1:56:A:LEU:N | 1:56:A:LEU:CA | 1:56:A:LEU:C | 3        | 6.63          |
| (1,48) | 1:55:A:THR:C | 1:56:A:LEU:N | 1:56:A:LEU:CA | 1:56:A:LEU:C | 7        | 6.62          |
| (1,5)  | 1:6:A:LYS:C  | 1:7:A:THR:N  | 1:7:A:THR:CA  | 1:7:A:THR:C  | 15       | 6.62          |
| (1,48) | 1:55:A:THR:C | 1:56:A:LEU:N | 1:56:A:LEU:CA | 1:56:A:LEU:C | 6        | 6.61          |
| (1,48) | 1:55:A:THR:C | 1:56:A:LEU:N | 1:56:A:LEU:CA | 1:56:A:LEU:C | 2        | 6.59          |
| (1,48) | 1:55:A:THR:C | 1:56:A:LEU:N | 1:56:A:LEU:CA | 1:56:A:LEU:C | 10       | 6.51          |
| (1,48) | 1:55:A:THR:C | 1:56:A:LEU:N | 1:56:A:LEU:CA | 1:56:A:LEU:C | 20       | 6.5           |
| (1,5)  | 1:6:A:LYS:C  | 1:7:A:THR:N  | 1:7:A:THR:CA  | 1:7:A:THR:C  | 1        | 6.5           |
| (1,48) | 1:55:A:THR:C | 1:56:A:LEU:N | 1:56:A:LEU:CA | 1:56:A:LEU:C | 9        | 6.48          |
| (1,48) | 1:55:A:THR:C | 1:56:A:LEU:N | 1:56:A:LEU:CA | 1:56:A:LEU:C | 13       | 6.45          |
| (1,48) | 1:55:A:THR:C | 1:56:A:LEU:N | 1:56:A:LEU:CA | 1:56:A:LEU:C | 8        | 6.44          |
| (1,48) | 1:55:A:THR:C | 1:56:A:LEU:N | 1:56:A:LEU:CA | 1:56:A:LEU:C | 1        | 6.43          |
| (1,48) | 1:55:A:THR:C | 1:56:A:LEU:N | 1:56:A:LEU:CA | 1:56:A:LEU:C | 12       | 6.43          |
| (1,5)  | 1:6:A:LYS:C  | 1:7:A:THR:N  | 1:7:A:THR:CA  | 1:7:A:THR:C  | 5        | 6.42          |
| (1,48) | 1:55:A:THR:C | 1:56:A:LEU:N | 1:56:A:LEU:CA | 1:56:A:LEU:C | 5        | 6.41          |
| (1,8)  | 1:10:A:GLY:C | 1:11:A:LYS:N | 1:11:A:LYS:CA | 1:11:A:LYS:C | 4        | 6.41          |
| (1,5)  | 1:6:A:LYS:C  | 1:7:A:THR:N  | 1:7:A:THR:CA  | 1:7:A:THR:C  | 8        | 6.4           |

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| Key    | Atom-1       | Atom-2       | Atom-3        | Atom-4       | Model ID | Violation (°) |
|--------|--------------|--------------|---------------|--------------|----------|---------------|
| (1,5)  | 1:6:A:LYS:C  | 1:7:A:THR:N  | 1:7:A:THR:CA  | 1:7:A:THR:C  | 16       | 6.4           |
| (1,48) | 1:55:A:THR:C | 1:56:A:LEU:N | 1:56:A:LEU:CA | 1:56:A:LEU:C | 4        | 6.39          |
| (1,5)  | 1:6:A:LYS:C  | 1:7:A:THR:N  | 1:7:A:THR:CA  | 1:7:A:THR:C  | 6        | 6.39          |
| (1,5)  | 1:6:A:LYS:C  | 1:7:A:THR:N  | 1:7:A:THR:CA  | 1:7:A:THR:C  | 19       | 6.39          |
| (1,27) | 1:31:A:GLN:C | 1:32:A:ASP:N | 1:32:A:ASP:CA | 1:32:A:ASP:C | 13       | 6.38          |
| (1,63) | 1:70:A:VAL:C | 1:71:A:LEU:N | 1:71:A:LEU:CA | 1:71:A:LEU:C | 6        | 6.37          |
| (1,48) | 1:55:A:THR:C | 1:56:A:LEU:N | 1:56:A:LEU:CA | 1:56:A:LEU:C | 18       | 6.33          |
| (1,48) | 1:55:A:THR:C | 1:56:A:LEU:N | 1:56:A:LEU:CA | 1:56:A:LEU:C | 11       | 6.32          |
| (1,48) | 1:55:A:THR:C | 1:56:A:LEU:N | 1:56:A:LEU:CA | 1:56:A:LEU:C | 14       | 6.32          |
| (1,48) | 1:55:A:THR:C | 1:56:A:LEU:N | 1:56:A:LEU:CA | 1:56:A:LEU:C | 17       | 6.32          |
| (1,52) | 1:59:A:TYR:C | 1:60:A:ASN:N | 1:60:A:ASN:CA | 1:60:A:ASN:C | 12       | 6.3           |
| (1,48) | 1:55:A:THR:C | 1:56:A:LEU:N | 1:56:A:LEU:CA | 1:56:A:LEU:C | 19       | 6.3           |
| (1,5)  | 1:6:A:LYS:C  | 1:7:A:THR:N  | 1:7:A:THR:CA  | 1:7:A:THR:C  | 14       | 6.3           |
| (1,48) | 1:55:A:THR:C | 1:56:A:LEU:N | 1:56:A:LEU:CA | 1:56:A:LEU:C | 15       | 6.29          |
| (1,48) | 1:55:A:THR:C | 1:56:A:LEU:N | 1:56:A:LEU:CA | 1:56:A:LEU:C | 16       | 6.23          |
| (1,27) | 1:31:A:GLN:C | 1:32:A:ASP:N | 1:32:A:ASP:CA | 1:32:A:ASP:C | 4        | 6.19          |
| (1,5)  | 1:6:A:LYS:C  | 1:7:A:THR:N  | 1:7:A:THR:CA  | 1:7:A:THR:C  | 18       | 6.19          |
| (1,27) | 1:31:A:GLN:C | 1:32:A:ASP:N | 1:32:A:ASP:CA | 1:32:A:ASP:C | 17       | 6.18          |
| (1,30) | 1:35:A:GLY:C | 1:36:A:ILE:N | 1:36:A:ILE:CA | 1:36:A:ILE:C | 9        | 6.17          |
| (1,5)  | 1:6:A:LYS:C  | 1:7:A:THR:N  | 1:7:A:THR:CA  | 1:7:A:THR:C  | 12       | 6.14          |
| (1,27) | 1:31:A:GLN:C | 1:32:A:ASP:N | 1:32:A:ASP:CA | 1:32:A:ASP:C | 15       | 6.12          |
| (1,27) | 1:31:A:GLN:C | 1:32:A:ASP:N | 1:32:A:ASP:CA | 1:32:A:ASP:C | 16       | 6.12          |
| (1,52) | 1:59:A:TYR:C | 1:60:A:ASN:N | 1:60:A:ASN:CA | 1:60:A:ASN:C | 18       | 6.11          |
| (1,27) | 1:31:A:GLN:C | 1:32:A:ASP:N | 1:32:A:ASP:CA | 1:32:A:ASP:C | 10       | 6.11          |
| (1,27) | 1:31:A:GLN:C | 1:32:A:ASP:N | 1:32:A:ASP:CA | 1:32:A:ASP:C | 19       | 6.1           |
| (1,27) | 1:31:A:GLN:C | 1:32:A:ASP:N | 1:32:A:ASP:CA | 1:32:A:ASP:C | 3        | 6.07          |
| (1,63) | 1:70:A:VAL:C | 1:71:A:LEU:N | 1:71:A:LEU:CA | 1:71:A:LEU:C | 3        | 6.06          |
| (1,27) | 1:31:A:GLN:C | 1:32:A:ASP:N | 1:32:A:ASP:CA | 1:32:A:ASP:C | 2        | 6.05          |
| (1,5)  | 1:6:A:LYS:C  | 1:7:A:THR:N  | 1:7:A:THR:CA  | 1:7:A:THR:C  | 11       | 6.05          |
| (1,27) | 1:31:A:GLN:C | 1:32:A:ASP:N | 1:32:A:ASP:CA | 1:32:A:ASP:C | 18       | 6.04          |
| (1,27) | 1:31:A:GLN:C | 1:32:A:ASP:N | 1:32:A:ASP:CA | 1:32:A:ASP:C | 5        | 6.03          |
| (1,27) | 1:31:A:GLN:C | 1:32:A:ASP:N | 1:32:A:ASP:CA | 1:32:A:ASP:C | 14       | 6.03          |
| (1,52) | 1:59:A:TYR:C | 1:60:A:ASN:N | 1:60:A:ASN:CA | 1:60:A:ASN:C | 15       | 6.02          |
| (1,52) | 1:59:A:TYR:C | 1:60:A:ASN:N | 1:60:A:ASN:CA | 1:60:A:ASN:C | 13       | 6.0           |
| (1,57) | 1:64:A:GLU:C | 1:65:A:SER:N | 1:65:A:SER:CA | 1:65:A:SER:C | 20       | 5.98          |
| (1,52) | 1:59:A:TYR:C | 1:60:A:ASN:N | 1:60:A:ASN:CA | 1:60:A:ASN:C | 4        | 5.96          |
| (1,27) | 1:31:A:GLN:C | 1:32:A:ASP:N | 1:32:A:ASP:CA | 1:32:A:ASP:C | 11       | 5.96          |
| (1,30) | 1:35:A:GLY:C | 1:36:A:ILE:N | 1:36:A:ILE:CA | 1:36:A:ILE:C | 4        | 5.93          |
| (1,30) | 1:35:A:GLY:C | 1:36:A:ILE:N | 1:36:A:ILE:CA | 1:36:A:ILE:C | 5        | 5.91          |
| (1,38) | 1:44:A:ILE:C | 1:45:A:PHE:N | 1:45:A:PHE:CA | 1:45:A:PHE:C | 14       | 5.9           |
| (1,30) | 1:35:A:GLY:C | 1:36:A:ILE:N | 1:36:A:ILE:CA | 1:36:A:ILE:C | 2        | 5.9           |
| (1,27) | 1:31:A:GLN:C | 1:32:A:ASP:N | 1:32:A:ASP:CA | 1:32:A:ASP:C | 1        | 5.9           |
| (1,30) | 1:35:A:GLY:C | 1:36:A:ILE:N | 1:36:A:ILE:CA | 1:36:A:ILE:C | 8        | 5.88          |
| (1,27) | 1:31:A:GLN:C | 1:32:A:ASP:N | 1:32:A:ASP:CA | 1:32:A:ASP:C | 7        | 5.88          |
| (1,52) | 1:59:A:TYR:C | 1:60:A:ASN:N | 1:60:A:ASN:CA | 1:60:A:ASN:C | 7        | 5.87          |
| (1,30) | 1:35:A:GLY:C | 1:36:A:ILE:N | 1:36:A:ILE:CA | 1:36:A:ILE:C | 10       | 5.87          |
| (1,27) | 1:31:A:GLN:C | 1:32:A:ASP:N | 1:32:A:ASP:CA | 1:32:A:ASP:C | 6        | 5.87          |
| (1,57) | 1:64:A:GLU:C | 1:65:A:SER:N | 1:65:A:SER:CA | 1:65:A:SER:C | 3        | 5.86          |
| (1,52) | 1:59:A:TYR:C | 1:60:A:ASN:N | 1:60:A:ASN:CA | 1:60:A:ASN:C | 1        | 5.86          |
| (1,27) | 1:31:A:GLN:C | 1:32:A:ASP:N | 1:32:A:ASP:CA | 1:32:A:ASP:C | 8        | 5.84          |
| (1,57) | 1:64:A:GLU:C | 1:65:A:SER:N | 1:65:A:SER:CA | 1:65:A:SER:C | 17       | 5.83          |

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| Key    | Atom-1       | Atom-2       | Atom-3        | Atom-4       | Model ID | Violation (°) |
|--------|--------------|--------------|---------------|--------------|----------|---------------|
| (1,27) | 1:31:A:GLN:C | 1:32:A:ASP:N | 1:32:A:ASP:CA | 1:32:A:ASP:C | 12       | 5.83          |
| (1,30) | 1:35:A:GLY:C | 1:36:A:ILE:N | 1:36:A:ILE:CA | 1:36:A:ILE:C | 17       | 5.82          |
| (1,57) | 1:64:A:GLU:C | 1:65:A:SER:N | 1:65:A:SER:CA | 1:65:A:SER:C | 2        | 5.8           |
| (1,57) | 1:64:A:GLU:C | 1:65:A:SER:N | 1:65:A:SER:CA | 1:65:A:SER:C | 13       | 5.8           |
| (1,38) | 1:44:A:ILE:C | 1:45:A:PHE:N | 1:45:A:PHE:CA | 1:45:A:PHE:C | 3        | 5.8           |
| (1,52) | 1:59:A:TYR:C | 1:60:A:ASN:N | 1:60:A:ASN:CA | 1:60:A:ASN:C | 10       | 5.79          |
| (1,30) | 1:35:A:GLY:C | 1:36:A:ILE:N | 1:36:A:ILE:CA | 1:36:A:ILE:C | 7        | 5.75          |
| (1,30) | 1:35:A:GLY:C | 1:36:A:ILE:N | 1:36:A:ILE:CA | 1:36:A:ILE:C | 12       | 5.74          |
| (1,57) | 1:64:A:GLU:C | 1:65:A:SER:N | 1:65:A:SER:CA | 1:65:A:SER:C | 10       | 5.73          |
| (1,52) | 1:59:A:TYR:C | 1:60:A:ASN:N | 1:60:A:ASN:CA | 1:60:A:ASN:C | 5        | 5.73          |
| (1,52) | 1:59:A:TYR:C | 1:60:A:ASN:N | 1:60:A:ASN:CA | 1:60:A:ASN:C | 8        | 5.73          |
| (1,52) | 1:59:A:TYR:C | 1:60:A:ASN:N | 1:60:A:ASN:CA | 1:60:A:ASN:C | 9        | 5.73          |
| (1,30) | 1:35:A:GLY:C | 1:36:A:ILE:N | 1:36:A:ILE:CA | 1:36:A:ILE:C | 11       | 5.73          |
| (1,30) | 1:35:A:GLY:C | 1:36:A:ILE:N | 1:36:A:ILE:CA | 1:36:A:ILE:C | 3        | 5.72          |
| (1,57) | 1:64:A:GLU:C | 1:65:A:SER:N | 1:65:A:SER:CA | 1:65:A:SER:C | 7        | 5.7           |
| (1,30) | 1:35:A:GLY:C | 1:36:A:ILE:N | 1:36:A:ILE:CA | 1:36:A:ILE:C | 6        | 5.7           |
| (1,30) | 1:35:A:GLY:C | 1:36:A:ILE:N | 1:36:A:ILE:CA | 1:36:A:ILE:C | 13       | 5.7           |
| (1,30) | 1:35:A:GLY:C | 1:36:A:ILE:N | 1:36:A:ILE:CA | 1:36:A:ILE:C | 19       | 5.7           |
| (1,57) | 1:64:A:GLU:C | 1:65:A:SER:N | 1:65:A:SER:CA | 1:65:A:SER:C | 15       | 5.69          |
| (1,57) | 1:64:A:GLU:C | 1:65:A:SER:N | 1:65:A:SER:CA | 1:65:A:SER:C | 4        | 5.68          |
| (1,52) | 1:59:A:TYR:C | 1:60:A:ASN:N | 1:60:A:ASN:CA | 1:60:A:ASN:C | 19       | 5.68          |
| (1,38) | 1:44:A:ILE:C | 1:45:A:PHE:N | 1:45:A:PHE:CA | 1:45:A:PHE:C | 10       | 5.67          |
| (1,52) | 1:59:A:TYR:C | 1:60:A:ASN:N | 1:60:A:ASN:CA | 1:60:A:ASN:C | 2        | 5.66          |
| (1,52) | 1:59:A:TYR:C | 1:60:A:ASN:N | 1:60:A:ASN:CA | 1:60:A:ASN:C | 3        | 5.66          |
| (1,52) | 1:59:A:TYR:C | 1:60:A:ASN:N | 1:60:A:ASN:CA | 1:60:A:ASN:C | 11       | 5.66          |
| (1,57) | 1:64:A:GLU:C | 1:65:A:SER:N | 1:65:A:SER:CA | 1:65:A:SER:C | 14       | 5.64          |
| (1,52) | 1:59:A:TYR:C | 1:60:A:ASN:N | 1:60:A:ASN:CA | 1:60:A:ASN:C | 6        | 5.64          |
| (1,38) | 1:44:A:ILE:C | 1:45:A:PHE:N | 1:45:A:PHE:CA | 1:45:A:PHE:C | 13       | 5.64          |
| (1,52) | 1:59:A:TYR:C | 1:60:A:ASN:N | 1:60:A:ASN:CA | 1:60:A:ASN:C | 14       | 5.63          |
| (1,52) | 1:59:A:TYR:C | 1:60:A:ASN:N | 1:60:A:ASN:CA | 1:60:A:ASN:C | 20       | 5.63          |
| (1,57) | 1:64:A:GLU:C | 1:65:A:SER:N | 1:65:A:SER:CA | 1:65:A:SER:C | 19       | 5.62          |
| (1,27) | 1:31:A:GLN:C | 1:32:A:ASP:N | 1:32:A:ASP:CA | 1:32:A:ASP:C | 20       | 5.62          |
| (1,30) | 1:35:A:GLY:C | 1:36:A:ILE:N | 1:36:A:ILE:CA | 1:36:A:ILE:C | 18       | 5.61          |
| (1,57) | 1:64:A:GLU:C | 1:65:A:SER:N | 1:65:A:SER:CA | 1:65:A:SER:C | 18       | 5.58          |
| (1,30) | 1:35:A:GLY:C | 1:36:A:ILE:N | 1:36:A:ILE:CA | 1:36:A:ILE:C | 15       | 5.58          |
| (1,57) | 1:64:A:GLU:C | 1:65:A:SER:N | 1:65:A:SER:CA | 1:65:A:SER:C | 9        | 5.57          |
| (1,57) | 1:64:A:GLU:C | 1:65:A:SER:N | 1:65:A:SER:CA | 1:65:A:SER:C | 11       | 5.56          |
| (1,52) | 1:59:A:TYR:C | 1:60:A:ASN:N | 1:60:A:ASN:CA | 1:60:A:ASN:C | 16       | 5.55          |
| (1,30) | 1:35:A:GLY:C | 1:36:A:ILE:N | 1:36:A:ILE:CA | 1:36:A:ILE:C | 20       | 5.55          |
| (1,30) | 1:35:A:GLY:C | 1:36:A:ILE:N | 1:36:A:ILE:CA | 1:36:A:ILE:C | 1        | 5.53          |
| (1,30) | 1:35:A:GLY:C | 1:36:A:ILE:N | 1:36:A:ILE:CA | 1:36:A:ILE:C | 16       | 5.53          |
| (1,57) | 1:64:A:GLU:C | 1:65:A:SER:N | 1:65:A:SER:CA | 1:65:A:SER:C | 5        | 5.51          |
| (1,30) | 1:35:A:GLY:C | 1:36:A:ILE:N | 1:36:A:ILE:CA | 1:36:A:ILE:C | 14       | 5.5           |
| (1,57) | 1:64:A:GLU:C | 1:65:A:SER:N | 1:65:A:SER:CA | 1:65:A:SER:C | 16       | 5.48          |
| (1,57) | 1:64:A:GLU:C | 1:65:A:SER:N | 1:65:A:SER:CA | 1:65:A:SER:C | 6        | 5.47          |
| (1,52) | 1:59:A:TYR:C | 1:60:A:ASN:N | 1:60:A:ASN:CA | 1:60:A:ASN:C | 17       | 5.46          |
| (1,57) | 1:64:A:GLU:C | 1:65:A:SER:N | 1:65:A:SER:CA | 1:65:A:SER:C | 12       | 5.45          |
| (1,62) | 1:69:A:LEU:C | 1:70:A:VAL:N | 1:70:A:VAL:CA | 1:70:A:VAL:C | 9        | 5.44          |
| (1,62) | 1:69:A:LEU:C | 1:70:A:VAL:N | 1:70:A:VAL:CA | 1:70:A:VAL:C | 14       | 5.44          |
| (1,57) | 1:64:A:GLU:C | 1:65:A:SER:N | 1:65:A:SER:CA | 1:65:A:SER:C | 1        | 5.43          |
| (1,57) | 1:64:A:GLU:C | 1:65:A:SER:N | 1:65:A:SER:CA | 1:65:A:SER:C | 8        | 5.43          |

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Continued from previous page...

| Key    | Atom-1       | Atom-2       | Atom-3        | Atom-4       | Model ID | Violation (°) |
|--------|--------------|--------------|---------------|--------------|----------|---------------|
| (1,39) | 1:45:A:PHE:C | 1:46:A:ALA:N | 1:46:A:ALA:CA | 1:46:A:ALA:C | 10       | 5.43          |
| (1,37) | 1:43:A:LEU:C | 1:44:A:ILE:N | 1:44:A:ILE:CA | 1:44:A:ILE:C | 7        | 5.43          |
| (1,39) | 1:45:A:PHE:C | 1:46:A:ALA:N | 1:46:A:ALA:CA | 1:46:A:ALA:C | 3        | 5.41          |
| (1,37) | 1:43:A:LEU:C | 1:44:A:ILE:N | 1:44:A:ILE:CA | 1:44:A:ILE:C | 9        | 5.41          |
| (1,39) | 1:45:A:PHE:C | 1:46:A:ALA:N | 1:46:A:ALA:CA | 1:46:A:ALA:C | 2        | 5.4           |
| (1,39) | 1:45:A:PHE:C | 1:46:A:ALA:N | 1:46:A:ALA:CA | 1:46:A:ALA:C | 20       | 5.4           |
| (1,62) | 1:69:A:LEU:C | 1:70:A:VAL:N | 1:70:A:VAL:CA | 1:70:A:VAL:C | 4        | 5.39          |
| (1,39) | 1:45:A:PHE:C | 1:46:A:ALA:N | 1:46:A:ALA:CA | 1:46:A:ALA:C | 6        | 5.38          |
| (1,39) | 1:45:A:PHE:C | 1:46:A:ALA:N | 1:46:A:ALA:CA | 1:46:A:ALA:C | 19       | 5.36          |
| (1,36) | 1:42:A:ARG:C | 1:43:A:LEU:N | 1:43:A:LEU:CA | 1:43:A:LEU:C | 17       | 5.35          |
| (1,8)  | 1:10:A:GLY:C | 1:11:A:LYS:N | 1:11:A:LYS:CA | 1:11:A:LYS:C | 2        | 5.35          |
| (1,39) | 1:45:A:PHE:C | 1:46:A:ALA:N | 1:46:A:ALA:CA | 1:46:A:ALA:C | 12       | 5.34          |
| (1,39) | 1:45:A:PHE:C | 1:46:A:ALA:N | 1:46:A:ALA:CA | 1:46:A:ALA:C | 15       | 5.34          |
| (1,62) | 1:69:A:LEU:C | 1:70:A:VAL:N | 1:70:A:VAL:CA | 1:70:A:VAL:C | 10       | 5.33          |
| (1,39) | 1:45:A:PHE:C | 1:46:A:ALA:N | 1:46:A:ALA:CA | 1:46:A:ALA:C | 11       | 5.33          |
| (1,8)  | 1:10:A:GLY:C | 1:11:A:LYS:N | 1:11:A:LYS:CA | 1:11:A:LYS:C | 10       | 5.33          |
| (1,62) | 1:69:A:LEU:C | 1:70:A:VAL:N | 1:70:A:VAL:CA | 1:70:A:VAL:C | 3        | 5.31          |
| (1,39) | 1:45:A:PHE:C | 1:46:A:ALA:N | 1:46:A:ALA:CA | 1:46:A:ALA:C | 18       | 5.31          |
| (1,5)  | 1:6:A:LYS:C  | 1:7:A:THR:N  | 1:7:A:THR:CA  | 1:7:A:THR:C  | 17       | 5.31          |
| (1,39) | 1:45:A:PHE:C | 1:46:A:ALA:N | 1:46:A:ALA:CA | 1:46:A:ALA:C | 1        | 5.3           |
| (1,39) | 1:45:A:PHE:C | 1:46:A:ALA:N | 1:46:A:ALA:CA | 1:46:A:ALA:C | 5        | 5.29          |
| (1,8)  | 1:10:A:GLY:C | 1:11:A:LYS:N | 1:11:A:LYS:CA | 1:11:A:LYS:C | 7        | 5.27          |
| (1,39) | 1:45:A:PHE:C | 1:46:A:ALA:N | 1:46:A:ALA:CA | 1:46:A:ALA:C | 16       | 5.25          |
| (1,39) | 1:45:A:PHE:C | 1:46:A:ALA:N | 1:46:A:ALA:CA | 1:46:A:ALA:C | 17       | 5.24          |
| (1,27) | 1:31:A:GLN:C | 1:32:A:ASP:N | 1:32:A:ASP:CA | 1:32:A:ASP:C | 9        | 5.24          |
| (1,36) | 1:42:A:ARG:C | 1:43:A:LEU:N | 1:43:A:LEU:CA | 1:43:A:LEU:C | 19       | 5.22          |
| (1,39) | 1:45:A:PHE:C | 1:46:A:ALA:N | 1:46:A:ALA:CA | 1:46:A:ALA:C | 13       | 5.18          |
| (1,39) | 1:45:A:PHE:C | 1:46:A:ALA:N | 1:46:A:ALA:CA | 1:46:A:ALA:C | 14       | 5.18          |
| (1,39) | 1:45:A:PHE:C | 1:46:A:ALA:N | 1:46:A:ALA:CA | 1:46:A:ALA:C | 8        | 5.15          |
| (1,36) | 1:42:A:ARG:C | 1:43:A:LEU:N | 1:43:A:LEU:CA | 1:43:A:LEU:C | 4        | 5.15          |
| (1,38) | 1:44:A:ILE:C | 1:45:A:PHE:N | 1:45:A:PHE:CA | 1:45:A:PHE:C | 8        | 5.12          |
| (1,36) | 1:42:A:ARG:C | 1:43:A:LEU:N | 1:43:A:LEU:CA | 1:43:A:LEU:C | 11       | 5.12          |
| (1,62) | 1:69:A:LEU:C | 1:70:A:VAL:N | 1:70:A:VAL:CA | 1:70:A:VAL:C | 2        | 5.08          |
| (1,36) | 1:42:A:ARG:C | 1:43:A:LEU:N | 1:43:A:LEU:CA | 1:43:A:LEU:C | 15       | 5.07          |
| (1,36) | 1:42:A:ARG:C | 1:43:A:LEU:N | 1:43:A:LEU:CA | 1:43:A:LEU:C | 20       | 5.06          |
| (1,38) | 1:44:A:ILE:C | 1:45:A:PHE:N | 1:45:A:PHE:CA | 1:45:A:PHE:C | 17       | 5.05          |
| (1,1)  | 1:2:A:GLN:C  | 1:3:A:ILE:N  | 1:3:A:ILE:CA  | 1:3:A:ILE:C  | 12       | 5.05          |
| (1,36) | 1:42:A:ARG:C | 1:43:A:LEU:N | 1:43:A:LEU:CA | 1:43:A:LEU:C | 7        | 5.04          |
| (1,36) | 1:42:A:ARG:C | 1:43:A:LEU:N | 1:43:A:LEU:CA | 1:43:A:LEU:C | 16       | 5.04          |
| (1,62) | 1:69:A:LEU:C | 1:70:A:VAL:N | 1:70:A:VAL:CA | 1:70:A:VAL:C | 7        | 5.03          |
| (1,38) | 1:44:A:ILE:C | 1:45:A:PHE:N | 1:45:A:PHE:CA | 1:45:A:PHE:C | 6        | 5.03          |
| (1,38) | 1:44:A:ILE:C | 1:45:A:PHE:N | 1:45:A:PHE:CA | 1:45:A:PHE:C | 16       | 5.03          |
| (1,36) | 1:42:A:ARG:C | 1:43:A:LEU:N | 1:43:A:LEU:CA | 1:43:A:LEU:C | 18       | 5.03          |
| (1,62) | 1:69:A:LEU:C | 1:70:A:VAL:N | 1:70:A:VAL:CA | 1:70:A:VAL:C | 12       | 5.01          |
| (1,63) | 1:70:A:VAL:C | 1:71:A:LEU:N | 1:71:A:LEU:CA | 1:71:A:LEU:C | 18       | 5.0           |
| (1,38) | 1:44:A:ILE:C | 1:45:A:PHE:N | 1:45:A:PHE:CA | 1:45:A:PHE:C | 12       | 5.0           |
| (1,58) | 1:65:A:SER:C | 1:66:A:THR:N | 1:66:A:THR:CA | 1:66:A:THR:C | 7        | 4.98          |
| (1,38) | 1:44:A:ILE:C | 1:45:A:PHE:N | 1:45:A:PHE:CA | 1:45:A:PHE:C | 5        | 4.96          |
| (1,36) | 1:42:A:ARG:C | 1:43:A:LEU:N | 1:43:A:LEU:CA | 1:43:A:LEU:C | 12       | 4.96          |
| (1,62) | 1:69:A:LEU:C | 1:70:A:VAL:N | 1:70:A:VAL:CA | 1:70:A:VAL:C | 5        | 4.95          |
| (1,62) | 1:69:A:LEU:C | 1:70:A:VAL:N | 1:70:A:VAL:CA | 1:70:A:VAL:C | 15       | 4.95          |

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Continued from previous page...

| Key    | Atom-1       | Atom-2       | Atom-3        | Atom-4       | Model ID | Violation (°) |
|--------|--------------|--------------|---------------|--------------|----------|---------------|
| (1,58) | 1:65:A:SER:C | 1:66:A:THR:N | 1:66:A:THR:CA | 1:66:A:THR:C | 10       | 4.95          |
| (1,37) | 1:43:A:LEU:C | 1:44:A:ILE:N | 1:44:A:ILE:CA | 1:44:A:ILE:C | 2        | 4.95          |
| (1,37) | 1:43:A:LEU:C | 1:44:A:ILE:N | 1:44:A:ILE:CA | 1:44:A:ILE:C | 8        | 4.94          |
| (1,62) | 1:69:A:LEU:C | 1:70:A:VAL:N | 1:70:A:VAL:CA | 1:70:A:VAL:C | 1        | 4.93          |
| (1,38) | 1:44:A:ILE:C | 1:45:A:PHE:N | 1:45:A:PHE:CA | 1:45:A:PHE:C | 15       | 4.93          |
| (1,38) | 1:44:A:ILE:C | 1:45:A:PHE:N | 1:45:A:PHE:CA | 1:45:A:PHE:C | 1        | 4.91          |
| (1,36) | 1:42:A:ARG:C | 1:43:A:LEU:N | 1:43:A:LEU:CA | 1:43:A:LEU:C | 9        | 4.9           |
| (1,36) | 1:42:A:ARG:C | 1:43:A:LEU:N | 1:43:A:LEU:CA | 1:43:A:LEU:C | 1        | 4.87          |
| (1,36) | 1:42:A:ARG:C | 1:43:A:LEU:N | 1:43:A:LEU:CA | 1:43:A:LEU:C | 6        | 4.86          |
| (1,5)  | 1:6:A:LYS:C  | 1:7:A:THR:N  | 1:7:A:THR:CA  | 1:7:A:THR:C  | 13       | 4.86          |
| (1,62) | 1:69:A:LEU:C | 1:70:A:VAL:N | 1:70:A:VAL:CA | 1:70:A:VAL:C | 20       | 4.83          |
| (1,5)  | 1:6:A:LYS:C  | 1:7:A:THR:N  | 1:7:A:THR:CA  | 1:7:A:THR:C  | 20       | 4.83          |
| (1,62) | 1:69:A:LEU:C | 1:70:A:VAL:N | 1:70:A:VAL:CA | 1:70:A:VAL:C | 6        | 4.82          |
| (1,62) | 1:69:A:LEU:C | 1:70:A:VAL:N | 1:70:A:VAL:CA | 1:70:A:VAL:C | 19       | 4.8           |
| (1,58) | 1:65:A:SER:C | 1:66:A:THR:N | 1:66:A:THR:CA | 1:66:A:THR:C | 3        | 4.79          |
| (1,36) | 1:42:A:ARG:C | 1:43:A:LEU:N | 1:43:A:LEU:CA | 1:43:A:LEU:C | 2        | 4.78          |
| (1,37) | 1:43:A:LEU:C | 1:44:A:ILE:N | 1:44:A:ILE:CA | 1:44:A:ILE:C | 11       | 4.76          |
| (1,58) | 1:65:A:SER:C | 1:66:A:THR:N | 1:66:A:THR:CA | 1:66:A:THR:C | 20       | 4.75          |
| (1,62) | 1:69:A:LEU:C | 1:70:A:VAL:N | 1:70:A:VAL:CA | 1:70:A:VAL:C | 18       | 4.74          |
| (1,5)  | 1:6:A:LYS:C  | 1:7:A:THR:N  | 1:7:A:THR:CA  | 1:7:A:THR:C  | 9        | 4.73          |
| (1,58) | 1:65:A:SER:C | 1:66:A:THR:N | 1:66:A:THR:CA | 1:66:A:THR:C | 2        | 4.72          |
| (1,38) | 1:44:A:ILE:C | 1:45:A:PHE:N | 1:45:A:PHE:CA | 1:45:A:PHE:C | 18       | 4.72          |
| (1,36) | 1:42:A:ARG:C | 1:43:A:LEU:N | 1:43:A:LEU:CA | 1:43:A:LEU:C | 5        | 4.71          |
| (1,38) | 1:44:A:ILE:C | 1:45:A:PHE:N | 1:45:A:PHE:CA | 1:45:A:PHE:C | 20       | 4.69          |
| (1,1)  | 1:2:A:GLN:C  | 1:3:A:ILE:N  | 1:3:A:ILE:CA  | 1:3:A:ILE:C  | 18       | 4.68          |
| (1,62) | 1:69:A:LEU:C | 1:70:A:VAL:N | 1:70:A:VAL:CA | 1:70:A:VAL:C | 13       | 4.67          |
| (1,58) | 1:65:A:SER:C | 1:66:A:THR:N | 1:66:A:THR:CA | 1:66:A:THR:C | 1        | 4.66          |
| (1,38) | 1:44:A:ILE:C | 1:45:A:PHE:N | 1:45:A:PHE:CA | 1:45:A:PHE:C | 19       | 4.65          |
| (1,37) | 1:43:A:LEU:C | 1:44:A:ILE:N | 1:44:A:ILE:CA | 1:44:A:ILE:C | 19       | 4.65          |
| (1,58) | 1:65:A:SER:C | 1:66:A:THR:N | 1:66:A:THR:CA | 1:66:A:THR:C | 5        | 4.63          |
| (1,1)  | 1:2:A:GLN:C  | 1:3:A:ILE:N  | 1:3:A:ILE:CA  | 1:3:A:ILE:C  | 16       | 4.63          |
| (1,62) | 1:69:A:LEU:C | 1:70:A:VAL:N | 1:70:A:VAL:CA | 1:70:A:VAL:C | 8        | 4.62          |
| (1,58) | 1:65:A:SER:C | 1:66:A:THR:N | 1:66:A:THR:CA | 1:66:A:THR:C | 4        | 4.62          |
| (1,62) | 1:69:A:LEU:C | 1:70:A:VAL:N | 1:70:A:VAL:CA | 1:70:A:VAL:C | 11       | 4.61          |
| (1,38) | 1:44:A:ILE:C | 1:45:A:PHE:N | 1:45:A:PHE:CA | 1:45:A:PHE:C | 11       | 4.6           |
| (1,37) | 1:43:A:LEU:C | 1:44:A:ILE:N | 1:44:A:ILE:CA | 1:44:A:ILE:C | 4        | 4.59          |
| (1,37) | 1:43:A:LEU:C | 1:44:A:ILE:N | 1:44:A:ILE:CA | 1:44:A:ILE:C | 18       | 4.59          |
| (1,1)  | 1:2:A:GLN:C  | 1:3:A:ILE:N  | 1:3:A:ILE:CA  | 1:3:A:ILE:C  | 20       | 4.58          |
| (1,39) | 1:45:A:PHE:C | 1:46:A:ALA:N | 1:46:A:ALA:CA | 1:46:A:ALA:C | 9        | 4.53          |
| (1,8)  | 1:10:A:GLY:C | 1:11:A:LYS:N | 1:11:A:LYS:CA | 1:11:A:LYS:C | 3        | 4.53          |
| (1,58) | 1:65:A:SER:C | 1:66:A:THR:N | 1:66:A:THR:CA | 1:66:A:THR:C | 6        | 4.52          |
| (1,58) | 1:65:A:SER:C | 1:66:A:THR:N | 1:66:A:THR:CA | 1:66:A:THR:C | 18       | 4.52          |
| (1,39) | 1:45:A:PHE:C | 1:46:A:ALA:N | 1:46:A:ALA:CA | 1:46:A:ALA:C | 7        | 4.52          |
| (1,39) | 1:45:A:PHE:C | 1:46:A:ALA:N | 1:46:A:ALA:CA | 1:46:A:ALA:C | 4        | 4.51          |
| (1,37) | 1:43:A:LEU:C | 1:44:A:ILE:N | 1:44:A:ILE:CA | 1:44:A:ILE:C | 17       | 4.51          |
| (1,58) | 1:65:A:SER:C | 1:66:A:THR:N | 1:66:A:THR:CA | 1:66:A:THR:C | 17       | 4.47          |
| (1,58) | 1:65:A:SER:C | 1:66:A:THR:N | 1:66:A:THR:CA | 1:66:A:THR:C | 16       | 4.46          |
| (1,58) | 1:65:A:SER:C | 1:66:A:THR:N | 1:66:A:THR:CA | 1:66:A:THR:C | 19       | 4.46          |
| (1,36) | 1:42:A:ARG:C | 1:43:A:LEU:N | 1:43:A:LEU:CA | 1:43:A:LEU:C | 8        | 4.46          |
| (1,62) | 1:69:A:LEU:C | 1:70:A:VAL:N | 1:70:A:VAL:CA | 1:70:A:VAL:C | 16       | 4.44          |
| (1,58) | 1:65:A:SER:C | 1:66:A:THR:N | 1:66:A:THR:CA | 1:66:A:THR:C | 14       | 4.44          |

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| Key    | Atom-1       | Atom-2       | Atom-3        | Atom-4       | Model ID | Violation (°) |
|--------|--------------|--------------|---------------|--------------|----------|---------------|
| (1,38) | 1:44:A:ILE:C | 1:45:A:PHE:N | 1:45:A:PHE:CA | 1:45:A:PHE:C | 2        | 4.44          |
| (1,58) | 1:65:A:SER:C | 1:66:A:THR:N | 1:66:A:THR:CA | 1:66:A:THR:C | 9        | 4.43          |
| (1,1)  | 1:2:A:GLN:C  | 1:3:A:ILE:N  | 1:3:A:ILE:CA  | 1:3:A:ILE:C  | 5        | 4.43          |
| (1,1)  | 1:2:A:GLN:C  | 1:3:A:ILE:N  | 1:3:A:ILE:CA  | 1:3:A:ILE:C  | 1        | 4.42          |
| (1,58) | 1:65:A:SER:C | 1:66:A:THR:N | 1:66:A:THR:CA | 1:66:A:THR:C | 11       | 4.39          |
| (1,58) | 1:65:A:SER:C | 1:66:A:THR:N | 1:66:A:THR:CA | 1:66:A:THR:C | 8        | 4.35          |
| (1,58) | 1:65:A:SER:C | 1:66:A:THR:N | 1:66:A:THR:CA | 1:66:A:THR:C | 15       | 4.35          |
| (1,5)  | 1:6:A:LYS:C  | 1:7:A:THR:N  | 1:7:A:THR:CA  | 1:7:A:THR:C  | 3        | 4.35          |
| (1,58) | 1:65:A:SER:C | 1:66:A:THR:N | 1:66:A:THR:CA | 1:66:A:THR:C | 13       | 4.3           |
| (1,43) | 1:50:A:LEU:C | 1:51:A:GLU:N | 1:51:A:GLU:CA | 1:51:A:GLU:C | 20       | 4.3           |
| (1,1)  | 1:2:A:GLN:C  | 1:3:A:ILE:N  | 1:3:A:ILE:CA  | 1:3:A:ILE:C  | 14       | 4.3           |
| (1,58) | 1:65:A:SER:C | 1:66:A:THR:N | 1:66:A:THR:CA | 1:66:A:THR:C | 12       | 4.28          |
| (1,15) | 1:17:A:VAL:C | 1:18:A:GLU:N | 1:18:A:GLU:CA | 1:18:A:GLU:C | 6        | 4.28          |
| (1,28) | 1:32:A:ASP:C | 1:33:A:LYS:N | 1:33:A:LYS:CA | 1:33:A:LYS:C | 6        | 4.26          |
| (1,28) | 1:32:A:ASP:C | 1:33:A:LYS:N | 1:33:A:LYS:CA | 1:33:A:LYS:C | 13       | 4.22          |
| (1,28) | 1:32:A:ASP:C | 1:33:A:LYS:N | 1:33:A:LYS:CA | 1:33:A:LYS:C | 11       | 4.21          |
| (1,28) | 1:32:A:ASP:C | 1:33:A:LYS:N | 1:33:A:LYS:CA | 1:33:A:LYS:C | 19       | 4.21          |
| (1,15) | 1:17:A:VAL:C | 1:18:A:GLU:N | 1:18:A:GLU:CA | 1:18:A:GLU:C | 9        | 4.21          |
| (1,36) | 1:42:A:ARG:C | 1:43:A:LEU:N | 1:43:A:LEU:CA | 1:43:A:LEU:C | 13       | 4.2           |
| (1,28) | 1:32:A:ASP:C | 1:33:A:LYS:N | 1:33:A:LYS:CA | 1:33:A:LYS:C | 17       | 4.2           |
| (1,15) | 1:17:A:VAL:C | 1:18:A:GLU:N | 1:18:A:GLU:CA | 1:18:A:GLU:C | 19       | 4.2           |
| (1,43) | 1:50:A:LEU:C | 1:51:A:GLU:N | 1:51:A:GLU:CA | 1:51:A:GLU:C | 10       | 4.19          |
| (1,28) | 1:32:A:ASP:C | 1:33:A:LYS:N | 1:33:A:LYS:CA | 1:33:A:LYS:C | 15       | 4.19          |
| (1,28) | 1:32:A:ASP:C | 1:33:A:LYS:N | 1:33:A:LYS:CA | 1:33:A:LYS:C | 16       | 4.18          |
| (1,28) | 1:32:A:ASP:C | 1:33:A:LYS:N | 1:33:A:LYS:CA | 1:33:A:LYS:C | 14       | 4.17          |
| (1,15) | 1:17:A:VAL:C | 1:18:A:GLU:N | 1:18:A:GLU:CA | 1:18:A:GLU:C | 11       | 4.17          |
| (1,28) | 1:32:A:ASP:C | 1:33:A:LYS:N | 1:33:A:LYS:CA | 1:33:A:LYS:C | 8        | 4.16          |
| (1,28) | 1:32:A:ASP:C | 1:33:A:LYS:N | 1:33:A:LYS:CA | 1:33:A:LYS:C | 10       | 4.15          |
| (1,28) | 1:32:A:ASP:C | 1:33:A:LYS:N | 1:33:A:LYS:CA | 1:33:A:LYS:C | 7        | 4.14          |
| (1,1)  | 1:2:A:GLN:C  | 1:3:A:ILE:N  | 1:3:A:ILE:CA  | 1:3:A:ILE:C  | 11       | 4.14          |
| (1,43) | 1:50:A:LEU:C | 1:51:A:GLU:N | 1:51:A:GLU:CA | 1:51:A:GLU:C | 7        | 4.13          |
| (1,15) | 1:17:A:VAL:C | 1:18:A:GLU:N | 1:18:A:GLU:CA | 1:18:A:GLU:C | 14       | 4.13          |
| (1,46) | 1:53:A:GLY:C | 1:54:A:ARG:N | 1:54:A:ARG:CA | 1:54:A:ARG:C | 5        | 4.12          |
| (1,60) | 1:67:A:LEU:C | 1:68:A:HIS:N | 1:68:A:HIS:CA | 1:68:A:HIS:C | 9        | 4.1           |
| (1,28) | 1:32:A:ASP:C | 1:33:A:LYS:N | 1:33:A:LYS:CA | 1:33:A:LYS:C | 18       | 4.1           |
| (1,43) | 1:50:A:LEU:C | 1:51:A:GLU:N | 1:51:A:GLU:CA | 1:51:A:GLU:C | 2        | 4.09          |
| (1,28) | 1:32:A:ASP:C | 1:33:A:LYS:N | 1:33:A:LYS:CA | 1:33:A:LYS:C | 12       | 4.09          |
| (1,36) | 1:42:A:ARG:C | 1:43:A:LEU:N | 1:43:A:LEU:CA | 1:43:A:LEU:C | 3        | 4.08          |
| (1,28) | 1:32:A:ASP:C | 1:33:A:LYS:N | 1:33:A:LYS:CA | 1:33:A:LYS:C | 1        | 4.07          |
| (1,15) | 1:17:A:VAL:C | 1:18:A:GLU:N | 1:18:A:GLU:CA | 1:18:A:GLU:C | 8        | 4.07          |
| (1,43) | 1:50:A:LEU:C | 1:51:A:GLU:N | 1:51:A:GLU:CA | 1:51:A:GLU:C | 13       | 4.06          |
| (1,43) | 1:50:A:LEU:C | 1:51:A:GLU:N | 1:51:A:GLU:CA | 1:51:A:GLU:C | 3        | 4.05          |
| (1,28) | 1:32:A:ASP:C | 1:33:A:LYS:N | 1:33:A:LYS:CA | 1:33:A:LYS:C | 2        | 4.05          |
| (1,28) | 1:32:A:ASP:C | 1:33:A:LYS:N | 1:33:A:LYS:CA | 1:33:A:LYS:C | 4        | 4.05          |
| (1,43) | 1:50:A:LEU:C | 1:51:A:GLU:N | 1:51:A:GLU:CA | 1:51:A:GLU:C | 1        | 4.04          |
| (1,43) | 1:50:A:LEU:C | 1:51:A:GLU:N | 1:51:A:GLU:CA | 1:51:A:GLU:C | 9        | 4.03          |
| (1,36) | 1:42:A:ARG:C | 1:43:A:LEU:N | 1:43:A:LEU:CA | 1:43:A:LEU:C | 10       | 4.03          |
| (1,18) | 1:21:A:ASP:C | 1:22:A:THR:N | 1:22:A:THR:CA | 1:22:A:THR:C | 6        | 4.03          |
| (1,5)  | 1:6:A:LYS:C  | 1:7:A:THR:N  | 1:7:A:THR:CA  | 1:7:A:THR:C  | 7        | 4.03          |
| (1,28) | 1:32:A:ASP:C | 1:33:A:LYS:N | 1:33:A:LYS:CA | 1:33:A:LYS:C | 9        | 4.02          |
| (1,15) | 1:17:A:VAL:C | 1:18:A:GLU:N | 1:18:A:GLU:CA | 1:18:A:GLU:C | 3        | 3.99          |

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| Key    | Atom-1       | Atom-2       | Atom-3        | Atom-4       | Model ID | Violation (°) |
|--------|--------------|--------------|---------------|--------------|----------|---------------|
| (1,62) | 1:69:A:LEU:C | 1:70:A:VAL:N | 1:70:A:VAL:CA | 1:70:A:VAL:C | 17       | 3.98          |
| (1,60) | 1:67:A:LEU:C | 1:68:A:HIS:N | 1:68:A:HIS:CA | 1:68:A:HIS:C | 17       | 3.98          |
| (1,43) | 1:50:A:LEU:C | 1:51:A:GLU:N | 1:51:A:GLU:CA | 1:51:A:GLU:C | 4        | 3.98          |
| (1,43) | 1:50:A:LEU:C | 1:51:A:GLU:N | 1:51:A:GLU:CA | 1:51:A:GLU:C | 16       | 3.98          |
| (1,28) | 1:32:A:ASP:C | 1:33:A:LYS:N | 1:33:A:LYS:CA | 1:33:A:LYS:C | 3        | 3.98          |
| (1,47) | 1:54:A:ARG:C | 1:55:A:THR:N | 1:55:A:THR:CA | 1:55:A:THR:C | 8        | 3.97          |
| (1,36) | 1:42:A:ARG:C | 1:43:A:LEU:N | 1:43:A:LEU:CA | 1:43:A:LEU:C | 14       | 3.97          |
| (1,18) | 1:21:A:ASP:C | 1:22:A:THR:N | 1:22:A:THR:CA | 1:22:A:THR:C | 5        | 3.97          |
| (1,1)  | 1:2:A:GLN:C  | 1:3:A:ILE:N  | 1:3:A:ILE:CA  | 1:3:A:ILE:C  | 19       | 3.97          |
| (1,59) | 1:66:A:THR:C | 1:67:A:LEU:N | 1:67:A:LEU:CA | 1:67:A:LEU:C | 12       | 3.96          |
| (1,28) | 1:32:A:ASP:C | 1:33:A:LYS:N | 1:33:A:LYS:CA | 1:33:A:LYS:C | 20       | 3.96          |
| (1,15) | 1:17:A:VAL:C | 1:18:A:GLU:N | 1:18:A:GLU:CA | 1:18:A:GLU:C | 18       | 3.96          |
| (1,43) | 1:50:A:LEU:C | 1:51:A:GLU:N | 1:51:A:GLU:CA | 1:51:A:GLU:C | 6        | 3.95          |
| (1,28) | 1:32:A:ASP:C | 1:33:A:LYS:N | 1:33:A:LYS:CA | 1:33:A:LYS:C | 5        | 3.95          |
| (1,43) | 1:50:A:LEU:C | 1:51:A:GLU:N | 1:51:A:GLU:CA | 1:51:A:GLU:C | 19       | 3.93          |
| (1,18) | 1:21:A:ASP:C | 1:22:A:THR:N | 1:22:A:THR:CA | 1:22:A:THR:C | 1        | 3.93          |
| (1,15) | 1:17:A:VAL:C | 1:18:A:GLU:N | 1:18:A:GLU:CA | 1:18:A:GLU:C | 15       | 3.93          |
| (1,59) | 1:66:A:THR:C | 1:67:A:LEU:N | 1:67:A:LEU:CA | 1:67:A:LEU:C | 18       | 3.92          |
| (1,43) | 1:50:A:LEU:C | 1:51:A:GLU:N | 1:51:A:GLU:CA | 1:51:A:GLU:C | 12       | 3.92          |
| (1,43) | 1:50:A:LEU:C | 1:51:A:GLU:N | 1:51:A:GLU:CA | 1:51:A:GLU:C | 14       | 3.92          |
| (1,37) | 1:43:A:LEU:C | 1:44:A:ILE:N | 1:44:A:ILE:CA | 1:44:A:ILE:C | 20       | 3.92          |
| (1,18) | 1:21:A:ASP:C | 1:22:A:THR:N | 1:22:A:THR:CA | 1:22:A:THR:C | 8        | 3.92          |
| (1,60) | 1:67:A:LEU:C | 1:68:A:HIS:N | 1:68:A:HIS:CA | 1:68:A:HIS:C | 20       | 3.91          |
| (1,1)  | 1:2:A:GLN:C  | 1:3:A:ILE:N  | 1:3:A:ILE:CA  | 1:3:A:ILE:C  | 13       | 3.91          |
| (1,59) | 1:66:A:THR:C | 1:67:A:LEU:N | 1:67:A:LEU:CA | 1:67:A:LEU:C | 19       | 3.9           |
| (1,43) | 1:50:A:LEU:C | 1:51:A:GLU:N | 1:51:A:GLU:CA | 1:51:A:GLU:C | 17       | 3.9           |
| (1,37) | 1:43:A:LEU:C | 1:44:A:ILE:N | 1:44:A:ILE:CA | 1:44:A:ILE:C | 12       | 3.9           |
| (1,18) | 1:21:A:ASP:C | 1:22:A:THR:N | 1:22:A:THR:CA | 1:22:A:THR:C | 14       | 3.9           |
| (1,15) | 1:17:A:VAL:C | 1:18:A:GLU:N | 1:18:A:GLU:CA | 1:18:A:GLU:C | 4        | 3.9           |
| (1,18) | 1:21:A:ASP:C | 1:22:A:THR:N | 1:22:A:THR:CA | 1:22:A:THR:C | 18       | 3.89          |
| (1,5)  | 1:6:A:LYS:C  | 1:7:A:THR:N  | 1:7:A:THR:CA  | 1:7:A:THR:C  | 2        | 3.89          |
| (1,1)  | 1:2:A:GLN:C  | 1:3:A:ILE:N  | 1:3:A:ILE:CA  | 1:3:A:ILE:C  | 6        | 3.89          |
| (1,59) | 1:66:A:THR:C | 1:67:A:LEU:N | 1:67:A:LEU:CA | 1:67:A:LEU:C | 11       | 3.88          |
| (1,43) | 1:50:A:LEU:C | 1:51:A:GLU:N | 1:51:A:GLU:CA | 1:51:A:GLU:C | 15       | 3.88          |
| (1,38) | 1:44:A:ILE:C | 1:45:A:PHE:N | 1:45:A:PHE:CA | 1:45:A:PHE:C | 4        | 3.88          |
| (1,59) | 1:66:A:THR:C | 1:67:A:LEU:N | 1:67:A:LEU:CA | 1:67:A:LEU:C | 15       | 3.87          |
| (1,5)  | 1:6:A:LYS:C  | 1:7:A:THR:N  | 1:7:A:THR:CA  | 1:7:A:THR:C  | 10       | 3.87          |
| (1,46) | 1:53:A:GLY:C | 1:54:A:ARG:N | 1:54:A:ARG:CA | 1:54:A:ARG:C | 15       | 3.86          |
| (1,43) | 1:50:A:LEU:C | 1:51:A:GLU:N | 1:51:A:GLU:CA | 1:51:A:GLU:C | 18       | 3.85          |
| (1,63) | 1:70:A:VAL:C | 1:71:A:LEU:N | 1:71:A:LEU:CA | 1:71:A:LEU:C | 20       | 3.84          |
| (1,47) | 1:54:A:ARG:C | 1:55:A:THR:N | 1:55:A:THR:CA | 1:55:A:THR:C | 10       | 3.84          |
| (1,18) | 1:21:A:ASP:C | 1:22:A:THR:N | 1:22:A:THR:CA | 1:22:A:THR:C | 3        | 3.84          |
| (1,43) | 1:50:A:LEU:C | 1:51:A:GLU:N | 1:51:A:GLU:CA | 1:51:A:GLU:C | 11       | 3.83          |
| (1,12) | 1:14:A:THR:C | 1:15:A:LEU:N | 1:15:A:LEU:CA | 1:15:A:LEU:C | 20       | 3.83          |
| (1,59) | 1:66:A:THR:C | 1:67:A:LEU:N | 1:67:A:LEU:CA | 1:67:A:LEU:C | 13       | 3.82          |
| (1,46) | 1:53:A:GLY:C | 1:54:A:ARG:N | 1:54:A:ARG:CA | 1:54:A:ARG:C | 17       | 3.82          |
| (1,18) | 1:21:A:ASP:C | 1:22:A:THR:N | 1:22:A:THR:CA | 1:22:A:THR:C | 15       | 3.82          |
| (1,15) | 1:17:A:VAL:C | 1:18:A:GLU:N | 1:18:A:GLU:CA | 1:18:A:GLU:C | 1        | 3.82          |
| (1,15) | 1:17:A:VAL:C | 1:18:A:GLU:N | 1:18:A:GLU:CA | 1:18:A:GLU:C | 10       | 3.82          |
| (1,60) | 1:67:A:LEU:C | 1:68:A:HIS:N | 1:68:A:HIS:CA | 1:68:A:HIS:C | 7        | 3.81          |
| (1,43) | 1:50:A:LEU:C | 1:51:A:GLU:N | 1:51:A:GLU:CA | 1:51:A:GLU:C | 5        | 3.81          |

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| Key    | Atom-1       | Atom-2       | Atom-3        | Atom-4       | Model ID | Violation (°) |
|--------|--------------|--------------|---------------|--------------|----------|---------------|
| (1,18) | 1:21:A:ASP:C | 1:22:A:THR:N | 1:22:A:THR:CA | 1:22:A:THR:C | 9        | 3.81          |
| (1,18) | 1:21:A:ASP:C | 1:22:A:THR:N | 1:22:A:THR:CA | 1:22:A:THR:C | 16       | 3.81          |
| (1,15) | 1:17:A:VAL:C | 1:18:A:GLU:N | 1:18:A:GLU:CA | 1:18:A:GLU:C | 17       | 3.81          |
| (1,60) | 1:67:A:LEU:C | 1:68:A:HIS:N | 1:68:A:HIS:CA | 1:68:A:HIS:C | 13       | 3.79          |
| (1,60) | 1:67:A:LEU:C | 1:68:A:HIS:N | 1:68:A:HIS:CA | 1:68:A:HIS:C | 4        | 3.78          |
| (1,47) | 1:54:A:ARG:C | 1:55:A:THR:N | 1:55:A:THR:CA | 1:55:A:THR:C | 15       | 3.78          |
| (1,46) | 1:53:A:GLY:C | 1:54:A:ARG:N | 1:54:A:ARG:CA | 1:54:A:ARG:C | 20       | 3.78          |
| (1,15) | 1:17:A:VAL:C | 1:18:A:GLU:N | 1:18:A:GLU:CA | 1:18:A:GLU:C | 13       | 3.78          |
| (1,46) | 1:53:A:GLY:C | 1:54:A:ARG:N | 1:54:A:ARG:CA | 1:54:A:ARG:C | 19       | 3.77          |
| (1,18) | 1:21:A:ASP:C | 1:22:A:THR:N | 1:22:A:THR:CA | 1:22:A:THR:C | 19       | 3.76          |
| (1,47) | 1:54:A:ARG:C | 1:55:A:THR:N | 1:55:A:THR:CA | 1:55:A:THR:C | 6        | 3.75          |
| (1,46) | 1:53:A:GLY:C | 1:54:A:ARG:N | 1:54:A:ARG:CA | 1:54:A:ARG:C | 8        | 3.75          |
| (1,37) | 1:43:A:LEU:C | 1:44:A:ILE:N | 1:44:A:ILE:CA | 1:44:A:ILE:C | 6        | 3.75          |
| (1,60) | 1:67:A:LEU:C | 1:68:A:HIS:N | 1:68:A:HIS:CA | 1:68:A:HIS:C | 19       | 3.74          |
| (1,59) | 1:66:A:THR:C | 1:67:A:LEU:N | 1:67:A:LEU:CA | 1:67:A:LEU:C | 16       | 3.74          |
| (1,46) | 1:53:A:GLY:C | 1:54:A:ARG:N | 1:54:A:ARG:CA | 1:54:A:ARG:C | 3        | 3.74          |
| (1,15) | 1:17:A:VAL:C | 1:18:A:GLU:N | 1:18:A:GLU:CA | 1:18:A:GLU:C | 16       | 3.74          |
| (1,12) | 1:14:A:THR:C | 1:15:A:LEU:N | 1:15:A:LEU:CA | 1:15:A:LEU:C | 17       | 3.73          |
| (1,59) | 1:66:A:THR:C | 1:67:A:LEU:N | 1:67:A:LEU:CA | 1:67:A:LEU:C | 1        | 3.72          |
| (1,59) | 1:66:A:THR:C | 1:67:A:LEU:N | 1:67:A:LEU:CA | 1:67:A:LEU:C | 5        | 3.72          |
| (1,47) | 1:54:A:ARG:C | 1:55:A:THR:N | 1:55:A:THR:CA | 1:55:A:THR:C | 1        | 3.72          |
| (1,12) | 1:14:A:THR:C | 1:15:A:LEU:N | 1:15:A:LEU:CA | 1:15:A:LEU:C | 13       | 3.72          |
| (1,46) | 1:53:A:GLY:C | 1:54:A:ARG:N | 1:54:A:ARG:CA | 1:54:A:ARG:C | 14       | 3.71          |
| (1,46) | 1:53:A:GLY:C | 1:54:A:ARG:N | 1:54:A:ARG:CA | 1:54:A:ARG:C | 16       | 3.71          |
| (1,37) | 1:43:A:LEU:C | 1:44:A:ILE:N | 1:44:A:ILE:CA | 1:44:A:ILE:C | 5        | 3.7           |
| (1,59) | 1:66:A:THR:C | 1:67:A:LEU:N | 1:67:A:LEU:CA | 1:67:A:LEU:C | 8        | 3.69          |
| (1,47) | 1:54:A:ARG:C | 1:55:A:THR:N | 1:55:A:THR:CA | 1:55:A:THR:C | 14       | 3.69          |
| (1,47) | 1:54:A:ARG:C | 1:55:A:THR:N | 1:55:A:THR:CA | 1:55:A:THR:C | 20       | 3.69          |
| (1,18) | 1:21:A:ASP:C | 1:22:A:THR:N | 1:22:A:THR:CA | 1:22:A:THR:C | 12       | 3.69          |
| (1,60) | 1:67:A:LEU:C | 1:68:A:HIS:N | 1:68:A:HIS:CA | 1:68:A:HIS:C | 18       | 3.68          |
| (1,59) | 1:66:A:THR:C | 1:67:A:LEU:N | 1:67:A:LEU:CA | 1:67:A:LEU:C | 6        | 3.68          |
| (1,47) | 1:54:A:ARG:C | 1:55:A:THR:N | 1:55:A:THR:CA | 1:55:A:THR:C | 13       | 3.68          |
| (1,47) | 1:54:A:ARG:C | 1:55:A:THR:N | 1:55:A:THR:CA | 1:55:A:THR:C | 19       | 3.68          |
| (1,15) | 1:17:A:VAL:C | 1:18:A:GLU:N | 1:18:A:GLU:CA | 1:18:A:GLU:C | 7        | 3.68          |
| (1,59) | 1:66:A:THR:C | 1:67:A:LEU:N | 1:67:A:LEU:CA | 1:67:A:LEU:C | 17       | 3.67          |
| (1,37) | 1:43:A:LEU:C | 1:44:A:ILE:N | 1:44:A:ILE:CA | 1:44:A:ILE:C | 1        | 3.67          |
| (1,24) | 1:28:A:ALA:C | 1:29:A:LYS:N | 1:29:A:LYS:CA | 1:29:A:LYS:C | 3        | 3.67          |
| (1,9)  | 1:11:A:LYS:C | 1:12:A:THR:N | 1:12:A:THR:CA | 1:12:A:THR:C | 17       | 3.67          |
| (1,46) | 1:53:A:GLY:C | 1:54:A:ARG:N | 1:54:A:ARG:CA | 1:54:A:ARG:C | 2        | 3.66          |
| (1,12) | 1:14:A:THR:C | 1:15:A:LEU:N | 1:15:A:LEU:CA | 1:15:A:LEU:C | 3        | 3.66          |
| (1,1)  | 1:2:A:GLN:C  | 1:3:A:ILE:N  | 1:3:A:ILE:CA  | 1:3:A:ILE:C  | 3        | 3.66          |
| (1,18) | 1:21:A:ASP:C | 1:22:A:THR:N | 1:22:A:THR:CA | 1:22:A:THR:C | 2        | 3.65          |
| (1,1)  | 1:2:A:GLN:C  | 1:3:A:ILE:N  | 1:3:A:ILE:CA  | 1:3:A:ILE:C  | 9        | 3.65          |
| (1,60) | 1:67:A:LEU:C | 1:68:A:HIS:N | 1:68:A:HIS:CA | 1:68:A:HIS:C | 12       | 3.64          |
| (1,59) | 1:66:A:THR:C | 1:67:A:LEU:N | 1:67:A:LEU:CA | 1:67:A:LEU:C | 10       | 3.64          |
| (1,18) | 1:21:A:ASP:C | 1:22:A:THR:N | 1:22:A:THR:CA | 1:22:A:THR:C | 10       | 3.64          |
| (1,15) | 1:17:A:VAL:C | 1:18:A:GLU:N | 1:18:A:GLU:CA | 1:18:A:GLU:C | 5        | 3.64          |
| (1,47) | 1:54:A:ARG:C | 1:55:A:THR:N | 1:55:A:THR:CA | 1:55:A:THR:C | 2        | 3.63          |
| (1,47) | 1:54:A:ARG:C | 1:55:A:THR:N | 1:55:A:THR:CA | 1:55:A:THR:C | 3        | 3.63          |
| (1,47) | 1:54:A:ARG:C | 1:55:A:THR:N | 1:55:A:THR:CA | 1:55:A:THR:C | 17       | 3.63          |
| (1,24) | 1:28:A:ALA:C | 1:29:A:LYS:N | 1:29:A:LYS:CA | 1:29:A:LYS:C | 10       | 3.63          |

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Continued from previous page...

| Key    | Atom-1       | Atom-2       | Atom-3        | Atom-4       | Model ID | Violation (°) |
|--------|--------------|--------------|---------------|--------------|----------|---------------|
| (1,60) | 1:67:A:LEU:C | 1:68:A:HIS:N | 1:68:A:HIS:CA | 1:68:A:HIS:C | 5        | 3.62          |
| (1,18) | 1:21:A:ASP:C | 1:22:A:THR:N | 1:22:A:THR:CA | 1:22:A:THR:C | 13       | 3.62          |
| (1,60) | 1:67:A:LEU:C | 1:68:A:HIS:N | 1:68:A:HIS:CA | 1:68:A:HIS:C | 2        | 3.61          |
| (1,60) | 1:67:A:LEU:C | 1:68:A:HIS:N | 1:68:A:HIS:CA | 1:68:A:HIS:C | 11       | 3.61          |
| (1,47) | 1:54:A:ARG:C | 1:55:A:THR:N | 1:55:A:THR:CA | 1:55:A:THR:C | 5        | 3.61          |
| (1,46) | 1:53:A:GLY:C | 1:54:A:ARG:N | 1:54:A:ARG:CA | 1:54:A:ARG:C | 1        | 3.61          |
| (1,43) | 1:50:A:LEU:C | 1:51:A:GLU:N | 1:51:A:GLU:CA | 1:51:A:GLU:C | 8        | 3.61          |
| (1,18) | 1:21:A:ASP:C | 1:22:A:THR:N | 1:22:A:THR:CA | 1:22:A:THR:C | 11       | 3.61          |
| (1,46) | 1:53:A:GLY:C | 1:54:A:ARG:N | 1:54:A:ARG:CA | 1:54:A:ARG:C | 13       | 3.6           |
| (1,18) | 1:21:A:ASP:C | 1:22:A:THR:N | 1:22:A:THR:CA | 1:22:A:THR:C | 4        | 3.6           |
| (1,12) | 1:14:A:THR:C | 1:15:A:LEU:N | 1:15:A:LEU:CA | 1:15:A:LEU:C | 1        | 3.6           |
| (1,12) | 1:14:A:THR:C | 1:15:A:LEU:N | 1:15:A:LEU:CA | 1:15:A:LEU:C | 14       | 3.6           |
| (1,59) | 1:66:A:THR:C | 1:67:A:LEU:N | 1:67:A:LEU:CA | 1:67:A:LEU:C | 2        | 3.59          |
| (1,47) | 1:54:A:ARG:C | 1:55:A:THR:N | 1:55:A:THR:CA | 1:55:A:THR:C | 12       | 3.59          |
| (1,24) | 1:28:A:ALA:C | 1:29:A:LYS:N | 1:29:A:LYS:CA | 1:29:A:LYS:C | 4        | 3.59          |
| (1,12) | 1:14:A:THR:C | 1:15:A:LEU:N | 1:15:A:LEU:CA | 1:15:A:LEU:C | 9        | 3.59          |
| (1,6)  | 1:7:A:THR:C  | 1:8:A:LEU:N  | 1:8:A:LEU:CA  | 1:8:A:LEU:C  | 16       | 3.59          |
| (1,59) | 1:66:A:THR:C | 1:67:A:LEU:N | 1:67:A:LEU:CA | 1:67:A:LEU:C | 4        | 3.58          |
| (1,12) | 1:14:A:THR:C | 1:15:A:LEU:N | 1:15:A:LEU:CA | 1:15:A:LEU:C | 7        | 3.58          |
| (1,12) | 1:14:A:THR:C | 1:15:A:LEU:N | 1:15:A:LEU:CA | 1:15:A:LEU:C | 10       | 3.58          |
| (1,60) | 1:67:A:LEU:C | 1:68:A:HIS:N | 1:68:A:HIS:CA | 1:68:A:HIS:C | 8        | 3.57          |
| (1,59) | 1:66:A:THR:C | 1:67:A:LEU:N | 1:67:A:LEU:CA | 1:67:A:LEU:C | 7        | 3.57          |
| (1,60) | 1:67:A:LEU:C | 1:68:A:HIS:N | 1:68:A:HIS:CA | 1:68:A:HIS:C | 6        | 3.56          |
| (1,46) | 1:53:A:GLY:C | 1:54:A:ARG:N | 1:54:A:ARG:CA | 1:54:A:ARG:C | 11       | 3.56          |
| (1,46) | 1:53:A:GLY:C | 1:54:A:ARG:N | 1:54:A:ARG:CA | 1:54:A:ARG:C | 18       | 3.56          |
| (1,18) | 1:21:A:ASP:C | 1:22:A:THR:N | 1:22:A:THR:CA | 1:22:A:THR:C | 20       | 3.56          |
| (1,12) | 1:14:A:THR:C | 1:15:A:LEU:N | 1:15:A:LEU:CA | 1:15:A:LEU:C | 12       | 3.56          |
| (1,12) | 1:14:A:THR:C | 1:15:A:LEU:N | 1:15:A:LEU:CA | 1:15:A:LEU:C | 19       | 3.56          |
| (1,59) | 1:66:A:THR:C | 1:67:A:LEU:N | 1:67:A:LEU:CA | 1:67:A:LEU:C | 9        | 3.55          |
| (1,37) | 1:43:A:LEU:C | 1:44:A:ILE:N | 1:44:A:ILE:CA | 1:44:A:ILE:C | 16       | 3.55          |
| (1,24) | 1:28:A:ALA:C | 1:29:A:LYS:N | 1:29:A:LYS:CA | 1:29:A:LYS:C | 8        | 3.55          |
| (1,24) | 1:28:A:ALA:C | 1:29:A:LYS:N | 1:29:A:LYS:CA | 1:29:A:LYS:C | 16       | 3.55          |
| (1,47) | 1:54:A:ARG:C | 1:55:A:THR:N | 1:55:A:THR:CA | 1:55:A:THR:C | 18       | 3.54          |
| (1,38) | 1:44:A:ILE:C | 1:45:A:PHE:N | 1:45:A:PHE:CA | 1:45:A:PHE:C | 7        | 3.54          |
| (1,12) | 1:14:A:THR:C | 1:15:A:LEU:N | 1:15:A:LEU:CA | 1:15:A:LEU:C | 2        | 3.54          |
| (1,12) | 1:14:A:THR:C | 1:15:A:LEU:N | 1:15:A:LEU:CA | 1:15:A:LEU:C | 11       | 3.54          |
| (1,12) | 1:14:A:THR:C | 1:15:A:LEU:N | 1:15:A:LEU:CA | 1:15:A:LEU:C | 16       | 3.54          |
| (1,59) | 1:66:A:THR:C | 1:67:A:LEU:N | 1:67:A:LEU:CA | 1:67:A:LEU:C | 14       | 3.53          |
| (1,24) | 1:28:A:ALA:C | 1:29:A:LYS:N | 1:29:A:LYS:CA | 1:29:A:LYS:C | 14       | 3.53          |
| (1,18) | 1:21:A:ASP:C | 1:22:A:THR:N | 1:22:A:THR:CA | 1:22:A:THR:C | 7        | 3.53          |
| (1,6)  | 1:7:A:THR:C  | 1:8:A:LEU:N  | 1:8:A:LEU:CA  | 1:8:A:LEU:C  | 15       | 3.53          |
| (1,24) | 1:28:A:ALA:C | 1:29:A:LYS:N | 1:29:A:LYS:CA | 1:29:A:LYS:C | 11       | 3.52          |
| (1,37) | 1:43:A:LEU:C | 1:44:A:ILE:N | 1:44:A:ILE:CA | 1:44:A:ILE:C | 15       | 3.51          |
| (1,24) | 1:28:A:ALA:C | 1:29:A:LYS:N | 1:29:A:LYS:CA | 1:29:A:LYS:C | 6        | 3.51          |
| (1,59) | 1:66:A:THR:C | 1:67:A:LEU:N | 1:67:A:LEU:CA | 1:67:A:LEU:C | 3        | 3.5           |
| (1,47) | 1:54:A:ARG:C | 1:55:A:THR:N | 1:55:A:THR:CA | 1:55:A:THR:C | 16       | 3.5           |
| (1,38) | 1:44:A:ILE:C | 1:45:A:PHE:N | 1:45:A:PHE:CA | 1:45:A:PHE:C | 9        | 3.49          |
| (1,24) | 1:28:A:ALA:C | 1:29:A:LYS:N | 1:29:A:LYS:CA | 1:29:A:LYS:C | 1        | 3.49          |
| (1,24) | 1:28:A:ALA:C | 1:29:A:LYS:N | 1:29:A:LYS:CA | 1:29:A:LYS:C | 9        | 3.48          |
| (1,24) | 1:28:A:ALA:C | 1:29:A:LYS:N | 1:29:A:LYS:CA | 1:29:A:LYS:C | 17       | 3.48          |
| (1,47) | 1:54:A:ARG:C | 1:55:A:THR:N | 1:55:A:THR:CA | 1:55:A:THR:C | 11       | 3.46          |

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| Key    | Atom-1       | Atom-2       | Atom-3        | Atom-4       | Model ID | Violation (°) |
|--------|--------------|--------------|---------------|--------------|----------|---------------|
| (1,12) | 1:14:A:THR:C | 1:15:A:LEU:N | 1:15:A:LEU:CA | 1:15:A:LEU:C | 18       | 3.46          |
| (1,47) | 1:54:A:ARG:C | 1:55:A:THR:N | 1:55:A:THR:CA | 1:55:A:THR:C | 4        | 3.45          |
| (1,47) | 1:54:A:ARG:C | 1:55:A:THR:N | 1:55:A:THR:CA | 1:55:A:THR:C | 7        | 3.45          |
| (1,6)  | 1:7:A:THR:C  | 1:8:A:LEU:N  | 1:8:A:LEU:CA  | 1:8:A:LEU:C  | 14       | 3.45          |
| (1,1)  | 1:2:A:GLN:C  | 1:3:A:ILE:N  | 1:3:A:ILE:CA  | 1:3:A:ILE:C  | 15       | 3.45          |
| (1,46) | 1:53:A:GLY:C | 1:54:A:ARG:N | 1:54:A:ARG:CA | 1:54:A:ARG:C | 10       | 3.44          |
| (1,24) | 1:28:A:ALA:C | 1:29:A:LYS:N | 1:29:A:LYS:CA | 1:29:A:LYS:C | 19       | 3.44          |
| (1,15) | 1:17:A:VAL:C | 1:18:A:GLU:N | 1:18:A:GLU:CA | 1:18:A:GLU:C | 2        | 3.44          |
| (1,46) | 1:53:A:GLY:C | 1:54:A:ARG:N | 1:54:A:ARG:CA | 1:54:A:ARG:C | 4        | 3.43          |
| (1,46) | 1:53:A:GLY:C | 1:54:A:ARG:N | 1:54:A:ARG:CA | 1:54:A:ARG:C | 12       | 3.42          |
| (1,18) | 1:21:A:ASP:C | 1:22:A:THR:N | 1:22:A:THR:CA | 1:22:A:THR:C | 17       | 3.42          |
| (1,46) | 1:53:A:GLY:C | 1:54:A:ARG:N | 1:54:A:ARG:CA | 1:54:A:ARG:C | 9        | 3.41          |
| (1,15) | 1:17:A:VAL:C | 1:18:A:GLU:N | 1:18:A:GLU:CA | 1:18:A:GLU:C | 12       | 3.4           |
| (1,60) | 1:67:A:LEU:C | 1:68:A:HIS:N | 1:68:A:HIS:CA | 1:68:A:HIS:C | 1        | 3.39          |
| (1,12) | 1:14:A:THR:C | 1:15:A:LEU:N | 1:15:A:LEU:CA | 1:15:A:LEU:C | 6        | 3.39          |
| (1,1)  | 1:2:A:GLN:C  | 1:3:A:ILE:N  | 1:3:A:ILE:CA  | 1:3:A:ILE:C  | 17       | 3.39          |
| (1,60) | 1:67:A:LEU:C | 1:68:A:HIS:N | 1:68:A:HIS:CA | 1:68:A:HIS:C | 15       | 3.38          |
| (1,60) | 1:67:A:LEU:C | 1:68:A:HIS:N | 1:68:A:HIS:CA | 1:68:A:HIS:C | 16       | 3.38          |
| (1,46) | 1:53:A:GLY:C | 1:54:A:ARG:N | 1:54:A:ARG:CA | 1:54:A:ARG:C | 6        | 3.38          |
| (1,12) | 1:14:A:THR:C | 1:15:A:LEU:N | 1:15:A:LEU:CA | 1:15:A:LEU:C | 5        | 3.38          |
| (1,24) | 1:28:A:ALA:C | 1:29:A:LYS:N | 1:29:A:LYS:CA | 1:29:A:LYS:C | 7        | 3.37          |
| (1,24) | 1:28:A:ALA:C | 1:29:A:LYS:N | 1:29:A:LYS:CA | 1:29:A:LYS:C | 2        | 3.36          |
| (1,24) | 1:28:A:ALA:C | 1:29:A:LYS:N | 1:29:A:LYS:CA | 1:29:A:LYS:C | 12       | 3.36          |
| (1,9)  | 1:11:A:LYS:C | 1:12:A:THR:N | 1:12:A:THR:CA | 1:12:A:THR:C | 4        | 3.36          |
| (1,6)  | 1:7:A:THR:C  | 1:8:A:LEU:N  | 1:8:A:LEU:CA  | 1:8:A:LEU:C  | 5        | 3.35          |
| (1,6)  | 1:7:A:THR:C  | 1:8:A:LEU:N  | 1:8:A:LEU:CA  | 1:8:A:LEU:C  | 1        | 3.34          |
| (1,5)  | 1:6:A:LYS:C  | 1:7:A:THR:N  | 1:7:A:THR:CA  | 1:7:A:THR:C  | 4        | 3.33          |
| (1,6)  | 1:7:A:THR:C  | 1:8:A:LEU:N  | 1:8:A:LEU:CA  | 1:8:A:LEU:C  | 6        | 3.32          |
| (1,15) | 1:17:A:VAL:C | 1:18:A:GLU:N | 1:18:A:GLU:CA | 1:18:A:GLU:C | 20       | 3.31          |
| (1,60) | 1:67:A:LEU:C | 1:68:A:HIS:N | 1:68:A:HIS:CA | 1:68:A:HIS:C | 10       | 3.3           |
| (1,47) | 1:54:A:ARG:C | 1:55:A:THR:N | 1:55:A:THR:CA | 1:55:A:THR:C | 9        | 3.3           |
| (1,24) | 1:28:A:ALA:C | 1:29:A:LYS:N | 1:29:A:LYS:CA | 1:29:A:LYS:C | 5        | 3.3           |
| (1,60) | 1:67:A:LEU:C | 1:68:A:HIS:N | 1:68:A:HIS:CA | 1:68:A:HIS:C | 14       | 3.29          |
| (1,1)  | 1:2:A:GLN:C  | 1:3:A:ILE:N  | 1:3:A:ILE:CA  | 1:3:A:ILE:C  | 2        | 3.28          |
| (1,60) | 1:67:A:LEU:C | 1:68:A:HIS:N | 1:68:A:HIS:CA | 1:68:A:HIS:C | 3        | 3.25          |
| (1,24) | 1:28:A:ALA:C | 1:29:A:LYS:N | 1:29:A:LYS:CA | 1:29:A:LYS:C | 20       | 3.25          |
| (1,24) | 1:28:A:ALA:C | 1:29:A:LYS:N | 1:29:A:LYS:CA | 1:29:A:LYS:C | 18       | 3.22          |
| (1,4)  | 1:5:A:VAL:C  | 1:6:A:LYS:N  | 1:6:A:LYS:CA  | 1:6:A:LYS:C  | 17       | 3.2           |
| (1,1)  | 1:2:A:GLN:C  | 1:3:A:ILE:N  | 1:3:A:ILE:CA  | 1:3:A:ILE:C  | 7        | 3.19          |
| (1,1)  | 1:2:A:GLN:C  | 1:3:A:ILE:N  | 1:3:A:ILE:CA  | 1:3:A:ILE:C  | 8        | 3.18          |
| (1,59) | 1:66:A:THR:C | 1:67:A:LEU:N | 1:67:A:LEU:CA | 1:67:A:LEU:C | 20       | 3.17          |
| (1,24) | 1:28:A:ALA:C | 1:29:A:LYS:N | 1:29:A:LYS:CA | 1:29:A:LYS:C | 15       | 3.14          |
| (1,24) | 1:28:A:ALA:C | 1:29:A:LYS:N | 1:29:A:LYS:CA | 1:29:A:LYS:C | 13       | 3.13          |
| (1,6)  | 1:7:A:THR:C  | 1:8:A:LEU:N  | 1:8:A:LEU:CA  | 1:8:A:LEU:C  | 18       | 3.11          |
| (1,6)  | 1:7:A:THR:C  | 1:8:A:LEU:N  | 1:8:A:LEU:CA  | 1:8:A:LEU:C  | 19       | 3.11          |
| (1,9)  | 1:11:A:LYS:C | 1:12:A:THR:N | 1:12:A:THR:CA | 1:12:A:THR:C | 3        | 3.09          |
| (1,8)  | 1:10:A:GLY:C | 1:11:A:LYS:N | 1:11:A:LYS:CA | 1:11:A:LYS:C | 20       | 3.08          |
| (1,9)  | 1:11:A:LYS:C | 1:12:A:THR:N | 1:12:A:THR:CA | 1:12:A:THR:C | 9        | 3.07          |
| (1,9)  | 1:11:A:LYS:C | 1:12:A:THR:N | 1:12:A:THR:CA | 1:12:A:THR:C | 13       | 3.06          |
| (1,1)  | 1:2:A:GLN:C  | 1:3:A:ILE:N  | 1:3:A:ILE:CA  | 1:3:A:ILE:C  | 10       | 3.06          |
| (1,45) | 1:52:A:ASP:C | 1:53:A:GLY:N | 1:53:A:GLY:CA | 1:53:A:GLY:C | 13       | 3.05          |

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| Key    | Atom-1       | Atom-2       | Atom-3        | Atom-4       | Model ID | Violation (°) |
|--------|--------------|--------------|---------------|--------------|----------|---------------|
| (1,9)  | 1:11:A:LYS:C | 1:12:A:THR:N | 1:12:A:THR:CA | 1:12:A:THR:C | 10       | 3.05          |
| (1,4)  | 1:5:A:VAL:C  | 1:6:A:LYS:N  | 1:6:A:LYS:CA  | 1:6:A:LYS:C  | 13       | 3.05          |
| (1,6)  | 1:7:A:THR:C  | 1:8:A:LEU:N  | 1:8:A:LEU:CA  | 1:8:A:LEU:C  | 8        | 3.04          |
| (1,9)  | 1:11:A:LYS:C | 1:12:A:THR:N | 1:12:A:THR:CA | 1:12:A:THR:C | 20       | 3.03          |
| (1,4)  | 1:5:A:VAL:C  | 1:6:A:LYS:N  | 1:6:A:LYS:CA  | 1:6:A:LYS:C  | 9        | 3.03          |
| (1,9)  | 1:11:A:LYS:C | 1:12:A:THR:N | 1:12:A:THR:CA | 1:12:A:THR:C | 2        | 3.01          |
| (1,46) | 1:53:A:GLY:C | 1:54:A:ARG:N | 1:54:A:ARG:CA | 1:54:A:ARG:C | 7        | 2.99          |
| (1,4)  | 1:5:A:VAL:C  | 1:6:A:LYS:N  | 1:6:A:LYS:CA  | 1:6:A:LYS:C  | 19       | 2.98          |
| (1,37) | 1:43:A:LEU:C | 1:44:A:ILE:N | 1:44:A:ILE:CA | 1:44:A:ILE:C | 13       | 2.94          |
| (1,4)  | 1:5:A:VAL:C  | 1:6:A:LYS:N  | 1:6:A:LYS:CA  | 1:6:A:LYS:C  | 1        | 2.91          |
| (1,4)  | 1:5:A:VAL:C  | 1:6:A:LYS:N  | 1:6:A:LYS:CA  | 1:6:A:LYS:C  | 12       | 2.9           |
| (1,31) | 1:37:A:PRO:C | 1:38:A:PRO:N | 1:38:A:PRO:CA | 1:38:A:PRO:C | 13       | 2.86          |
| (1,7)  | 1:8:A:LEU:C  | 1:9:A:THR:N  | 1:9:A:THR:CA  | 1:9:A:THR:C  | 16       | 2.84          |
| (1,4)  | 1:5:A:VAL:C  | 1:6:A:LYS:N  | 1:6:A:LYS:CA  | 1:6:A:LYS:C  | 11       | 2.84          |
| (1,9)  | 1:11:A:LYS:C | 1:12:A:THR:N | 1:12:A:THR:CA | 1:12:A:THR:C | 7        | 2.81          |
| (1,7)  | 1:8:A:LEU:C  | 1:9:A:THR:N  | 1:9:A:THR:CA  | 1:9:A:THR:C  | 14       | 2.81          |
| (1,7)  | 1:8:A:LEU:C  | 1:9:A:THR:N  | 1:9:A:THR:CA  | 1:9:A:THR:C  | 15       | 2.81          |
| (1,45) | 1:52:A:ASP:C | 1:53:A:GLY:N | 1:53:A:GLY:CA | 1:53:A:GLY:C | 14       | 2.79          |
| (1,8)  | 1:10:A:GLY:C | 1:11:A:LYS:N | 1:11:A:LYS:CA | 1:11:A:LYS:C | 13       | 2.79          |
| (1,4)  | 1:5:A:VAL:C  | 1:6:A:LYS:N  | 1:6:A:LYS:CA  | 1:6:A:LYS:C  | 15       | 2.79          |
| (1,8)  | 1:10:A:GLY:C | 1:11:A:LYS:N | 1:11:A:LYS:CA | 1:11:A:LYS:C | 9        | 2.77          |
| (1,4)  | 1:5:A:VAL:C  | 1:6:A:LYS:N  | 1:6:A:LYS:CA  | 1:6:A:LYS:C  | 8        | 2.75          |
| (1,45) | 1:52:A:ASP:C | 1:53:A:GLY:N | 1:53:A:GLY:CA | 1:53:A:GLY:C | 3        | 2.72          |
| (1,4)  | 1:5:A:VAL:C  | 1:6:A:LYS:N  | 1:6:A:LYS:CA  | 1:6:A:LYS:C  | 2        | 2.72          |
| (1,51) | 1:58:A:ASP:C | 1:59:A:TYR:N | 1:59:A:TYR:CA | 1:59:A:TYR:C | 3        | 2.71          |
| (1,6)  | 1:7:A:THR:C  | 1:8:A:LEU:N  | 1:8:A:LEU:CA  | 1:8:A:LEU:C  | 12       | 2.71          |
| (1,4)  | 1:5:A:VAL:C  | 1:6:A:LYS:N  | 1:6:A:LYS:CA  | 1:6:A:LYS:C  | 5        | 2.7           |
| (1,7)  | 1:8:A:LEU:C  | 1:9:A:THR:N  | 1:9:A:THR:CA  | 1:9:A:THR:C  | 8        | 2.69          |
| (1,7)  | 1:8:A:LEU:C  | 1:9:A:THR:N  | 1:9:A:THR:CA  | 1:9:A:THR:C  | 6        | 2.66          |
| (1,45) | 1:52:A:ASP:C | 1:53:A:GLY:N | 1:53:A:GLY:CA | 1:53:A:GLY:C | 10       | 2.65          |
| (1,6)  | 1:7:A:THR:C  | 1:8:A:LEU:N  | 1:8:A:LEU:CA  | 1:8:A:LEU:C  | 11       | 2.65          |
| (1,7)  | 1:8:A:LEU:C  | 1:9:A:THR:N  | 1:9:A:THR:CA  | 1:9:A:THR:C  | 5        | 2.64          |
| (1,37) | 1:43:A:LEU:C | 1:44:A:ILE:N | 1:44:A:ILE:CA | 1:44:A:ILE:C | 14       | 2.63          |
| (1,4)  | 1:5:A:VAL:C  | 1:6:A:LYS:N  | 1:6:A:LYS:CA  | 1:6:A:LYS:C  | 18       | 2.63          |
| (1,37) | 1:43:A:LEU:C | 1:44:A:ILE:N | 1:44:A:ILE:CA | 1:44:A:ILE:C | 3        | 2.59          |
| (1,4)  | 1:5:A:VAL:C  | 1:6:A:LYS:N  | 1:6:A:LYS:CA  | 1:6:A:LYS:C  | 16       | 2.56          |
| (1,7)  | 1:8:A:LEU:C  | 1:9:A:THR:N  | 1:9:A:THR:CA  | 1:9:A:THR:C  | 19       | 2.55          |
| (1,37) | 1:43:A:LEU:C | 1:44:A:ILE:N | 1:44:A:ILE:CA | 1:44:A:ILE:C | 10       | 2.54          |
| (1,42) | 1:49:A:GLN:C | 1:50:A:LEU:N | 1:50:A:LEU:CA | 1:50:A:LEU:C | 20       | 2.53          |
| (1,7)  | 1:8:A:LEU:C  | 1:9:A:THR:N  | 1:9:A:THR:CA  | 1:9:A:THR:C  | 1        | 2.53          |
| (1,51) | 1:58:A:ASP:C | 1:59:A:TYR:N | 1:59:A:TYR:CA | 1:59:A:TYR:C | 15       | 2.52          |
| (1,42) | 1:49:A:GLN:C | 1:50:A:LEU:N | 1:50:A:LEU:CA | 1:50:A:LEU:C | 10       | 2.52          |
| (1,7)  | 1:8:A:LEU:C  | 1:9:A:THR:N  | 1:9:A:THR:CA  | 1:9:A:THR:C  | 18       | 2.51          |
| (1,51) | 1:58:A:ASP:C | 1:59:A:TYR:N | 1:59:A:TYR:CA | 1:59:A:TYR:C | 10       | 2.5           |
| (1,51) | 1:58:A:ASP:C | 1:59:A:TYR:N | 1:59:A:TYR:CA | 1:59:A:TYR:C | 18       | 2.5           |
| (1,7)  | 1:8:A:LEU:C  | 1:9:A:THR:N  | 1:9:A:THR:CA  | 1:9:A:THR:C  | 9        | 2.47          |
| (1,4)  | 1:5:A:VAL:C  | 1:6:A:LYS:N  | 1:6:A:LYS:CA  | 1:6:A:LYS:C  | 10       | 2.47          |
| (1,4)  | 1:5:A:VAL:C  | 1:6:A:LYS:N  | 1:6:A:LYS:CA  | 1:6:A:LYS:C  | 7        | 2.46          |
| (1,4)  | 1:5:A:VAL:C  | 1:6:A:LYS:N  | 1:6:A:LYS:CA  | 1:6:A:LYS:C  | 14       | 2.46          |
| (1,51) | 1:58:A:ASP:C | 1:59:A:TYR:N | 1:59:A:TYR:CA | 1:59:A:TYR:C | 13       | 2.45          |
| (1,42) | 1:49:A:GLN:C | 1:50:A:LEU:N | 1:50:A:LEU:CA | 1:50:A:LEU:C | 9        | 2.44          |

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| Key    | Atom-1       | Atom-2       | Atom-3        | Atom-4       | Model ID | Violation (°) |
|--------|--------------|--------------|---------------|--------------|----------|---------------|
| (1,1)  | 1:2:A:GLN:C  | 1:3:A:ILE:N  | 1:3:A:ILE:CA  | 1:3:A:ILE:C  | 4        | 2.42          |
| (1,45) | 1:52:A:ASP:C | 1:53:A:GLY:N | 1:53:A:GLY:CA | 1:53:A:GLY:C | 6        | 2.41          |
| (1,51) | 1:58:A:ASP:C | 1:59:A:TYR:N | 1:59:A:TYR:CA | 1:59:A:TYR:C | 1        | 2.4           |
| (1,4)  | 1:5:A:VAL:C  | 1:6:A:LYS:N  | 1:6:A:LYS:CA  | 1:6:A:LYS:C  | 3        | 2.39          |
| (1,51) | 1:58:A:ASP:C | 1:59:A:TYR:N | 1:59:A:TYR:CA | 1:59:A:TYR:C | 2        | 2.36          |
| (1,4)  | 1:5:A:VAL:C  | 1:6:A:LYS:N  | 1:6:A:LYS:CA  | 1:6:A:LYS:C  | 6        | 2.34          |
| (1,42) | 1:49:A:GLN:C | 1:50:A:LEU:N | 1:50:A:LEU:CA | 1:50:A:LEU:C | 14       | 2.31          |
| (1,51) | 1:58:A:ASP:C | 1:59:A:TYR:N | 1:59:A:TYR:CA | 1:59:A:TYR:C | 8        | 2.3           |
| (1,51) | 1:58:A:ASP:C | 1:59:A:TYR:N | 1:59:A:TYR:CA | 1:59:A:TYR:C | 14       | 2.3           |
| (1,7)  | 1:8:A:LEU:C  | 1:9:A:THR:N  | 1:9:A:THR:CA  | 1:9:A:THR:C  | 12       | 2.3           |
| (1,4)  | 1:5:A:VAL:C  | 1:6:A:LYS:N  | 1:6:A:LYS:CA  | 1:6:A:LYS:C  | 4        | 2.27          |
| (1,11) | 1:13:A:ILE:C | 1:14:A:THR:N | 1:14:A:THR:CA | 1:14:A:THR:C | 7        | 2.26          |
| (1,51) | 1:58:A:ASP:C | 1:59:A:TYR:N | 1:59:A:TYR:CA | 1:59:A:TYR:C | 6        | 2.25          |
| (1,51) | 1:58:A:ASP:C | 1:59:A:TYR:N | 1:59:A:TYR:CA | 1:59:A:TYR:C | 11       | 2.25          |
| (1,42) | 1:49:A:GLN:C | 1:50:A:LEU:N | 1:50:A:LEU:CA | 1:50:A:LEU:C | 13       | 2.25          |
| (1,42) | 1:49:A:GLN:C | 1:50:A:LEU:N | 1:50:A:LEU:CA | 1:50:A:LEU:C | 2        | 2.24          |
| (1,42) | 1:49:A:GLN:C | 1:50:A:LEU:N | 1:50:A:LEU:CA | 1:50:A:LEU:C | 7        | 2.24          |
| (1,42) | 1:49:A:GLN:C | 1:50:A:LEU:N | 1:50:A:LEU:CA | 1:50:A:LEU:C | 17       | 2.23          |
| (1,11) | 1:13:A:ILE:C | 1:14:A:THR:N | 1:14:A:THR:CA | 1:14:A:THR:C | 10       | 2.23          |
| (1,11) | 1:13:A:ILE:C | 1:14:A:THR:N | 1:14:A:THR:CA | 1:14:A:THR:C | 2        | 2.22          |
| (1,7)  | 1:8:A:LEU:C  | 1:9:A:THR:N  | 1:9:A:THR:CA  | 1:9:A:THR:C  | 11       | 2.22          |
| (1,11) | 1:13:A:ILE:C | 1:14:A:THR:N | 1:14:A:THR:CA | 1:14:A:THR:C | 3        | 2.2           |
| (1,51) | 1:58:A:ASP:C | 1:59:A:TYR:N | 1:59:A:TYR:CA | 1:59:A:TYR:C | 19       | 2.19          |
| (1,20) | 1:24:A:GLU:C | 1:25:A:ASN:N | 1:25:A:ASN:CA | 1:25:A:ASN:C | 3        | 2.19          |
| (1,56) | 1:63:A:LYS:C | 1:64:A:GLU:N | 1:64:A:GLU:CA | 1:64:A:GLU:C | 4        | 2.18          |
| (1,42) | 1:49:A:GLN:C | 1:50:A:LEU:N | 1:50:A:LEU:CA | 1:50:A:LEU:C | 11       | 2.18          |
| (1,42) | 1:49:A:GLN:C | 1:50:A:LEU:N | 1:50:A:LEU:CA | 1:50:A:LEU:C | 19       | 2.18          |
| (1,26) | 1:30:A:ILE:C | 1:31:A:GLN:N | 1:31:A:GLN:CA | 1:31:A:GLN:C | 9        | 2.18          |
| (1,56) | 1:63:A:LYS:C | 1:64:A:GLU:N | 1:64:A:GLU:CA | 1:64:A:GLU:C | 20       | 2.17          |
| (1,26) | 1:30:A:ILE:C | 1:31:A:GLN:N | 1:31:A:GLN:CA | 1:31:A:GLN:C | 6        | 2.17          |
| (1,26) | 1:30:A:ILE:C | 1:31:A:GLN:N | 1:31:A:GLN:CA | 1:31:A:GLN:C | 20       | 2.17          |
| (1,22) | 1:26:A:VAL:C | 1:27:A:LYS:N | 1:27:A:LYS:CA | 1:27:A:LYS:C | 8        | 2.17          |
| (1,56) | 1:63:A:LYS:C | 1:64:A:GLU:N | 1:64:A:GLU:CA | 1:64:A:GLU:C | 3        | 2.16          |
| (1,16) | 1:19:A:PRO:C | 1:20:A:SER:N | 1:20:A:SER:CA | 1:20:A:SER:C | 4        | 2.16          |
| (1,7)  | 1:8:A:LEU:C  | 1:9:A:THR:N  | 1:9:A:THR:CA  | 1:9:A:THR:C  | 13       | 2.16          |
| (1,42) | 1:49:A:GLN:C | 1:50:A:LEU:N | 1:50:A:LEU:CA | 1:50:A:LEU:C | 18       | 2.15          |
| (1,56) | 1:63:A:LYS:C | 1:64:A:GLU:N | 1:64:A:GLU:CA | 1:64:A:GLU:C | 15       | 2.13          |
| (1,51) | 1:58:A:ASP:C | 1:59:A:TYR:N | 1:59:A:TYR:CA | 1:59:A:TYR:C | 5        | 2.13          |
| (1,42) | 1:49:A:GLN:C | 1:50:A:LEU:N | 1:50:A:LEU:CA | 1:50:A:LEU:C | 12       | 2.13          |
| (1,26) | 1:30:A:ILE:C | 1:31:A:GLN:N | 1:31:A:GLN:CA | 1:31:A:GLN:C | 12       | 2.12          |
| (1,26) | 1:30:A:ILE:C | 1:31:A:GLN:N | 1:31:A:GLN:CA | 1:31:A:GLN:C | 18       | 2.12          |
| (1,8)  | 1:10:A:GLY:C | 1:11:A:LYS:N | 1:11:A:LYS:CA | 1:11:A:LYS:C | 17       | 2.12          |
| (1,56) | 1:63:A:LYS:C | 1:64:A:GLU:N | 1:64:A:GLU:CA | 1:64:A:GLU:C | 2        | 2.11          |
| (1,42) | 1:49:A:GLN:C | 1:50:A:LEU:N | 1:50:A:LEU:CA | 1:50:A:LEU:C | 4        | 2.11          |
| (1,42) | 1:49:A:GLN:C | 1:50:A:LEU:N | 1:50:A:LEU:CA | 1:50:A:LEU:C | 16       | 2.11          |
| (1,26) | 1:30:A:ILE:C | 1:31:A:GLN:N | 1:31:A:GLN:CA | 1:31:A:GLN:C | 16       | 2.11          |
| (1,26) | 1:30:A:ILE:C | 1:31:A:GLN:N | 1:31:A:GLN:CA | 1:31:A:GLN:C | 1        | 2.1           |
| (1,11) | 1:13:A:ILE:C | 1:14:A:THR:N | 1:14:A:THR:CA | 1:14:A:THR:C | 13       | 2.1           |
| (1,11) | 1:13:A:ILE:C | 1:14:A:THR:N | 1:14:A:THR:CA | 1:14:A:THR:C | 20       | 2.1           |
| (1,56) | 1:63:A:LYS:C | 1:64:A:GLU:N | 1:64:A:GLU:CA | 1:64:A:GLU:C | 5        | 2.09          |
| (1,56) | 1:63:A:LYS:C | 1:64:A:GLU:N | 1:64:A:GLU:CA | 1:64:A:GLU:C | 10       | 2.09          |

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| Key    | Atom-1       | Atom-2       | Atom-3        | Atom-4       | Model ID | Violation (°) |
|--------|--------------|--------------|---------------|--------------|----------|---------------|
| (1,26) | 1:30:A:ILE:C | 1:31:A:GLN:N | 1:31:A:GLN:CA | 1:31:A:GLN:C | 7        | 2.09          |
| (1,26) | 1:30:A:ILE:C | 1:31:A:GLN:N | 1:31:A:GLN:CA | 1:31:A:GLN:C | 8        | 2.09          |
| (1,42) | 1:49:A:GLN:C | 1:50:A:LEU:N | 1:50:A:LEU:CA | 1:50:A:LEU:C | 5        | 2.08          |
| (1,42) | 1:49:A:GLN:C | 1:50:A:LEU:N | 1:50:A:LEU:CA | 1:50:A:LEU:C | 6        | 2.08          |
| (1,26) | 1:30:A:ILE:C | 1:31:A:GLN:N | 1:31:A:GLN:CA | 1:31:A:GLN:C | 15       | 2.08          |
| (1,26) | 1:30:A:ILE:C | 1:31:A:GLN:N | 1:31:A:GLN:CA | 1:31:A:GLN:C | 17       | 2.08          |
| (1,26) | 1:30:A:ILE:C | 1:31:A:GLN:N | 1:31:A:GLN:CA | 1:31:A:GLN:C | 11       | 2.07          |
| (1,26) | 1:30:A:ILE:C | 1:31:A:GLN:N | 1:31:A:GLN:CA | 1:31:A:GLN:C | 19       | 2.06          |
| (1,4)  | 1:5:A:VAL:C  | 1:6:A:LYS:N  | 1:6:A:LYS:CA  | 1:6:A:LYS:C  | 20       | 2.06          |
| (1,56) | 1:63:A:LYS:C | 1:64:A:GLU:N | 1:64:A:GLU:CA | 1:64:A:GLU:C | 18       | 2.05          |
| (1,51) | 1:58:A:ASP:C | 1:59:A:TYR:N | 1:59:A:TYR:CA | 1:59:A:TYR:C | 12       | 2.05          |
| (1,56) | 1:63:A:LYS:C | 1:64:A:GLU:N | 1:64:A:GLU:CA | 1:64:A:GLU:C | 8        | 2.04          |
| (1,56) | 1:63:A:LYS:C | 1:64:A:GLU:N | 1:64:A:GLU:CA | 1:64:A:GLU:C | 19       | 2.04          |
| (1,42) | 1:49:A:GLN:C | 1:50:A:LEU:N | 1:50:A:LEU:CA | 1:50:A:LEU:C | 8        | 2.04          |
| (1,16) | 1:19:A:PRO:C | 1:20:A:SER:N | 1:20:A:SER:CA | 1:20:A:SER:C | 16       | 2.04          |
| (1,51) | 1:58:A:ASP:C | 1:59:A:TYR:N | 1:59:A:TYR:CA | 1:59:A:TYR:C | 9        | 2.03          |
| (1,31) | 1:37:A:PRO:C | 1:38:A:PRO:N | 1:38:A:PRO:CA | 1:38:A:PRO:C | 6        | 2.03          |
| (1,56) | 1:63:A:LYS:C | 1:64:A:GLU:N | 1:64:A:GLU:CA | 1:64:A:GLU:C | 16       | 2.02          |
| (1,51) | 1:58:A:ASP:C | 1:59:A:TYR:N | 1:59:A:TYR:CA | 1:59:A:TYR:C | 17       | 2.02          |
| (1,42) | 1:49:A:GLN:C | 1:50:A:LEU:N | 1:50:A:LEU:CA | 1:50:A:LEU:C | 15       | 2.02          |
| (1,22) | 1:26:A:VAL:C | 1:27:A:LYS:N | 1:27:A:LYS:CA | 1:27:A:LYS:C | 4        | 2.02          |
| (1,22) | 1:26:A:VAL:C | 1:27:A:LYS:N | 1:27:A:LYS:CA | 1:27:A:LYS:C | 5        | 2.02          |
| (1,56) | 1:63:A:LYS:C | 1:64:A:GLU:N | 1:64:A:GLU:CA | 1:64:A:GLU:C | 9        | 2.01          |
| (1,56) | 1:63:A:LYS:C | 1:64:A:GLU:N | 1:64:A:GLU:CA | 1:64:A:GLU:C | 7        | 1.99          |
| (1,10) | 1:12:A:THR:C | 1:13:A:ILE:N | 1:13:A:ILE:CA | 1:13:A:ILE:C | 2        | 1.99          |
| (1,56) | 1:63:A:LYS:C | 1:64:A:GLU:N | 1:64:A:GLU:CA | 1:64:A:GLU:C | 6        | 1.98          |
| (1,56) | 1:63:A:LYS:C | 1:64:A:GLU:N | 1:64:A:GLU:CA | 1:64:A:GLU:C | 11       | 1.98          |
| (1,26) | 1:30:A:ILE:C | 1:31:A:GLN:N | 1:31:A:GLN:CA | 1:31:A:GLN:C | 2        | 1.98          |
| (1,16) | 1:19:A:PRO:C | 1:20:A:SER:N | 1:20:A:SER:CA | 1:20:A:SER:C | 15       | 1.98          |
| (1,56) | 1:63:A:LYS:C | 1:64:A:GLU:N | 1:64:A:GLU:CA | 1:64:A:GLU:C | 12       | 1.97          |
| (1,51) | 1:58:A:ASP:C | 1:59:A:TYR:N | 1:59:A:TYR:CA | 1:59:A:TYR:C | 16       | 1.97          |
| (1,51) | 1:58:A:ASP:C | 1:59:A:TYR:N | 1:59:A:TYR:CA | 1:59:A:TYR:C | 20       | 1.97          |
| (1,42) | 1:49:A:GLN:C | 1:50:A:LEU:N | 1:50:A:LEU:CA | 1:50:A:LEU:C | 1        | 1.96          |
| (1,42) | 1:49:A:GLN:C | 1:50:A:LEU:N | 1:50:A:LEU:CA | 1:50:A:LEU:C | 3        | 1.96          |
| (1,26) | 1:30:A:ILE:C | 1:31:A:GLN:N | 1:31:A:GLN:CA | 1:31:A:GLN:C | 5        | 1.95          |
| (1,26) | 1:30:A:ILE:C | 1:31:A:GLN:N | 1:31:A:GLN:CA | 1:31:A:GLN:C | 14       | 1.95          |
| (1,56) | 1:63:A:LYS:C | 1:64:A:GLU:N | 1:64:A:GLU:CA | 1:64:A:GLU:C | 13       | 1.94          |
| (1,22) | 1:26:A:VAL:C | 1:27:A:LYS:N | 1:27:A:LYS:CA | 1:27:A:LYS:C | 1        | 1.94          |
| (1,16) | 1:19:A:PRO:C | 1:20:A:SER:N | 1:20:A:SER:CA | 1:20:A:SER:C | 1        | 1.94          |
| (1,56) | 1:63:A:LYS:C | 1:64:A:GLU:N | 1:64:A:GLU:CA | 1:64:A:GLU:C | 1        | 1.93          |
| (1,56) | 1:63:A:LYS:C | 1:64:A:GLU:N | 1:64:A:GLU:CA | 1:64:A:GLU:C | 14       | 1.93          |
| (1,16) | 1:19:A:PRO:C | 1:20:A:SER:N | 1:20:A:SER:CA | 1:20:A:SER:C | 19       | 1.93          |
| (1,20) | 1:24:A:GLU:C | 1:25:A:ASN:N | 1:25:A:ASN:CA | 1:25:A:ASN:C | 5        | 1.91          |
| (1,16) | 1:19:A:PRO:C | 1:20:A:SER:N | 1:20:A:SER:CA | 1:20:A:SER:C | 7        | 1.91          |
| (1,16) | 1:19:A:PRO:C | 1:20:A:SER:N | 1:20:A:SER:CA | 1:20:A:SER:C | 12       | 1.91          |
| (1,56) | 1:63:A:LYS:C | 1:64:A:GLU:N | 1:64:A:GLU:CA | 1:64:A:GLU:C | 17       | 1.9           |
| (1,45) | 1:52:A:ASP:C | 1:53:A:GLY:N | 1:53:A:GLY:CA | 1:53:A:GLY:C | 9        | 1.9           |
| (1,26) | 1:30:A:ILE:C | 1:31:A:GLN:N | 1:31:A:GLN:CA | 1:31:A:GLN:C | 10       | 1.9           |
| (1,16) | 1:19:A:PRO:C | 1:20:A:SER:N | 1:20:A:SER:CA | 1:20:A:SER:C | 3        | 1.9           |
| (1,16) | 1:19:A:PRO:C | 1:20:A:SER:N | 1:20:A:SER:CA | 1:20:A:SER:C | 11       | 1.9           |
| (1,26) | 1:30:A:ILE:C | 1:31:A:GLN:N | 1:31:A:GLN:CA | 1:31:A:GLN:C | 4        | 1.89          |

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| Key    | Atom-1       | Atom-2       | Atom-3        | Atom-4       | Model ID | Violation (°) |
|--------|--------------|--------------|---------------|--------------|----------|---------------|
| (1,22) | 1:26:A:VAL:C | 1:27:A:LYS:N | 1:27:A:LYS:CA | 1:27:A:LYS:C | 19       | 1.89          |
| (1,16) | 1:19:A:PRO:C | 1:20:A:SER:N | 1:20:A:SER:CA | 1:20:A:SER:C | 2        | 1.89          |
| (1,16) | 1:19:A:PRO:C | 1:20:A:SER:N | 1:20:A:SER:CA | 1:20:A:SER:C | 10       | 1.88          |
| (1,26) | 1:30:A:ILE:C | 1:31:A:GLN:N | 1:31:A:GLN:CA | 1:31:A:GLN:C | 13       | 1.87          |
| (1,22) | 1:26:A:VAL:C | 1:27:A:LYS:N | 1:27:A:LYS:CA | 1:27:A:LYS:C | 14       | 1.87          |
| (1,22) | 1:26:A:VAL:C | 1:27:A:LYS:N | 1:27:A:LYS:CA | 1:27:A:LYS:C | 17       | 1.87          |
| (1,22) | 1:26:A:VAL:C | 1:27:A:LYS:N | 1:27:A:LYS:CA | 1:27:A:LYS:C | 16       | 1.86          |
| (1,11) | 1:13:A:ILE:C | 1:14:A:THR:N | 1:14:A:THR:CA | 1:14:A:THR:C | 9        | 1.86          |
| (1,45) | 1:52:A:ASP:C | 1:53:A:GLY:N | 1:53:A:GLY:CA | 1:53:A:GLY:C | 1        | 1.84          |
| (1,26) | 1:30:A:ILE:C | 1:31:A:GLN:N | 1:31:A:GLN:CA | 1:31:A:GLN:C | 3        | 1.84          |
| (1,22) | 1:26:A:VAL:C | 1:27:A:LYS:N | 1:27:A:LYS:CA | 1:27:A:LYS:C | 6        | 1.84          |
| (1,22) | 1:26:A:VAL:C | 1:27:A:LYS:N | 1:27:A:LYS:CA | 1:27:A:LYS:C | 10       | 1.84          |
| (1,11) | 1:13:A:ILE:C | 1:14:A:THR:N | 1:14:A:THR:CA | 1:14:A:THR:C | 17       | 1.84          |
| (1,16) | 1:19:A:PRO:C | 1:20:A:SER:N | 1:20:A:SER:CA | 1:20:A:SER:C | 18       | 1.83          |
| (1,16) | 1:19:A:PRO:C | 1:20:A:SER:N | 1:20:A:SER:CA | 1:20:A:SER:C | 20       | 1.83          |
| (1,22) | 1:26:A:VAL:C | 1:27:A:LYS:N | 1:27:A:LYS:CA | 1:27:A:LYS:C | 3        | 1.82          |
| (1,51) | 1:58:A:ASP:C | 1:59:A:TYR:N | 1:59:A:TYR:CA | 1:59:A:TYR:C | 7        | 1.8           |
| (1,20) | 1:24:A:GLU:C | 1:25:A:ASN:N | 1:25:A:ASN:CA | 1:25:A:ASN:C | 15       | 1.79          |
| (1,16) | 1:19:A:PRO:C | 1:20:A:SER:N | 1:20:A:SER:CA | 1:20:A:SER:C | 8        | 1.78          |
| (1,16) | 1:19:A:PRO:C | 1:20:A:SER:N | 1:20:A:SER:CA | 1:20:A:SER:C | 14       | 1.78          |
| (1,51) | 1:58:A:ASP:C | 1:59:A:TYR:N | 1:59:A:TYR:CA | 1:59:A:TYR:C | 4        | 1.77          |
| (1,45) | 1:52:A:ASP:C | 1:53:A:GLY:N | 1:53:A:GLY:CA | 1:53:A:GLY:C | 20       | 1.77          |
| (1,22) | 1:26:A:VAL:C | 1:27:A:LYS:N | 1:27:A:LYS:CA | 1:27:A:LYS:C | 18       | 1.77          |
| (1,16) | 1:19:A:PRO:C | 1:20:A:SER:N | 1:20:A:SER:CA | 1:20:A:SER:C | 5        | 1.77          |
| (1,10) | 1:12:A:THR:C | 1:13:A:ILE:N | 1:13:A:ILE:CA | 1:13:A:ILE:C | 7        | 1.76          |
| (1,10) | 1:12:A:THR:C | 1:13:A:ILE:N | 1:13:A:ILE:CA | 1:13:A:ILE:C | 10       | 1.75          |
| (1,16) | 1:19:A:PRO:C | 1:20:A:SER:N | 1:20:A:SER:CA | 1:20:A:SER:C | 6        | 1.74          |
| (1,20) | 1:24:A:GLU:C | 1:25:A:ASN:N | 1:25:A:ASN:CA | 1:25:A:ASN:C | 1        | 1.73          |
| (1,20) | 1:24:A:GLU:C | 1:25:A:ASN:N | 1:25:A:ASN:CA | 1:25:A:ASN:C | 19       | 1.71          |
| (1,22) | 1:26:A:VAL:C | 1:27:A:LYS:N | 1:27:A:LYS:CA | 1:27:A:LYS:C | 12       | 1.7           |
| (1,50) | 1:57:A:SER:C | 1:58:A:ASP:N | 1:58:A:ASP:CA | 1:58:A:ASP:C | 9        | 1.69          |
| (1,20) | 1:24:A:GLU:C | 1:25:A:ASN:N | 1:25:A:ASN:CA | 1:25:A:ASN:C | 12       | 1.69          |
| (1,12) | 1:14:A:THR:C | 1:15:A:LEU:N | 1:15:A:LEU:CA | 1:15:A:LEU:C | 15       | 1.69          |
| (1,20) | 1:24:A:GLU:C | 1:25:A:ASN:N | 1:25:A:ASN:CA | 1:25:A:ASN:C | 17       | 1.68          |
| (1,6)  | 1:7:A:THR:C  | 1:8:A:LEU:N  | 1:8:A:LEU:CA  | 1:8:A:LEU:C  | 9        | 1.68          |
| (1,22) | 1:26:A:VAL:C | 1:27:A:LYS:N | 1:27:A:LYS:CA | 1:27:A:LYS:C | 7        | 1.67          |
| (1,22) | 1:26:A:VAL:C | 1:27:A:LYS:N | 1:27:A:LYS:CA | 1:27:A:LYS:C | 15       | 1.67          |
| (1,22) | 1:26:A:VAL:C | 1:27:A:LYS:N | 1:27:A:LYS:CA | 1:27:A:LYS:C | 11       | 1.66          |
| (1,20) | 1:24:A:GLU:C | 1:25:A:ASN:N | 1:25:A:ASN:CA | 1:25:A:ASN:C | 8        | 1.66          |
| (1,20) | 1:24:A:GLU:C | 1:25:A:ASN:N | 1:25:A:ASN:CA | 1:25:A:ASN:C | 11       | 1.66          |
| (1,17) | 1:20:A:SER:C | 1:21:A:ASP:N | 1:21:A:ASP:CA | 1:21:A:ASP:C | 3        | 1.66          |
| (1,9)  | 1:11:A:LYS:C | 1:12:A:THR:N | 1:12:A:THR:CA | 1:12:A:THR:C | 14       | 1.65          |
| (1,45) | 1:52:A:ASP:C | 1:53:A:GLY:N | 1:53:A:GLY:CA | 1:53:A:GLY:C | 12       | 1.64          |
| (1,17) | 1:20:A:SER:C | 1:21:A:ASP:N | 1:21:A:ASP:CA | 1:21:A:ASP:C | 10       | 1.64          |
| (1,16) | 1:19:A:PRO:C | 1:20:A:SER:N | 1:20:A:SER:CA | 1:20:A:SER:C | 17       | 1.64          |
| (1,11) | 1:13:A:ILE:C | 1:14:A:THR:N | 1:14:A:THR:CA | 1:14:A:THR:C | 11       | 1.64          |
| (1,20) | 1:24:A:GLU:C | 1:25:A:ASN:N | 1:25:A:ASN:CA | 1:25:A:ASN:C | 13       | 1.63          |
| (1,11) | 1:13:A:ILE:C | 1:14:A:THR:N | 1:14:A:THR:CA | 1:14:A:THR:C | 1        | 1.63          |
| (1,11) | 1:13:A:ILE:C | 1:14:A:THR:N | 1:14:A:THR:CA | 1:14:A:THR:C | 19       | 1.63          |
| (1,50) | 1:57:A:SER:C | 1:58:A:ASP:N | 1:58:A:ASP:CA | 1:58:A:ASP:C | 11       | 1.62          |
| (1,22) | 1:26:A:VAL:C | 1:27:A:LYS:N | 1:27:A:LYS:CA | 1:27:A:LYS:C | 20       | 1.62          |

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| Key    | Atom-1       | Atom-2       | Atom-3        | Atom-4       | Model ID | Violation (°) |
|--------|--------------|--------------|---------------|--------------|----------|---------------|
| (1,17) | 1:20:A:SER:C | 1:21:A:ASP:N | 1:21:A:ASP:CA | 1:21:A:ASP:C | 18       | 1.62          |
| (1,16) | 1:19:A:PRO:C | 1:20:A:SER:N | 1:20:A:SER:CA | 1:20:A:SER:C | 9        | 1.62          |
| (1,9)  | 1:11:A:LYS:C | 1:12:A:THR:N | 1:12:A:THR:CA | 1:12:A:THR:C | 16       | 1.62          |
| (1,31) | 1:37:A:PRO:C | 1:38:A:PRO:N | 1:38:A:PRO:CA | 1:38:A:PRO:C | 17       | 1.61          |
| (1,20) | 1:24:A:GLU:C | 1:25:A:ASN:N | 1:25:A:ASN:CA | 1:25:A:ASN:C | 18       | 1.61          |
| (1,20) | 1:24:A:GLU:C | 1:25:A:ASN:N | 1:25:A:ASN:CA | 1:25:A:ASN:C | 14       | 1.6           |
| (1,16) | 1:19:A:PRO:C | 1:20:A:SER:N | 1:20:A:SER:CA | 1:20:A:SER:C | 13       | 1.6           |
| (1,22) | 1:26:A:VAL:C | 1:27:A:LYS:N | 1:27:A:LYS:CA | 1:27:A:LYS:C | 2        | 1.59          |
| (1,22) | 1:26:A:VAL:C | 1:27:A:LYS:N | 1:27:A:LYS:CA | 1:27:A:LYS:C | 9        | 1.59          |
| (1,12) | 1:14:A:THR:C | 1:15:A:LEU:N | 1:15:A:LEU:CA | 1:15:A:LEU:C | 8        | 1.58          |
| (1,9)  | 1:11:A:LYS:C | 1:12:A:THR:N | 1:12:A:THR:CA | 1:12:A:THR:C | 12       | 1.58          |
| (1,50) | 1:57:A:SER:C | 1:58:A:ASP:N | 1:58:A:ASP:CA | 1:58:A:ASP:C | 17       | 1.57          |
| (1,22) | 1:26:A:VAL:C | 1:27:A:LYS:N | 1:27:A:LYS:CA | 1:27:A:LYS:C | 13       | 1.57          |
| (1,17) | 1:20:A:SER:C | 1:21:A:ASP:N | 1:21:A:ASP:CA | 1:21:A:ASP:C | 2        | 1.56          |
| (1,17) | 1:20:A:SER:C | 1:21:A:ASP:N | 1:21:A:ASP:CA | 1:21:A:ASP:C | 7        | 1.56          |
| (1,50) | 1:57:A:SER:C | 1:58:A:ASP:N | 1:58:A:ASP:CA | 1:58:A:ASP:C | 19       | 1.55          |
| (1,45) | 1:52:A:ASP:C | 1:53:A:GLY:N | 1:53:A:GLY:CA | 1:53:A:GLY:C | 2        | 1.55          |
| (1,25) | 1:29:A:LYS:C | 1:30:A:ILE:N | 1:30:A:ILE:CA | 1:30:A:ILE:C | 4        | 1.55          |
| (1,20) | 1:24:A:GLU:C | 1:25:A:ASN:N | 1:25:A:ASN:CA | 1:25:A:ASN:C | 4        | 1.55          |
| (1,50) | 1:57:A:SER:C | 1:58:A:ASP:N | 1:58:A:ASP:CA | 1:58:A:ASP:C | 20       | 1.54          |
| (1,45) | 1:52:A:ASP:C | 1:53:A:GLY:N | 1:53:A:GLY:CA | 1:53:A:GLY:C | 15       | 1.54          |
| (1,31) | 1:37:A:PRO:C | 1:38:A:PRO:N | 1:38:A:PRO:CA | 1:38:A:PRO:C | 3        | 1.54          |
| (1,17) | 1:20:A:SER:C | 1:21:A:ASP:N | 1:21:A:ASP:CA | 1:21:A:ASP:C | 9        | 1.54          |
| (1,9)  | 1:11:A:LYS:C | 1:12:A:THR:N | 1:12:A:THR:CA | 1:12:A:THR:C | 11       | 1.54          |
| (1,50) | 1:57:A:SER:C | 1:58:A:ASP:N | 1:58:A:ASP:CA | 1:58:A:ASP:C | 1        | 1.53          |
| (1,50) | 1:57:A:SER:C | 1:58:A:ASP:N | 1:58:A:ASP:CA | 1:58:A:ASP:C | 4        | 1.53          |
| (1,50) | 1:57:A:SER:C | 1:58:A:ASP:N | 1:58:A:ASP:CA | 1:58:A:ASP:C | 8        | 1.53          |
| (1,45) | 1:52:A:ASP:C | 1:53:A:GLY:N | 1:53:A:GLY:CA | 1:53:A:GLY:C | 17       | 1.53          |
| (1,20) | 1:24:A:GLU:C | 1:25:A:ASN:N | 1:25:A:ASN:CA | 1:25:A:ASN:C | 6        | 1.52          |
| (1,17) | 1:20:A:SER:C | 1:21:A:ASP:N | 1:21:A:ASP:CA | 1:21:A:ASP:C | 4        | 1.52          |
| (1,17) | 1:20:A:SER:C | 1:21:A:ASP:N | 1:21:A:ASP:CA | 1:21:A:ASP:C | 6        | 1.52          |
| (1,17) | 1:20:A:SER:C | 1:21:A:ASP:N | 1:21:A:ASP:CA | 1:21:A:ASP:C | 8        | 1.52          |
| (1,17) | 1:20:A:SER:C | 1:21:A:ASP:N | 1:21:A:ASP:CA | 1:21:A:ASP:C | 12       | 1.52          |
| (1,50) | 1:57:A:SER:C | 1:58:A:ASP:N | 1:58:A:ASP:CA | 1:58:A:ASP:C | 7        | 1.51          |
| (1,11) | 1:13:A:ILE:C | 1:14:A:THR:N | 1:14:A:THR:CA | 1:14:A:THR:C | 5        | 1.51          |
| (1,25) | 1:29:A:LYS:C | 1:30:A:ILE:N | 1:30:A:ILE:CA | 1:30:A:ILE:C | 3        | 1.5           |
| (1,20) | 1:24:A:GLU:C | 1:25:A:ASN:N | 1:25:A:ASN:CA | 1:25:A:ASN:C | 9        | 1.5           |
| (1,20) | 1:24:A:GLU:C | 1:25:A:ASN:N | 1:25:A:ASN:CA | 1:25:A:ASN:C | 16       | 1.5           |
| (1,17) | 1:20:A:SER:C | 1:21:A:ASP:N | 1:21:A:ASP:CA | 1:21:A:ASP:C | 1        | 1.5           |
| (1,50) | 1:57:A:SER:C | 1:58:A:ASP:N | 1:58:A:ASP:CA | 1:58:A:ASP:C | 16       | 1.48          |
| (1,23) | 1:27:A:LYS:C | 1:28:A:ALA:N | 1:28:A:ALA:CA | 1:28:A:ALA:C | 9        | 1.48          |
| (1,50) | 1:57:A:SER:C | 1:58:A:ASP:N | 1:58:A:ASP:CA | 1:58:A:ASP:C | 15       | 1.47          |
| (1,40) | 1:47:A:GLY:C | 1:48:A:LYS:N | 1:48:A:LYS:CA | 1:48:A:LYS:C | 13       | 1.47          |
| (1,10) | 1:12:A:THR:C | 1:13:A:ILE:N | 1:13:A:ILE:CA | 1:13:A:ILE:C | 3        | 1.47          |
| (1,50) | 1:57:A:SER:C | 1:58:A:ASP:N | 1:58:A:ASP:CA | 1:58:A:ASP:C | 13       | 1.46          |
| (1,31) | 1:37:A:PRO:C | 1:38:A:PRO:N | 1:38:A:PRO:CA | 1:38:A:PRO:C | 7        | 1.46          |
| (1,11) | 1:13:A:ILE:C | 1:14:A:THR:N | 1:14:A:THR:CA | 1:14:A:THR:C | 12       | 1.46          |
| (1,10) | 1:12:A:THR:C | 1:13:A:ILE:N | 1:13:A:ILE:CA | 1:13:A:ILE:C | 4        | 1.46          |
| (1,9)  | 1:11:A:LYS:C | 1:12:A:THR:N | 1:12:A:THR:CA | 1:12:A:THR:C | 6        | 1.46          |
| (1,25) | 1:29:A:LYS:C | 1:30:A:ILE:N | 1:30:A:ILE:CA | 1:30:A:ILE:C | 17       | 1.45          |
| (1,17) | 1:20:A:SER:C | 1:21:A:ASP:N | 1:21:A:ASP:CA | 1:21:A:ASP:C | 11       | 1.44          |

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| Key    | Atom-1       | Atom-2       | Atom-3        | Atom-4       | Model ID | Violation (°) |
|--------|--------------|--------------|---------------|--------------|----------|---------------|
| (1,17) | 1:20:A:SER:C | 1:21:A:ASP:N | 1:21:A:ASP:CA | 1:21:A:ASP:C | 13       | 1.44          |
| (1,11) | 1:13:A:ILE:C | 1:14:A:THR:N | 1:14:A:THR:CA | 1:14:A:THR:C | 18       | 1.43          |
| (1,25) | 1:29:A:LYS:C | 1:30:A:ILE:N | 1:30:A:ILE:CA | 1:30:A:ILE:C | 11       | 1.42          |
| (1,17) | 1:20:A:SER:C | 1:21:A:ASP:N | 1:21:A:ASP:CA | 1:21:A:ASP:C | 5        | 1.42          |
| (1,10) | 1:12:A:THR:C | 1:13:A:ILE:N | 1:13:A:ILE:CA | 1:13:A:ILE:C | 20       | 1.4           |
| (1,31) | 1:37:A:PRO:C | 1:38:A:PRO:N | 1:38:A:PRO:CA | 1:38:A:PRO:C | 9        | 1.39          |
| (1,25) | 1:29:A:LYS:C | 1:30:A:ILE:N | 1:30:A:ILE:CA | 1:30:A:ILE:C | 15       | 1.39          |
| (1,17) | 1:20:A:SER:C | 1:21:A:ASP:N | 1:21:A:ASP:CA | 1:21:A:ASP:C | 19       | 1.39          |
| (1,11) | 1:13:A:ILE:C | 1:14:A:THR:N | 1:14:A:THR:CA | 1:14:A:THR:C | 14       | 1.39          |
| (1,50) | 1:57:A:SER:C | 1:58:A:ASP:N | 1:58:A:ASP:CA | 1:58:A:ASP:C | 3        | 1.38          |
| (1,50) | 1:57:A:SER:C | 1:58:A:ASP:N | 1:58:A:ASP:CA | 1:58:A:ASP:C | 14       | 1.38          |
| (1,25) | 1:29:A:LYS:C | 1:30:A:ILE:N | 1:30:A:ILE:CA | 1:30:A:ILE:C | 6        | 1.38          |
| (1,25) | 1:29:A:LYS:C | 1:30:A:ILE:N | 1:30:A:ILE:CA | 1:30:A:ILE:C | 19       | 1.38          |
| (1,50) | 1:57:A:SER:C | 1:58:A:ASP:N | 1:58:A:ASP:CA | 1:58:A:ASP:C | 18       | 1.37          |
| (1,25) | 1:29:A:LYS:C | 1:30:A:ILE:N | 1:30:A:ILE:CA | 1:30:A:ILE:C | 16       | 1.37          |
| (1,17) | 1:20:A:SER:C | 1:21:A:ASP:N | 1:21:A:ASP:CA | 1:21:A:ASP:C | 14       | 1.37          |
| (1,50) | 1:57:A:SER:C | 1:58:A:ASP:N | 1:58:A:ASP:CA | 1:58:A:ASP:C | 5        | 1.36          |
| (1,25) | 1:29:A:LYS:C | 1:30:A:ILE:N | 1:30:A:ILE:CA | 1:30:A:ILE:C | 8        | 1.35          |
| (1,50) | 1:57:A:SER:C | 1:58:A:ASP:N | 1:58:A:ASP:CA | 1:58:A:ASP:C | 12       | 1.34          |
| (1,11) | 1:13:A:ILE:C | 1:14:A:THR:N | 1:14:A:THR:CA | 1:14:A:THR:C | 6        | 1.33          |
| (1,50) | 1:57:A:SER:C | 1:58:A:ASP:N | 1:58:A:ASP:CA | 1:58:A:ASP:C | 2        | 1.32          |
| (1,25) | 1:29:A:LYS:C | 1:30:A:ILE:N | 1:30:A:ILE:CA | 1:30:A:ILE:C | 2        | 1.32          |
| (1,14) | 1:16:A:GLU:C | 1:17:A:VAL:N | 1:17:A:VAL:CA | 1:17:A:VAL:C | 2        | 1.32          |
| (1,40) | 1:47:A:GLY:C | 1:48:A:LYS:N | 1:48:A:LYS:CA | 1:48:A:LYS:C | 11       | 1.31          |
| (1,40) | 1:47:A:GLY:C | 1:48:A:LYS:N | 1:48:A:LYS:CA | 1:48:A:LYS:C | 14       | 1.31          |
| (1,31) | 1:37:A:PRO:C | 1:38:A:PRO:N | 1:38:A:PRO:CA | 1:38:A:PRO:C | 16       | 1.31          |
| (1,23) | 1:27:A:LYS:C | 1:28:A:ALA:N | 1:28:A:ALA:CA | 1:28:A:ALA:C | 12       | 1.31          |
| (1,23) | 1:27:A:LYS:C | 1:28:A:ALA:N | 1:28:A:ALA:CA | 1:28:A:ALA:C | 20       | 1.31          |
| (1,11) | 1:13:A:ILE:C | 1:14:A:THR:N | 1:14:A:THR:CA | 1:14:A:THR:C | 16       | 1.31          |
| (1,31) | 1:37:A:PRO:C | 1:38:A:PRO:N | 1:38:A:PRO:CA | 1:38:A:PRO:C | 19       | 1.3           |
| (1,25) | 1:29:A:LYS:C | 1:30:A:ILE:N | 1:30:A:ILE:CA | 1:30:A:ILE:C | 5        | 1.3           |
| (1,25) | 1:29:A:LYS:C | 1:30:A:ILE:N | 1:30:A:ILE:CA | 1:30:A:ILE:C | 14       | 1.3           |
| (1,20) | 1:24:A:GLU:C | 1:25:A:ASN:N | 1:25:A:ASN:CA | 1:25:A:ASN:C | 20       | 1.3           |
| (1,17) | 1:20:A:SER:C | 1:21:A:ASP:N | 1:21:A:ASP:CA | 1:21:A:ASP:C | 20       | 1.3           |
| (1,25) | 1:29:A:LYS:C | 1:30:A:ILE:N | 1:30:A:ILE:CA | 1:30:A:ILE:C | 7        | 1.29          |
| (1,23) | 1:27:A:LYS:C | 1:28:A:ALA:N | 1:28:A:ALA:CA | 1:28:A:ALA:C | 16       | 1.29          |
| (1,20) | 1:24:A:GLU:C | 1:25:A:ASN:N | 1:25:A:ASN:CA | 1:25:A:ASN:C | 7        | 1.29          |
| (1,25) | 1:29:A:LYS:C | 1:30:A:ILE:N | 1:30:A:ILE:CA | 1:30:A:ILE:C | 10       | 1.28          |
| (1,25) | 1:29:A:LYS:C | 1:30:A:ILE:N | 1:30:A:ILE:CA | 1:30:A:ILE:C | 12       | 1.28          |
| (1,25) | 1:29:A:LYS:C | 1:30:A:ILE:N | 1:30:A:ILE:CA | 1:30:A:ILE:C | 13       | 1.28          |
| (1,23) | 1:27:A:LYS:C | 1:28:A:ALA:N | 1:28:A:ALA:CA | 1:28:A:ALA:C | 11       | 1.28          |
| (1,9)  | 1:11:A:LYS:C | 1:12:A:THR:N | 1:12:A:THR:CA | 1:12:A:THR:C | 18       | 1.28          |
| (1,23) | 1:27:A:LYS:C | 1:28:A:ALA:N | 1:28:A:ALA:CA | 1:28:A:ALA:C | 1        | 1.27          |
| (1,23) | 1:27:A:LYS:C | 1:28:A:ALA:N | 1:28:A:ALA:CA | 1:28:A:ALA:C | 2        | 1.27          |
| (1,23) | 1:27:A:LYS:C | 1:28:A:ALA:N | 1:28:A:ALA:CA | 1:28:A:ALA:C | 4        | 1.27          |
| (1,17) | 1:20:A:SER:C | 1:21:A:ASP:N | 1:21:A:ASP:CA | 1:21:A:ASP:C | 15       | 1.27          |
| (1,17) | 1:20:A:SER:C | 1:21:A:ASP:N | 1:21:A:ASP:CA | 1:21:A:ASP:C | 16       | 1.27          |
| (1,12) | 1:14:A:THR:C | 1:15:A:LEU:N | 1:15:A:LEU:CA | 1:15:A:LEU:C | 4        | 1.27          |
| (1,25) | 1:29:A:LYS:C | 1:30:A:ILE:N | 1:30:A:ILE:CA | 1:30:A:ILE:C | 1        | 1.26          |
| (1,23) | 1:27:A:LYS:C | 1:28:A:ALA:N | 1:28:A:ALA:CA | 1:28:A:ALA:C | 6        | 1.26          |
| (1,20) | 1:24:A:GLU:C | 1:25:A:ASN:N | 1:25:A:ASN:CA | 1:25:A:ASN:C | 10       | 1.26          |

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| Key    | Atom-1       | Atom-2       | Atom-3        | Atom-4       | Model ID | Violation (°) |
|--------|--------------|--------------|---------------|--------------|----------|---------------|
| (1,33) | 1:39:A:ASP:C | 1:40:A:GLN:N | 1:40:A:GLN:CA | 1:40:A:GLN:C | 20       | 1.25          |
| (1,23) | 1:27:A:LYS:C | 1:28:A:ALA:N | 1:28:A:ALA:CA | 1:28:A:ALA:C | 5        | 1.25          |
| (1,23) | 1:27:A:LYS:C | 1:28:A:ALA:N | 1:28:A:ALA:CA | 1:28:A:ALA:C | 10       | 1.25          |
| (1,20) | 1:24:A:GLU:C | 1:25:A:ASN:N | 1:25:A:ASN:CA | 1:25:A:ASN:C | 2        | 1.25          |
| (1,23) | 1:27:A:LYS:C | 1:28:A:ALA:N | 1:28:A:ALA:CA | 1:28:A:ALA:C | 3        | 1.24          |
| (1,23) | 1:27:A:LYS:C | 1:28:A:ALA:N | 1:28:A:ALA:CA | 1:28:A:ALA:C | 18       | 1.24          |
| (1,10) | 1:12:A:THR:C | 1:13:A:ILE:N | 1:13:A:ILE:CA | 1:13:A:ILE:C | 6        | 1.24          |
| (1,31) | 1:37:A:PRO:C | 1:38:A:PRO:N | 1:38:A:PRO:CA | 1:38:A:PRO:C | 18       | 1.23          |
| (1,25) | 1:29:A:LYS:C | 1:30:A:ILE:N | 1:30:A:ILE:CA | 1:30:A:ILE:C | 18       | 1.23          |
| (1,9)  | 1:11:A:LYS:C | 1:12:A:THR:N | 1:12:A:THR:CA | 1:12:A:THR:C | 1        | 1.23          |
| (1,23) | 1:27:A:LYS:C | 1:28:A:ALA:N | 1:28:A:ALA:CA | 1:28:A:ALA:C | 13       | 1.22          |
| (1,50) | 1:57:A:SER:C | 1:58:A:ASP:N | 1:58:A:ASP:CA | 1:58:A:ASP:C | 6        | 1.21          |
| (1,50) | 1:57:A:SER:C | 1:58:A:ASP:N | 1:58:A:ASP:CA | 1:58:A:ASP:C | 10       | 1.21          |
| (1,31) | 1:37:A:PRO:C | 1:38:A:PRO:N | 1:38:A:PRO:CA | 1:38:A:PRO:C | 10       | 1.21          |
| (1,31) | 1:37:A:PRO:C | 1:38:A:PRO:N | 1:38:A:PRO:CA | 1:38:A:PRO:C | 14       | 1.21          |
| (1,23) | 1:27:A:LYS:C | 1:28:A:ALA:N | 1:28:A:ALA:CA | 1:28:A:ALA:C | 7        | 1.21          |
| (1,40) | 1:47:A:GLY:C | 1:48:A:LYS:N | 1:48:A:LYS:CA | 1:48:A:LYS:C | 20       | 1.2           |
| (1,33) | 1:39:A:ASP:C | 1:40:A:GLN:N | 1:40:A:GLN:CA | 1:40:A:GLN:C | 9        | 1.2           |
| (1,31) | 1:37:A:PRO:C | 1:38:A:PRO:N | 1:38:A:PRO:CA | 1:38:A:PRO:C | 15       | 1.2           |
| (1,45) | 1:52:A:ASP:C | 1:53:A:GLY:N | 1:53:A:GLY:CA | 1:53:A:GLY:C | 16       | 1.19          |
| (1,31) | 1:37:A:PRO:C | 1:38:A:PRO:N | 1:38:A:PRO:CA | 1:38:A:PRO:C | 1        | 1.19          |
| (1,31) | 1:37:A:PRO:C | 1:38:A:PRO:N | 1:38:A:PRO:CA | 1:38:A:PRO:C | 4        | 1.18          |
| (1,23) | 1:27:A:LYS:C | 1:28:A:ALA:N | 1:28:A:ALA:CA | 1:28:A:ALA:C | 17       | 1.18          |
| (1,9)  | 1:11:A:LYS:C | 1:12:A:THR:N | 1:12:A:THR:CA | 1:12:A:THR:C | 19       | 1.18          |
| (1,23) | 1:27:A:LYS:C | 1:28:A:ALA:N | 1:28:A:ALA:CA | 1:28:A:ALA:C | 8        | 1.17          |
| (1,10) | 1:12:A:THR:C | 1:13:A:ILE:N | 1:13:A:ILE:CA | 1:13:A:ILE:C | 11       | 1.17          |
| (1,45) | 1:52:A:ASP:C | 1:53:A:GLY:N | 1:53:A:GLY:CA | 1:53:A:GLY:C | 19       | 1.16          |
| (1,40) | 1:47:A:GLY:C | 1:48:A:LYS:N | 1:48:A:LYS:CA | 1:48:A:LYS:C | 3        | 1.16          |
| (1,40) | 1:47:A:GLY:C | 1:48:A:LYS:N | 1:48:A:LYS:CA | 1:48:A:LYS:C | 10       | 1.16          |
| (1,6)  | 1:7:A:THR:C  | 1:8:A:LEU:N  | 1:8:A:LEU:CA  | 1:8:A:LEU:C  | 13       | 1.16          |
| (1,23) | 1:27:A:LYS:C | 1:28:A:ALA:N | 1:28:A:ALA:CA | 1:28:A:ALA:C | 15       | 1.15          |
| (1,23) | 1:27:A:LYS:C | 1:28:A:ALA:N | 1:28:A:ALA:CA | 1:28:A:ALA:C | 14       | 1.14          |
| (1,40) | 1:47:A:GLY:C | 1:48:A:LYS:N | 1:48:A:LYS:CA | 1:48:A:LYS:C | 15       | 1.13          |
| (1,17) | 1:20:A:SER:C | 1:21:A:ASP:N | 1:21:A:ASP:CA | 1:21:A:ASP:C | 17       | 1.13          |
| (1,45) | 1:52:A:ASP:C | 1:53:A:GLY:N | 1:53:A:GLY:CA | 1:53:A:GLY:C | 5        | 1.11          |
| (1,14) | 1:16:A:GLU:C | 1:17:A:VAL:N | 1:17:A:VAL:CA | 1:17:A:VAL:C | 9        | 1.11          |
| (1,9)  | 1:11:A:LYS:C | 1:12:A:THR:N | 1:12:A:THR:CA | 1:12:A:THR:C | 15       | 1.11          |
| (1,40) | 1:47:A:GLY:C | 1:48:A:LYS:N | 1:48:A:LYS:CA | 1:48:A:LYS:C | 18       | 1.1           |
| (1,31) | 1:37:A:PRO:C | 1:38:A:PRO:N | 1:38:A:PRO:CA | 1:38:A:PRO:C | 2        | 1.1           |
| (1,23) | 1:27:A:LYS:C | 1:28:A:ALA:N | 1:28:A:ALA:CA | 1:28:A:ALA:C | 19       | 1.1           |
| (1,61) | 1:68:A:HIS:C | 1:69:A:LEU:N | 1:69:A:LEU:CA | 1:69:A:LEU:C | 12       | 1.09          |
| (1,61) | 1:68:A:HIS:C | 1:69:A:LEU:N | 1:69:A:LEU:CA | 1:69:A:LEU:C | 20       | 1.08          |
| (1,40) | 1:47:A:GLY:C | 1:48:A:LYS:N | 1:48:A:LYS:CA | 1:48:A:LYS:C | 19       | 1.08          |
| (1,40) | 1:47:A:GLY:C | 1:48:A:LYS:N | 1:48:A:LYS:CA | 1:48:A:LYS:C | 17       | 1.07          |
| (1,10) | 1:12:A:THR:C | 1:13:A:ILE:N | 1:13:A:ILE:CA | 1:13:A:ILE:C | 18       | 1.07          |
| (1,41) | 1:48:A:LYS:C | 1:49:A:GLN:N | 1:49:A:GLN:CA | 1:49:A:GLN:C | 10       | 1.06          |
| (1,31) | 1:37:A:PRO:C | 1:38:A:PRO:N | 1:38:A:PRO:CA | 1:38:A:PRO:C | 11       | 1.06          |
| (1,14) | 1:16:A:GLU:C | 1:17:A:VAL:N | 1:17:A:VAL:CA | 1:17:A:VAL:C | 16       | 1.04          |
| (1,14) | 1:16:A:GLU:C | 1:17:A:VAL:N | 1:17:A:VAL:CA | 1:17:A:VAL:C | 20       | 1.04          |
| (1,10) | 1:12:A:THR:C | 1:13:A:ILE:N | 1:13:A:ILE:CA | 1:13:A:ILE:C | 14       | 1.04          |
| (1,7)  | 1:8:A:LEU:C  | 1:9:A:THR:N  | 1:9:A:THR:CA  | 1:9:A:THR:C  | 17       | 1.04          |

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| Key    | Atom-1       | Atom-2       | Atom-3        | Atom-4       | Model ID | Violation (°) |
|--------|--------------|--------------|---------------|--------------|----------|---------------|
| (1,41) | 1:48:A:LYS:C | 1:49:A:GLN:N | 1:49:A:GLN:CA | 1:49:A:GLN:C | 20       | 1.03          |
| (1,40) | 1:47:A:GLY:C | 1:48:A:LYS:N | 1:48:A:LYS:CA | 1:48:A:LYS:C | 9        | 1.03          |
| (1,40) | 1:47:A:GLY:C | 1:48:A:LYS:N | 1:48:A:LYS:CA | 1:48:A:LYS:C | 16       | 1.03          |
| (1,14) | 1:16:A:GLU:C | 1:17:A:VAL:N | 1:17:A:VAL:CA | 1:17:A:VAL:C | 18       | 1.03          |
| (1,10) | 1:12:A:THR:C | 1:13:A:ILE:N | 1:13:A:ILE:CA | 1:13:A:ILE:C | 8        | 1.03          |
| (1,9)  | 1:11:A:LYS:C | 1:12:A:THR:N | 1:12:A:THR:CA | 1:12:A:THR:C | 5        | 1.02          |
| (1,14) | 1:16:A:GLU:C | 1:17:A:VAL:N | 1:17:A:VAL:CA | 1:17:A:VAL:C | 10       | 1.01          |
| (1,40) | 1:47:A:GLY:C | 1:48:A:LYS:N | 1:48:A:LYS:CA | 1:48:A:LYS:C | 6        | 1.0           |
| (1,25) | 1:29:A:LYS:C | 1:30:A:ILE:N | 1:30:A:ILE:CA | 1:30:A:ILE:C | 9        | 1.0           |
| (1,25) | 1:29:A:LYS:C | 1:30:A:ILE:N | 1:30:A:ILE:CA | 1:30:A:ILE:C | 20       | 1.0           |