



# Full wwPDB NMR Structure Validation Report ⓘ

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PDB ID : 6OBW / pdb\_00006obw  
BMRB ID : 30593  
Title : CSP1-cyc(K6D10)  
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This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

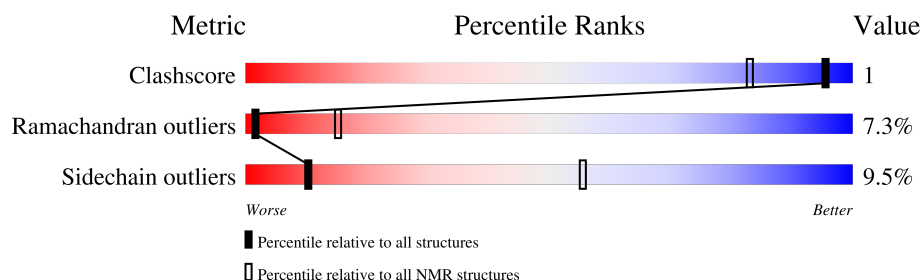
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 52%.

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     | 17     | <div> <div>53%</div> <div>12%</div> <div>35%</div> </div> |

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 13 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

| Well-defined (core) protein residues |                       |                   |              |
|--------------------------------------|-----------------------|-------------------|--------------|
| Well-defined core                    | Residue range (total) | Backbone RMSD (Å) | Medoid model |
| 1                                    | A:3-A:13 (11)         | 0.20              | 13           |

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

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

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

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

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 327 atoms, of which 170 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Competence-stimulating peptide type 1.

| Mol | Chain | Residues | Atoms |     |     |    |    |   | Trace |
|-----|-------|----------|-------|-----|-----|----|----|---|-------|
| 1   | A     | 17       | Total | C   | H   | N  | O  | S | 0     |
|     |       |          | 327   | 103 | 170 | 30 | 23 | 1 |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| A     | 10      | ASN      | ASP    | conflict | UNP P60242 |

## 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: Competence-stimulating peptide type 1



### 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: Competence-stimulating peptide type 1



#### 4.2.2 Score per residue for model 2

- Molecule 1: Competence-stimulating peptide type 1



### 4.2.3 Score per residue for model 3

- Molecule 1: Competence-stimulating peptide type 1



### 4.2.4 Score per residue for model 4

- Molecule 1: Competence-stimulating peptide type 1



### 4.2.5 Score per residue for model 5

- Molecule 1: Competence-stimulating peptide type 1



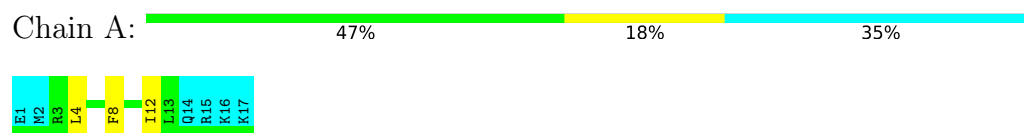
### 4.2.6 Score per residue for model 6

- Molecule 1: Competence-stimulating peptide type 1



### 4.2.7 Score per residue for model 7

- Molecule 1: Competence-stimulating peptide type 1



#### 4.2.8 Score per residue for model 8

- Molecule 1: Competence-stimulating peptide type 1



#### 4.2.9 Score per residue for model 9

- Molecule 1: Competence-stimulating peptide type 1



#### 4.2.10 Score per residue for model 10

- Molecule 1: Competence-stimulating peptide type 1



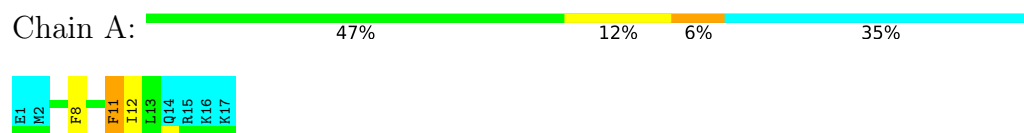
#### 4.2.11 Score per residue for model 11

- Molecule 1: Competence-stimulating peptide type 1



#### 4.2.12 Score per residue for model 12

- Molecule 1: Competence-stimulating peptide type 1



#### 4.2.13 Score per residue for model 13 (medoid)

- Molecule 1: Competence-stimulating peptide type 1



#### 4.2.14 Score per residue for model 14

- Molecule 1: Competence-stimulating peptide type 1



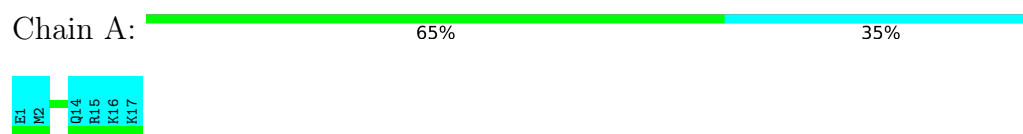
#### 4.2.15 Score per residue for model 15

- Molecule 1: Competence-stimulating peptide type 1



#### 4.2.16 Score per residue for model 16

- Molecule 1: Competence-stimulating peptide type 1



#### 4.2.17 Score per residue for model 17

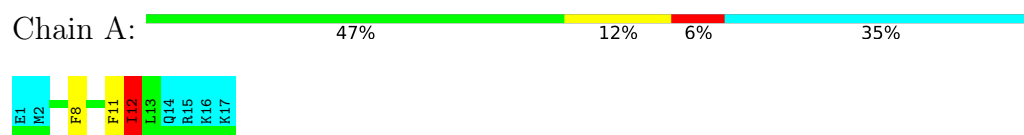
- Molecule 1: Competence-stimulating peptide type 1





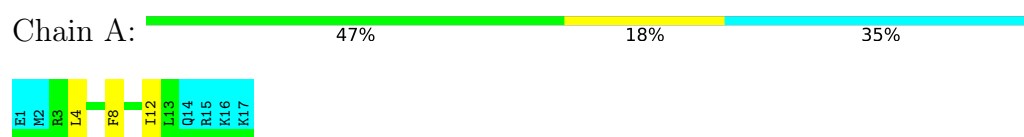
#### 4.2.18 Score per residue for model 18

- Molecule 1: Competence-stimulating peptide type 1



#### 4.2.19 Score per residue for model 19

- Molecule 1: Competence-stimulating peptide type 1



#### 4.2.20 Score per residue for model 20

- Molecule 1: Competence-stimulating peptide type 1



## 5 Refinement protocol and experimental data overview

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

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

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

| Software name | Classification        | Version |
|---------------|-----------------------|---------|
| X-PLOR NIH    | structure calculation |         |
| 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                       | 139            |
| Number of shifts mapped to atoms             | 139            |
| Number of unparsed shifts                    | 0              |
| Number of shifts with mapping errors         | 0              |
| Number of shifts with mapping warnings       | 0              |
| Assignment completeness (well-defined parts) | 52%            |

## 6 Model quality [i](#)

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

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes |
|-----|-------|-------|----------|----------|---------|
| 1   | A     | 101   | 106      | 104      | 0±0     |
| All | All   | 2020  | 2120     | 2080     | 4       |

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 1.

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

| Atom-1       | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|--------------|-----------------|----------|-------------|--------|-------|
|              |                 |          |             | Worst  | Total |
| 1:A:11:PHE:O | 1:A:12:ILE:HG23 | 0.67     | 1.89        | 4      | 2     |
| 1:A:11:PHE:O | 1:A:12:ILE:HD13 | 0.46     | 2.10        | 12     | 1     |
| 1:A:4:LEU:O  | 1:A:4:LEU:HD13  | 0.45     | 2.12        | 14     | 1     |

### 6.3 Torsion angles [i](#)

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

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

| Mol | Chain | Analysed      | Favoured    | Allowed     | Outliers   | Percentiles |    |
|-----|-------|---------------|-------------|-------------|------------|-------------|----|
| 1   | A     | 11/17 (65%)   | 9±0 (80±4%) | 1±1 (12±7%) | 1±0 (7±4%) | 1           | 15 |
| All | All   | 220/340 (65%) | 177 (80%)   | 27 (12%)    | 16 (7%)    | 1           | 15 |

All 2 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 12  | ILE  | 15             |
| 1   | A     | 11  | PHE  | 1              |

### 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     | 10/17 (59%)   | 9±1 (91±6%) | 1±1 (10±6%) | 10          | 55 |
| All | All   | 200/340 (59%) | 181 (90%)   | 19 (10%)    | 10          | 55 |

All 3 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     | 4   | LEU  | 10             |
| 1   | A     | 8   | PHE  | 7              |
| 1   | A     | 12  | ILE  | 2              |

### 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

There are no ligands in this entry.

## 6.7 Other polymers

There are no such molecules in this entry.

## 6.8 Polymer linkage issues

There are no chain breaks in this entry.

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

The completeness of assignment taking into account all chemical shift lists is 52% for the well-defined parts and 47% for the entire structure.

### 7.1 Chemical shift list 1

File name: `working_cs.cif`

Chemical shift list name: `shiftFile_1`

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

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

|                                         |     |
|-----------------------------------------|-----|
| Total number of shifts                  | 139 |
| Number of shifts mapped to atoms        | 139 |
| Number of unparsed shifts               | 0   |
| Number of shifts with mapping errors    | 0   |
| Number of shifts with mapping warnings  | 0   |
| Number of shift outliers (ShiftChecker) | 0   |

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

No chemical shift referencing corrections were calculated (not enough data).

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

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 52%, i.e. 99 atoms were assigned a chemical shift out of a possible 192. 0 out of 2 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total        | <sup>1</sup> H | <sup>13</sup> C | <sup>15</sup> N |
|-----------|--------------|----------------|-----------------|-----------------|
| Backbone  | 38/55 (69%)  | 22/22 (100%)   | 7/22 (32%)      | 9/11 (82%)      |
| Sidechain | 56/107 (52%) | 50/69 (72%)    | 6/30 (20%)      | 0/8 (0%)        |
| Aromatic  | 5/30 (17%)   | 5/15 (33%)     | 0/15 (0%)       | 0/0 (—%)        |
| Overall   | 99/192 (52%) | 77/106 (73%)   | 13/67 (19%)     | 9/19 (47%)      |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 47%, i.e. 139 atoms were assigned a chemical shift out of a possible 293. 0 out of 2 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total         | <sup>1</sup> H | <sup>13</sup> C | <sup>15</sup> N |
|-----------|---------------|----------------|-----------------|-----------------|
| Backbone  | 56/85 (66%)   | 31/34 (91%)    | 12/34 (35%)     | 13/17 (76%)     |
| Sidechain | 78/178 (44%)  | 67/113 (59%)   | 11/51 (22%)     | 0/14 (0%)       |
| Aromatic  | 5/30 (17%)    | 5/15 (33%)     | 0/15 (0%)       | 0/0 (—%)        |
| Overall   | 139/293 (47%) | 103/162 (64%)  | 23/100 (23%)    | 13/31 (42%)     |

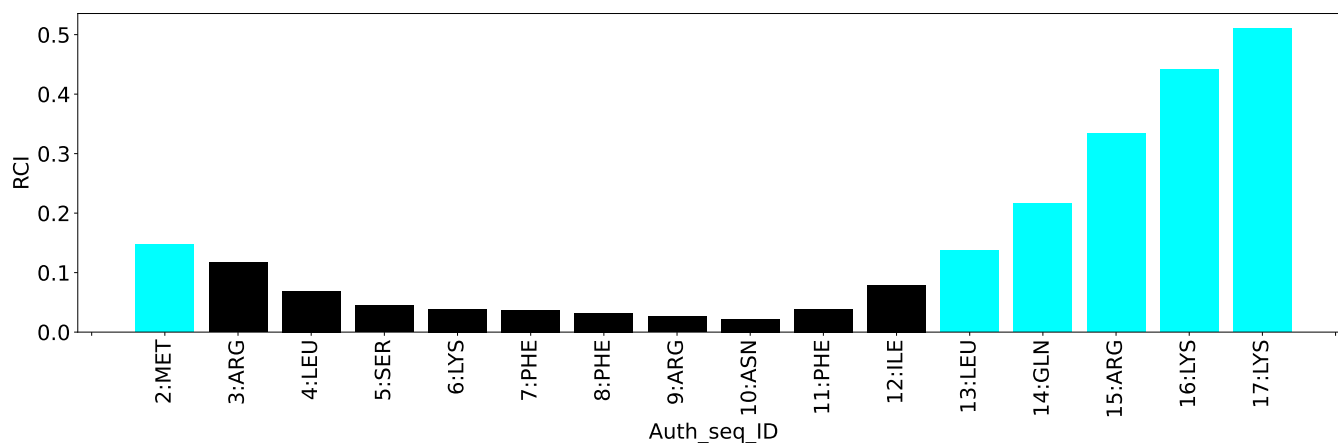
### 7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

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

Random coil index (RCI) for chain A:



## 8 NMR restraints analysis

### 8.1 Conformationally restricting restraints

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

| Description                                              | Value |
|----------------------------------------------------------|-------|
| Total distance restraints                                | 251   |
| Intra-residue ( $ i-j =0$ )                              | 149   |
| Sequential ( $ i-j =1$ )                                 | 58    |
| Medium range ( $ i-j >1$ and $ i-j <5$ )                 | 40    |
| Long range ( $ i-j \geq 5$ )                             | 4     |
| Inter-chain                                              | 0     |
| Hydrogen bond restraints                                 | 0     |
| Disulfide bond restraints                                | 0     |
| Total dihedral-angle restraints                          | 19    |
| Number of unmapped restraints                            | 0     |
| Number of restraints per residue                         | 15.9  |
| Number of long range restraints per residue <sup>1</sup> | 0.2   |

<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)  | 9.9                                    | 0.2     |
| 0.2-0.5 (Medium) | 17.9                                   | 0.5     |
| >0.5 (Large)     | 0.9                                    | 0.62    |



### 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)   | 2.1                                    | 9.48    |
| 10.0-20.0 (Medium) | 0.7                                    | 13.79   |
| >20.0 (Large)      | 6.0                                    | 142.57  |

## 9 Distance violation analysis ⓘ

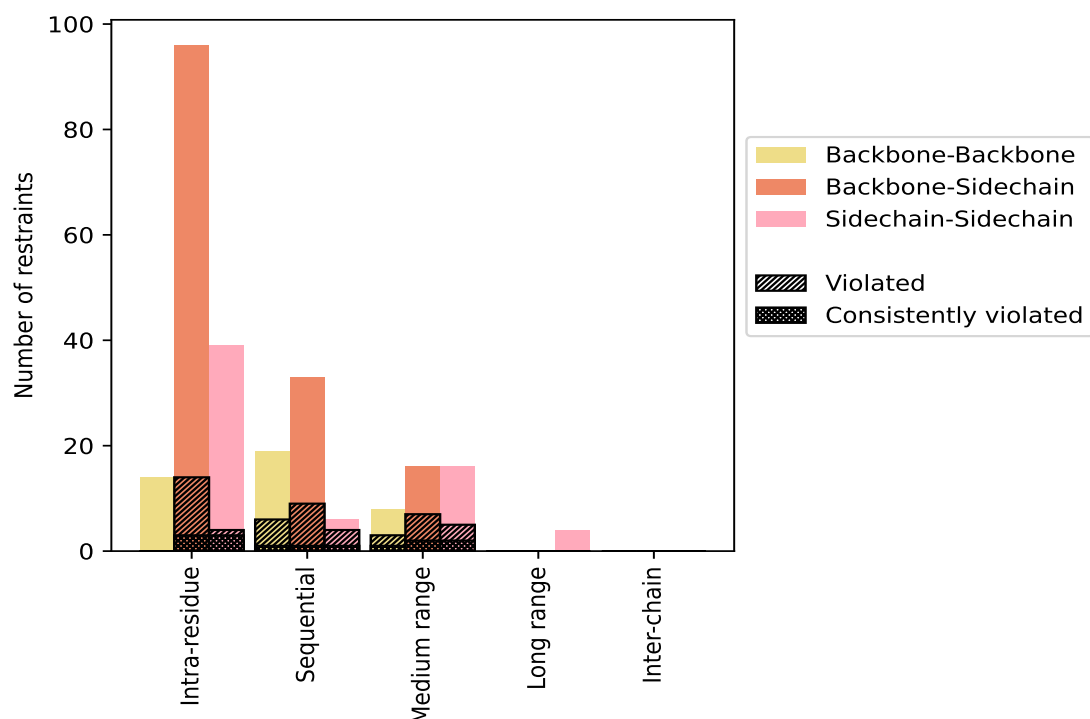
### 9.1 Summary of distance violations ⓘ

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>149</b> | <b>59.4</b>    | <b>18</b>             | <b>12.1</b>    | <b>7.2</b>     | <b>6</b>                           | <b>4.0</b>     | <b>2.4</b>     |
| Backbone-Backbone                                                           | 14         | 5.6            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 96         | 38.2           | 14                    | 14.6           | 5.6            | 3                                  | 3.1            | 1.2            |
| Sidechain-Sidechain                                                         | 39         | 15.5           | 4                     | 10.3           | 1.6            | 3                                  | 7.7            | 1.2            |
| <b>Sequential (<math> i-j =1</math>)</b>                                    | <b>58</b>  | <b>23.1</b>    | <b>19</b>             | <b>32.8</b>    | <b>7.6</b>     | <b>3</b>                           | <b>5.2</b>     | <b>1.2</b>     |
| Backbone-Backbone                                                           | 19         | 7.6            | 6                     | 31.6           | 2.4            | 1                                  | 5.3            | 0.4            |
| Backbone-Sidechain                                                          | 33         | 13.1           | 9                     | 27.3           | 3.6            | 1                                  | 3.0            | 0.4            |
| Sidechain-Sidechain                                                         | 6          | 2.4            | 4                     | 66.7           | 1.6            | 1                                  | 16.7           | 0.4            |
| <b>Medium range (<math> i-j &gt;1</math> &amp; <math> i-j &lt;5</math>)</b> | <b>40</b>  | <b>15.9</b>    | <b>15</b>             | <b>37.5</b>    | <b>6.0</b>     | <b>5</b>                           | <b>12.5</b>    | <b>2.0</b>     |
| Backbone-Backbone                                                           | 8          | 3.2            | 3                     | 37.5           | 1.2            | 1                                  | 12.5           | 0.4            |
| Backbone-Sidechain                                                          | 16         | 6.4            | 7                     | 43.8           | 2.8            | 2                                  | 12.5           | 0.8            |
| Sidechain-Sidechain                                                         | 16         | 6.4            | 5                     | 31.2           | 2.0            | 2                                  | 12.5           | 0.8            |
| <b>Long range (<math> i-j \geq 5</math>)</b>                                | <b>4</b>   | <b>1.6</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                                                         | 4          | 1.6            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| <b>Inter-chain</b>                                                          | <b>0</b>   | <b>0.0</b>     | <b>0</b>              | <b>0.0</b>     | <b>0.0</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| Backbone-Backbone                                                           | 0          | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 0          | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Sidechain-Sidechain                                                         | 0          | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| <b>Hydrogen bond</b>                                                        | <b>0</b>   | <b>0.0</b>     | <b>0</b>              | <b>0.0</b>     | <b>0.0</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| <b>Disulfide bond</b>                                                       | <b>0</b>   | <b>0.0</b>     | <b>0</b>              | <b>0.0</b>     | <b>0.0</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| <b>Total</b>                                                                | <b>251</b> | <b>100.0</b>   | <b>52</b>             | <b>20.7</b>    | <b>20.7</b>    | <b>14</b>                          | <b>5.6</b>     | <b>5.6</b>     |
| Backbone-Backbone                                                           | 41         | 16.3           | 9                     | 22.0           | 3.6            | 2                                  | 4.9            | 0.8            |
| Backbone-Sidechain                                                          | 145        | 57.8           | 30                    | 20.7           | 12.0           | 6                                  | 4.1            | 2.4            |
| Sidechain-Sidechain                                                         | 65         | 25.9           | 13                    | 20.0           | 5.2            | 6                                  | 9.2            | 2.4            |

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

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



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

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

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

| Model ID | Number of violations |                 |                 |                 |                 |       | Mean (Å) | Max (Å) | SD <sup>6</sup> (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
|          | IR <sup>1</sup>      | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total |          |         |                     |            |
| 1        | 10                   | 9               | 7               | 0               | 0               | 26    | 0.29     | 0.52    | 0.11                | 0.29       |
| 2        | 10                   | 13              | 9               | 0               | 0               | 32    | 0.26     | 0.53    | 0.12                | 0.26       |
| 3        | 9                    | 10              | 8               | 0               | 0               | 27    | 0.28     | 0.59    | 0.12                | 0.23       |
| 4        | 12                   | 10              | 9               | 0               | 0               | 31    | 0.26     | 0.54    | 0.12                | 0.24       |
| 5        | 11                   | 9               | 8               | 0               | 0               | 28    | 0.27     | 0.52    | 0.12                | 0.29       |
| 6        | 14                   | 11              | 9               | 0               | 0               | 34    | 0.25     | 0.5     | 0.12                | 0.22       |
| 7        | 10                   | 7               | 8               | 0               | 0               | 25    | 0.27     | 0.56    | 0.12                | 0.26       |
| 8        | 12                   | 11              | 10              | 0               | 0               | 33    | 0.25     | 0.52    | 0.11                | 0.23       |
| 9        | 14                   | 10              | 9               | 0               | 0               | 33    | 0.25     | 0.62    | 0.12                | 0.21       |
| 10       | 14                   | 10              | 7               | 0               | 0               | 31    | 0.26     | 0.62    | 0.13                | 0.22       |

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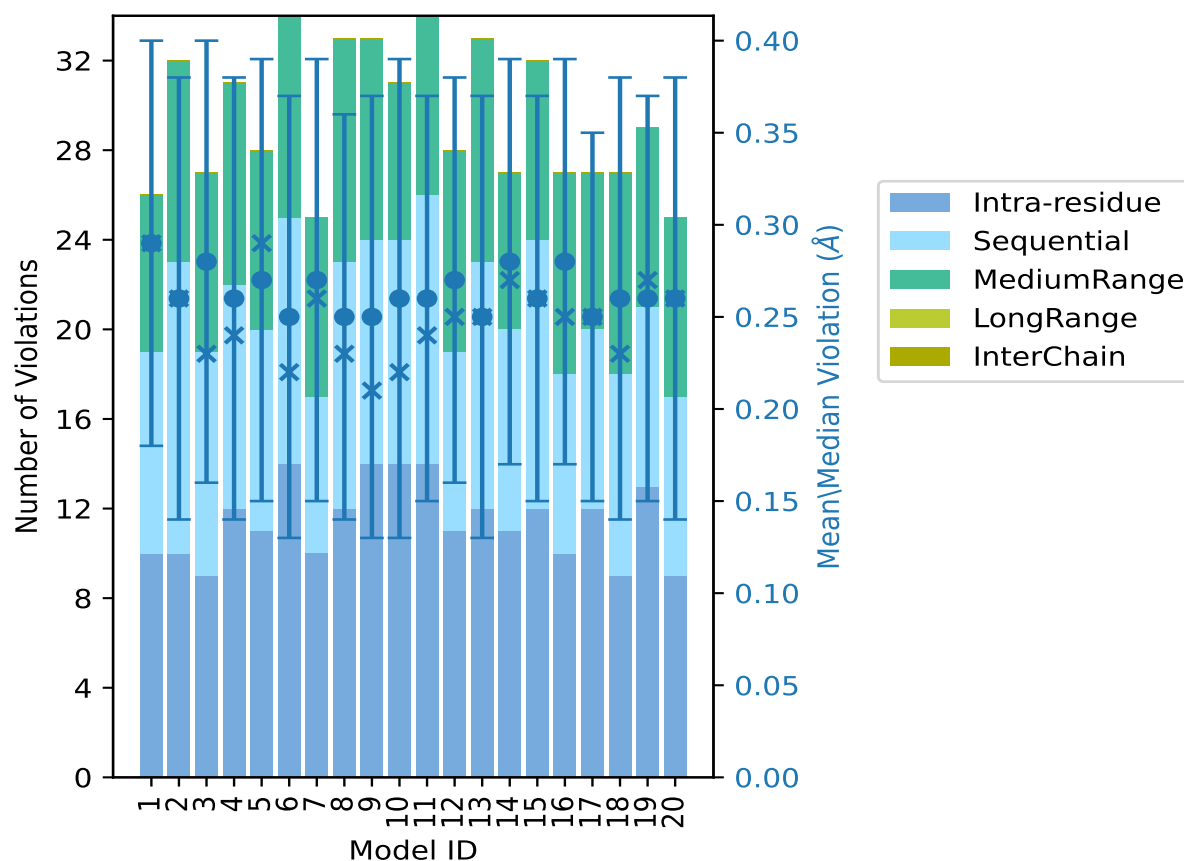
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| Model ID | Number of violations |                 |                 |                 |                 |       | Mean (Å) | Max (Å) | SD <sup>6</sup> (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
|          | IR <sup>1</sup>      | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total |          |         |                     |            |
| 11       | 14                   | 12              | 8               | 0               | 0               | 34    | 0.26     | 0.54    | 0.11                | 0.24       |
| 12       | 11                   | 8               | 9               | 0               | 0               | 28    | 0.27     | 0.49    | 0.11                | 0.25       |
| 13       | 12                   | 11              | 10              | 0               | 0               | 33    | 0.25     | 0.54    | 0.12                | 0.25       |
| 14       | 11                   | 9               | 7               | 0               | 0               | 27    | 0.28     | 0.53    | 0.11                | 0.27       |
| 15       | 12                   | 12              | 8               | 0               | 0               | 32    | 0.26     | 0.53    | 0.11                | 0.26       |
| 16       | 10                   | 8               | 9               | 0               | 0               | 27    | 0.28     | 0.58    | 0.11                | 0.25       |
| 17       | 12                   | 8               | 7               | 0               | 0               | 27    | 0.25     | 0.48    | 0.1                 | 0.25       |
| 18       | 9                    | 9               | 9               | 0               | 0               | 27    | 0.26     | 0.52    | 0.12                | 0.23       |
| 19       | 13                   | 8               | 8               | 0               | 0               | 29    | 0.26     | 0.46    | 0.11                | 0.27       |
| 20       | 9                    | 8               | 8               | 0               | 0               | 25    | 0.26     | 0.53    | 0.12                | 0.26       |

<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 ⓘ

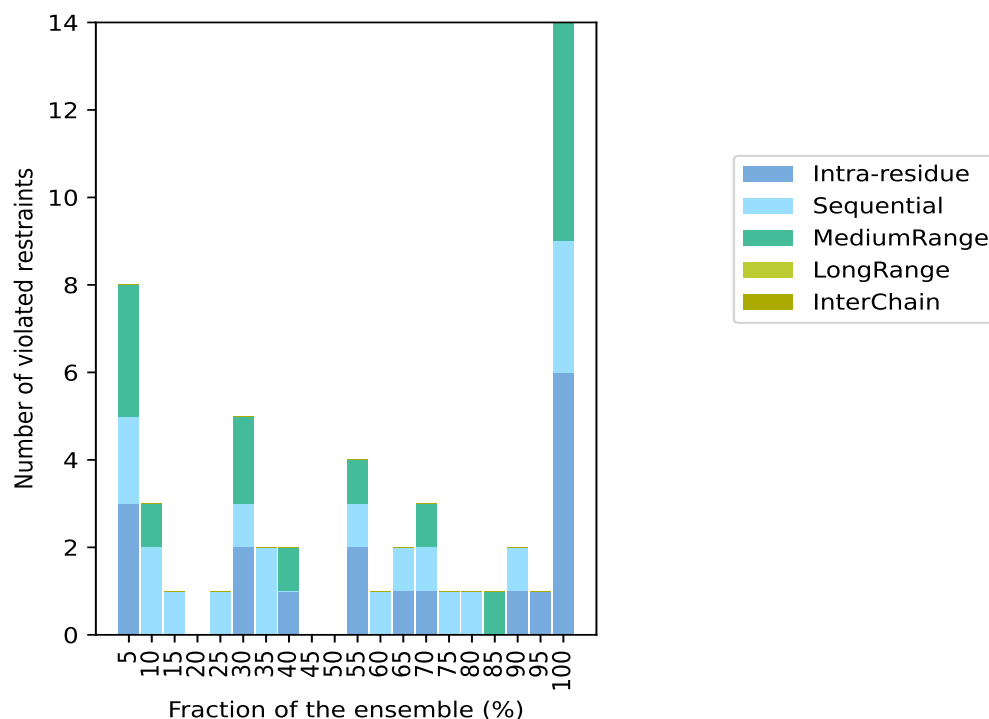
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 199(IR:131, SQ:39, MR:25, LR:4, IC:0) restraints are not 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                             | 2               | 3               | 0               | 0               | 8     | 1                        | 5.0   |
| 0                             | 2               | 1               | 0               | 0               | 3     | 2                        | 10.0  |
| 0                             | 1               | 0               | 0               | 0               | 1     | 3                        | 15.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 4                        | 20.0  |
| 0                             | 1               | 0               | 0               | 0               | 1     | 5                        | 25.0  |
| 2                             | 1               | 2               | 0               | 0               | 5     | 6                        | 30.0  |
| 0                             | 2               | 0               | 0               | 0               | 2     | 7                        | 35.0  |
| 1                             | 0               | 1               | 0               | 0               | 2     | 8                        | 40.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 9                        | 45.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 10                       | 50.0  |
| 2                             | 1               | 1               | 0               | 0               | 4     | 11                       | 55.0  |
| 0                             | 1               | 0               | 0               | 0               | 1     | 12                       | 60.0  |
| 1                             | 1               | 0               | 0               | 0               | 2     | 13                       | 65.0  |
| 1                             | 1               | 1               | 0               | 0               | 3     | 14                       | 70.0  |
| 0                             | 1               | 0               | 0               | 0               | 1     | 15                       | 75.0  |
| 0                             | 1               | 0               | 0               | 0               | 1     | 16                       | 80.0  |
| 0                             | 0               | 1               | 0               | 0               | 1     | 17                       | 85.0  |
| 1                             | 1               | 0               | 0               | 0               | 2     | 18                       | 90.0  |
| 1                             | 0               | 0               | 0               | 0               | 1     | 19                       | 95.0  |
| 6                             | 3               | 5               | 0               | 0               | 14    | 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

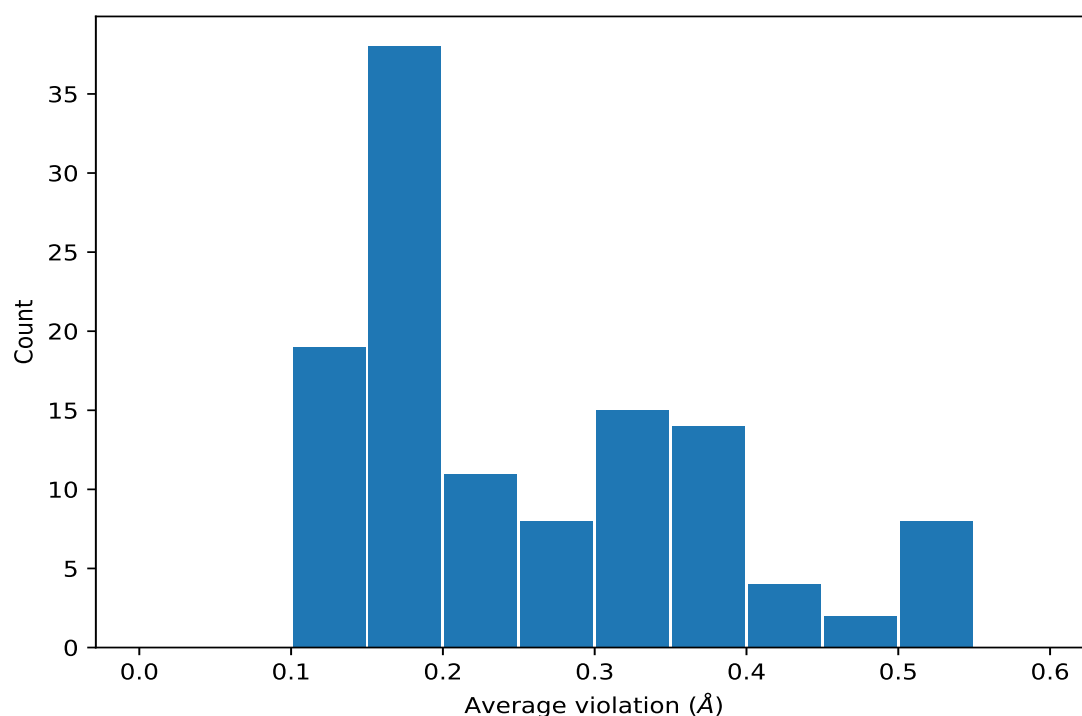
### 9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



## 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) |
|---------|----------------|---------------|---------------------|----------|---------------------|------------|
| (1,120) | 1:8:A:PHE:HA   | 1:8:A:PHE:HE1 | 20                  | 0.48     | 0.07                | 0.5        |
| (1,120) | 1:8:A:PHE:HA   | 1:8:A:PHE:HE2 | 20                  | 0.48     | 0.07                | 0.5        |
| (1,112) | 1:7:A:PHE:HB2  | 1:7:A:PHE:HZ  | 20                  | 0.44     | 0.0                 | 0.44       |
| (1,112) | 1:7:A:PHE:HB3  | 1:7:A:PHE:HZ  | 20                  | 0.44     | 0.0                 | 0.44       |
| (1,115) | 1:7:A:PHE:HB2  | 1:7:A:PHE:HZ  | 20                  | 0.44     | 0.0                 | 0.44       |
| (1,115) | 1:7:A:PHE:HB3  | 1:7:A:PHE:HZ  | 20                  | 0.44     | 0.0                 | 0.44       |
| (1,93)  | 1:6:A:LYS:HA   | 1:7:A:PHE:HB2 | 20                  | 0.36     | 0.02                | 0.36       |
| (1,93)  | 1:6:A:LYS:HA   | 1:7:A:PHE:HB3 | 20                  | 0.36     | 0.02                | 0.36       |
| (1,53)  | 1:4:A:LEU:HD11 | 1:6:A:LYS:HB2 | 20                  | 0.35     | 0.06                | 0.34       |
| (1,53)  | 1:4:A:LEU:HD11 | 1:6:A:LYS:HB3 | 20                  | 0.35     | 0.06                | 0.34       |
| (1,53)  | 1:4:A:LEU:HD12 | 1:6:A:LYS:HB2 | 20                  | 0.35     | 0.06                | 0.34       |
| (1,53)  | 1:4:A:LEU:HD12 | 1:6:A:LYS:HB3 | 20                  | 0.35     | 0.06                | 0.34       |
| (1,53)  | 1:4:A:LEU:HD13 | 1:6:A:LYS:HB2 | 20                  | 0.35     | 0.06                | 0.34       |
| (1,53)  | 1:4:A:LEU:HD13 | 1:6:A:LYS:HB3 | 20                  | 0.35     | 0.06                | 0.34       |
| (1,53)  | 1:4:A:LEU:HD21 | 1:6:A:LYS:HB2 | 20                  | 0.35     | 0.06                | 0.34       |
| (1,53)  | 1:4:A:LEU:HD21 | 1:6:A:LYS:HB3 | 20                  | 0.35     | 0.06                | 0.34       |

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| Key     | Atom-1          | Atom-2         | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|-----------------|----------------|---------------------|----------|---------------------|------------|
| (1,53)  | 1:4:A:LEU:HD22  | 1:6:A:LYS:HB2  | 20                  | 0.35     | 0.06                | 0.34       |
| (1,53)  | 1:4:A:LEU:HD22  | 1:6:A:LYS:HB3  | 20                  | 0.35     | 0.06                | 0.34       |
| (1,53)  | 1:4:A:LEU:HD23  | 1:6:A:LYS:HB2  | 20                  | 0.35     | 0.06                | 0.34       |
| (1,53)  | 1:4:A:LEU:HD23  | 1:6:A:LYS:HB3  | 20                  | 0.35     | 0.06                | 0.34       |
| (1,95)  | 1:6:A:LYS:HB2   | 1:7:A:PHE:HB2  | 20                  | 0.33     | 0.03                | 0.33       |
| (1,95)  | 1:6:A:LYS:HB2   | 1:7:A:PHE:HB3  | 20                  | 0.33     | 0.03                | 0.33       |
| (1,95)  | 1:6:A:LYS:HB3   | 1:7:A:PHE:HB2  | 20                  | 0.33     | 0.03                | 0.33       |
| (1,95)  | 1:6:A:LYS:HB3   | 1:7:A:PHE:HB3  | 20                  | 0.33     | 0.03                | 0.33       |
| (1,132) | 1:8:A:PHE:HB2   | 1:11:A:PHE:HB2 | 20                  | 0.31     | 0.05                | 0.31       |
| (1,132) | 1:8:A:PHE:HB2   | 1:11:A:PHE:HB3 | 20                  | 0.31     | 0.05                | 0.31       |
| (1,132) | 1:8:A:PHE:HB3   | 1:11:A:PHE:HB2 | 20                  | 0.31     | 0.05                | 0.31       |
| (1,132) | 1:8:A:PHE:HB3   | 1:11:A:PHE:HB3 | 20                  | 0.31     | 0.05                | 0.31       |
| (1,31)  | 1:3:A:ARG:HG2   | 1:6:A:LYS:HA   | 20                  | 0.28     | 0.04                | 0.28       |
| (1,31)  | 1:3:A:ARG:HG3   | 1:6:A:LYS:HA   | 20                  | 0.28     | 0.04                | 0.28       |
| (1,103) | 1:6:A:LYS:HA    | 1:8:A:PHE:HA   | 20                  | 0.27     | 0.02                | 0.28       |
| (1,116) | 1:7:A:PHE:H     | 1:7:A:PHE:HZ   | 20                  | 0.27     | 0.02                | 0.28       |
| (1,215) | 1:14:A:GLN:H    | 1:15:A:ARG:HA  | 20                  | 0.27     | 0.06                | 0.27       |
| (1,106) | 1:6:A:LYS:HA    | 1:9:A:ARG:HG2  | 20                  | 0.24     | 0.05                | 0.23       |
| (1,106) | 1:6:A:LYS:HA    | 1:9:A:ARG:HG3  | 20                  | 0.24     | 0.05                | 0.23       |
| (1,124) | 1:8:A:PHE:HB2   | 1:8:A:PHE:HZ   | 20                  | 0.21     | 0.0                 | 0.21       |
| (1,124) | 1:8:A:PHE:HB3   | 1:8:A:PHE:HZ   | 20                  | 0.21     | 0.0                 | 0.21       |
| (1,157) | 1:11:A:PHE:HA   | 1:11:A:PHE:HE1 | 20                  | 0.15     | 0.04                | 0.13       |
| (1,157) | 1:11:A:PHE:HA   | 1:11:A:PHE:HE2 | 20                  | 0.15     | 0.04                | 0.13       |
| (1,18)  | 1:3:A:ARG:HB2   | 1:3:A:ARG:H    | 19                  | 0.33     | 0.02                | 0.33       |
| (1,18)  | 1:3:A:ARG:HB3   | 1:3:A:ARG:H    | 19                  | 0.33     | 0.02                | 0.33       |
| (1,139) | 1:9:A:ARG:HA    | 1:9:A:ARG:HD2  | 18                  | 0.3      | 0.09                | 0.31       |
| (1,139) | 1:9:A:ARG:HA    | 1:9:A:ARG:HD3  | 18                  | 0.3      | 0.09                | 0.31       |
| (1,26)  | 1:3:A:ARG:HB2   | 1:4:A:LEU:H    | 18                  | 0.22     | 0.09                | 0.19       |
| (1,26)  | 1:3:A:ARG:HB3   | 1:4:A:LEU:H    | 18                  | 0.22     | 0.09                | 0.19       |
| (1,150) | 1:9:A:ARG:HG2   | 1:12:A:ILE:HA  | 17                  | 0.23     | 0.07                | 0.24       |
| (1,150) | 1:9:A:ARG:HG3   | 1:12:A:ILE:HA  | 17                  | 0.23     | 0.07                | 0.24       |
| (1,184) | 1:12:A:ILE:HB   | 1:13:A:LEU:H   | 16                  | 0.22     | 0.02                | 0.23       |
| (1,99)  | 1:6:A:LYS:HD2   | 1:7:A:PHE:HB2  | 15                  | 0.51     | 0.06                | 0.48       |
| (1,99)  | 1:6:A:LYS:HD2   | 1:7:A:PHE:HB3  | 15                  | 0.51     | 0.06                | 0.48       |
| (1,99)  | 1:6:A:LYS:HD3   | 1:7:A:PHE:HB2  | 15                  | 0.51     | 0.06                | 0.48       |
| (1,99)  | 1:6:A:LYS:HD3   | 1:7:A:PHE:HB3  | 15                  | 0.51     | 0.06                | 0.48       |
| (1,179) | 1:12:A:ILE:HG12 | 1:12:A:ILE:H   | 14                  | 0.27     | 0.05                | 0.24       |
| (1,179) | 1:12:A:ILE:HG13 | 1:12:A:ILE:H   | 14                  | 0.27     | 0.05                | 0.24       |
| (1,201) | 1:13:A:LEU:H    | 1:14:A:GLN:H   | 14                  | 0.15     | 0.03                | 0.14       |
| (1,57)  | 1:4:A:LEU:HA    | 1:7:A:PHE:HZ   | 14                  | 0.13     | 0.02                | 0.14       |
| (1,214) | 1:14:A:GLN:HG2  | 1:15:A:ARG:H   | 13                  | 0.21     | 0.02                | 0.22       |
| (1,214) | 1:14:A:GLN:HG3  | 1:15:A:ARG:H   | 13                  | 0.21     | 0.02                | 0.22       |

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| Key     | Atom-1          | Atom-2         | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|-----------------|----------------|---------------------|----------|---------------------|------------|
| (1,196) | 1:13:A:LEU:HD11 | 1:13:A:LEU:H   | 13                  | 0.15     | 0.02                | 0.15       |
| (1,196) | 1:13:A:LEU:HD12 | 1:13:A:LEU:H   | 13                  | 0.15     | 0.02                | 0.15       |
| (1,196) | 1:13:A:LEU:HD13 | 1:13:A:LEU:H   | 13                  | 0.15     | 0.02                | 0.15       |
| (1,196) | 1:13:A:LEU:HD21 | 1:13:A:LEU:H   | 13                  | 0.15     | 0.02                | 0.15       |
| (1,196) | 1:13:A:LEU:HD22 | 1:13:A:LEU:H   | 13                  | 0.15     | 0.02                | 0.15       |
| (1,196) | 1:13:A:LEU:HD23 | 1:13:A:LEU:H   | 13                  | 0.15     | 0.02                | 0.15       |
| (1,185) | 1:12:A:ILE:HD11 | 1:13:A:LEU:H   | 12                  | 0.15     | 0.05                | 0.13       |
| (1,185) | 1:12:A:ILE:HD12 | 1:13:A:LEU:H   | 12                  | 0.15     | 0.05                | 0.13       |
| (1,185) | 1:12:A:ILE:HD13 | 1:13:A:LEU:H   | 12                  | 0.15     | 0.05                | 0.13       |
| (1,146) | 1:9:A:ARG:HD2   | 1:9:A:ARG:H    | 11                  | 0.17     | 0.03                | 0.17       |
| (1,146) | 1:9:A:ARG:HD3   | 1:9:A:ARG:H    | 11                  | 0.17     | 0.03                | 0.17       |
| (1,27)  | 1:3:A:ARG:HG2   | 1:4:A:LEU:HD11 | 11                  | 0.17     | 0.02                | 0.17       |
| (1,27)  | 1:3:A:ARG:HG2   | 1:4:A:LEU:HD12 | 11                  | 0.17     | 0.02                | 0.17       |
| (1,27)  | 1:3:A:ARG:HG2   | 1:4:A:LEU:HD13 | 11                  | 0.17     | 0.02                | 0.17       |
| (1,27)  | 1:3:A:ARG:HG2   | 1:4:A:LEU:HD21 | 11                  | 0.17     | 0.02                | 0.17       |
| (1,27)  | 1:3:A:ARG:HG2   | 1:4:A:LEU:HD22 | 11                  | 0.17     | 0.02                | 0.17       |
| (1,27)  | 1:3:A:ARG:HG2   | 1:4:A:LEU:HD23 | 11                  | 0.17     | 0.02                | 0.17       |
| (1,27)  | 1:3:A:ARG:HG3   | 1:4:A:LEU:HD11 | 11                  | 0.17     | 0.02                | 0.17       |
| (1,27)  | 1:3:A:ARG:HG3   | 1:4:A:LEU:HD12 | 11                  | 0.17     | 0.02                | 0.17       |
| (1,27)  | 1:3:A:ARG:HG3   | 1:4:A:LEU:HD13 | 11                  | 0.17     | 0.02                | 0.17       |
| (1,27)  | 1:3:A:ARG:HG3   | 1:4:A:LEU:HD21 | 11                  | 0.17     | 0.02                | 0.17       |
| (1,27)  | 1:3:A:ARG:HG3   | 1:4:A:LEU:HD22 | 11                  | 0.17     | 0.02                | 0.17       |
| (1,27)  | 1:3:A:ARG:HG3   | 1:4:A:LEU:HD23 | 11                  | 0.17     | 0.02                | 0.17       |
| (1,203) | 1:13:A:LEU:HD11 | 1:15:A:ARG:HA  | 11                  | 0.16     | 0.03                | 0.18       |
| (1,203) | 1:13:A:LEU:HD12 | 1:15:A:ARG:HA  | 11                  | 0.16     | 0.03                | 0.18       |
| (1,203) | 1:13:A:LEU:HD13 | 1:15:A:ARG:HA  | 11                  | 0.16     | 0.03                | 0.18       |
| (1,203) | 1:13:A:LEU:HD21 | 1:15:A:ARG:HA  | 11                  | 0.16     | 0.03                | 0.18       |
| (1,203) | 1:13:A:LEU:HD22 | 1:15:A:ARG:HA  | 11                  | 0.16     | 0.03                | 0.18       |
| (1,203) | 1:13:A:LEU:HD23 | 1:15:A:ARG:HA  | 11                  | 0.16     | 0.03                | 0.18       |
| (1,240) | 1:16:A:LYS:HG2  | 1:16:A:LYS:H   | 11                  | 0.14     | 0.01                | 0.14       |
| (1,240) | 1:16:A:LYS:HG3  | 1:16:A:LYS:H   | 11                  | 0.14     | 0.01                | 0.14       |
| (1,177) | 1:12:A:ILE:HD11 | 1:12:A:ILE:H   | 8                   | 0.33     | 0.03                | 0.35       |
| (1,177) | 1:12:A:ILE:HD12 | 1:12:A:ILE:H   | 8                   | 0.33     | 0.03                | 0.35       |
| (1,177) | 1:12:A:ILE:HD13 | 1:12:A:ILE:H   | 8                   | 0.33     | 0.03                | 0.35       |
| (1,154) | 1:9:A:ARG:HG2   | 1:13:A:LEU:H   | 8                   | 0.15     | 0.05                | 0.12       |
| (1,154) | 1:9:A:ARG:HG3   | 1:13:A:LEU:H   | 8                   | 0.15     | 0.05                | 0.12       |
| (2,1)   | 1:12:A:ILE:HG22 | 1:13:A:LEU:H   | 7                   | 0.17     | 0.03                | 0.16       |
| (2,1)   | 1:12:A:ILE:HG23 | 1:13:A:LEU:H   | 7                   | 0.17     | 0.03                | 0.16       |
| (2,1)   | 1:12:A:ILE:HG21 | 1:13:A:LEU:H   | 7                   | 0.17     | 0.03                | 0.16       |
| (1,187) | 1:12:A:ILE:HG12 | 1:13:A:LEU:H   | 7                   | 0.12     | 0.01                | 0.12       |
| (1,187) | 1:12:A:ILE:HG13 | 1:13:A:LEU:H   | 7                   | 0.12     | 0.01                | 0.12       |
| (1,217) | 1:14:A:GLN:HA   | 1:16:A:LYS:H   | 6                   | 0.19     | 0.01                | 0.18       |

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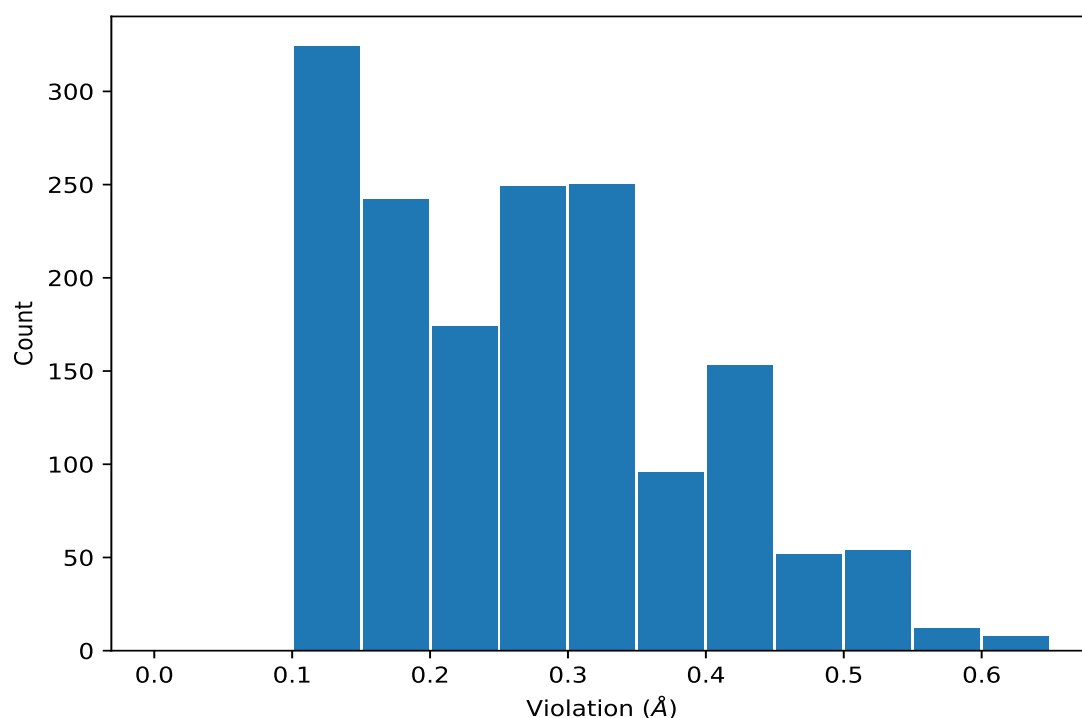
| Key     | Atom-1         | Atom-2        | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|----------------|---------------|---------------------|----------|---------------------|------------|
| (1,232) | 1:15:A:ARG:HA  | 1:17:A:LYS:H  | 6                   | 0.12     | 0.01                | 0.12       |
| (1,250) | 1:17:A:LYS:HG2 | 1:17:A:LYS:H  | 6                   | 0.12     | 0.03                | 0.12       |
| (1,250) | 1:17:A:LYS:HG3 | 1:17:A:LYS:H  | 6                   | 0.12     | 0.03                | 0.12       |
| (1,19)  | 1:3:A:ARG:HD2  | 1:3:A:ARG:HE  | 6                   | 0.11     | 0.0                 | 0.11       |
| (1,19)  | 1:3:A:ARG:HD3  | 1:3:A:ARG:HE  | 6                   | 0.11     | 0.0                 | 0.11       |
| (1,241) | 1:16:A:LYS:HA  | 1:17:A:LYS:H  | 6                   | 0.1      | 0.01                | 0.1        |
| (1,100) | 1:6:A:LYS:HG2  | 1:7:A:PHE:HB2 | 5                   | 0.53     | 0.02                | 0.53       |
| (1,100) | 1:6:A:LYS:HG2  | 1:7:A:PHE:HB3 | 5                   | 0.53     | 0.02                | 0.53       |
| (1,100) | 1:6:A:LYS:HG3  | 1:7:A:PHE:HB2 | 5                   | 0.53     | 0.02                | 0.53       |
| (1,100) | 1:6:A:LYS:HG3  | 1:7:A:PHE:HB3 | 5                   | 0.53     | 0.02                | 0.53       |
| (1,102) | 1:6:A:LYS:H    | 1:7:A:PHE:H   | 3                   | 0.11     | 0.0                 | 0.11       |
| (1,188) | 1:12:A:ILE:H   | 1:13:A:LEU:H  | 2                   | 0.26     | 0.02                | 0.26       |
| (1,65)  | 1:4:A:LEU:HD11 | 1:8:A:PHE:HZ  | 2                   | 0.13     | 0.02                | 0.13       |
| (1,65)  | 1:4:A:LEU:HD12 | 1:8:A:PHE:HZ  | 2                   | 0.13     | 0.02                | 0.13       |
| (1,65)  | 1:4:A:LEU:HD13 | 1:8:A:PHE:HZ  | 2                   | 0.13     | 0.02                | 0.13       |
| (1,65)  | 1:4:A:LEU:HD21 | 1:8:A:PHE:HZ  | 2                   | 0.13     | 0.02                | 0.13       |
| (1,65)  | 1:4:A:LEU:HD22 | 1:8:A:PHE:HZ  | 2                   | 0.13     | 0.02                | 0.13       |
| (1,65)  | 1:4:A:LEU:HD23 | 1:8:A:PHE:HZ  | 2                   | 0.13     | 0.02                | 0.13       |
| (1,28)  | 1:3:A:ARG:H    | 1:4:A:LEU:H   | 2                   | 0.12     | 0.02                | 0.12       |

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

## 9.5 All violated distance restraints ⓘ

### 9.5.1 Histogram : Distribution of distance violations ⓘ

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) |
|--------|---------------|---------------|----------|---------------|
| (1,99) | 1:6:A:LYS:HD2 | 1:7:A:PHE:HB2 | 9        | 0.62          |
| (1,99) | 1:6:A:LYS:HD2 | 1:7:A:PHE:HB3 | 9        | 0.62          |
| (1,99) | 1:6:A:LYS:HD3 | 1:7:A:PHE:HB2 | 9        | 0.62          |
| (1,99) | 1:6:A:LYS:HD3 | 1:7:A:PHE:HB3 | 9        | 0.62          |
| (1,99) | 1:6:A:LYS:HD2 | 1:7:A:PHE:HB2 | 10       | 0.62          |
| (1,99) | 1:6:A:LYS:HD2 | 1:7:A:PHE:HB3 | 10       | 0.62          |
| (1,99) | 1:6:A:LYS:HD3 | 1:7:A:PHE:HB2 | 10       | 0.62          |
| (1,99) | 1:6:A:LYS:HD3 | 1:7:A:PHE:HB3 | 10       | 0.62          |
| (1,99) | 1:6:A:LYS:HD2 | 1:7:A:PHE:HB2 | 3        | 0.59          |
| (1,99) | 1:6:A:LYS:HD2 | 1:7:A:PHE:HB3 | 3        | 0.59          |
| (1,99) | 1:6:A:LYS:HD3 | 1:7:A:PHE:HB2 | 3        | 0.59          |
| (1,99) | 1:6:A:LYS:HD3 | 1:7:A:PHE:HB3 | 3        | 0.59          |
| (1,99) | 1:6:A:LYS:HD2 | 1:7:A:PHE:HB2 | 16       | 0.58          |
| (1,99) | 1:6:A:LYS:HD2 | 1:7:A:PHE:HB3 | 16       | 0.58          |
| (1,99) | 1:6:A:LYS:HD3 | 1:7:A:PHE:HB2 | 16       | 0.58          |
| (1,99) | 1:6:A:LYS:HD3 | 1:7:A:PHE:HB3 | 16       | 0.58          |

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| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,100) | 1:6:A:LYS:HG2 | 1:7:A:PHE:HB2 | 7        | 0.56          |
| (1,100) | 1:6:A:LYS:HG2 | 1:7:A:PHE:HB3 | 7        | 0.56          |
| (1,100) | 1:6:A:LYS:HG3 | 1:7:A:PHE:HB2 | 7        | 0.56          |
| (1,100) | 1:6:A:LYS:HG3 | 1:7:A:PHE:HB3 | 7        | 0.56          |
| (1,120) | 1:8:A:PHE:HA  | 1:8:A:PHE:HE1 | 3        | 0.54          |
| (1,120) | 1:8:A:PHE:HA  | 1:8:A:PHE:HE2 | 3        | 0.54          |
| (1,120) | 1:8:A:PHE:HA  | 1:8:A:PHE:HE1 | 4        | 0.54          |
| (1,120) | 1:8:A:PHE:HA  | 1:8:A:PHE:HE2 | 4        | 0.54          |
| (1,120) | 1:8:A:PHE:HA  | 1:8:A:PHE:HE1 | 13       | 0.54          |
| (1,120) | 1:8:A:PHE:HA  | 1:8:A:PHE:HE2 | 13       | 0.54          |
| (1,100) | 1:6:A:LYS:HG2 | 1:7:A:PHE:HB2 | 11       | 0.54          |
| (1,100) | 1:6:A:LYS:HG2 | 1:7:A:PHE:HB3 | 11       | 0.54          |
| (1,100) | 1:6:A:LYS:HG3 | 1:7:A:PHE:HB2 | 11       | 0.54          |
| (1,100) | 1:6:A:LYS:HG3 | 1:7:A:PHE:HB3 | 11       | 0.54          |
| (1,120) | 1:8:A:PHE:HA  | 1:8:A:PHE:HE1 | 2        | 0.53          |
| (1,120) | 1:8:A:PHE:HA  | 1:8:A:PHE:HE2 | 2        | 0.53          |
| (1,120) | 1:8:A:PHE:HA  | 1:8:A:PHE:HE1 | 15       | 0.53          |
| (1,120) | 1:8:A:PHE:HA  | 1:8:A:PHE:HE2 | 15       | 0.53          |
| (1,120) | 1:8:A:PHE:HA  | 1:8:A:PHE:HE1 | 20       | 0.53          |
| (1,120) | 1:8:A:PHE:HA  | 1:8:A:PHE:HE2 | 20       | 0.53          |
| (1,100) | 1:6:A:LYS:HG2 | 1:7:A:PHE:HB2 | 14       | 0.53          |
| (1,100) | 1:6:A:LYS:HG2 | 1:7:A:PHE:HB3 | 14       | 0.53          |
| (1,100) | 1:6:A:LYS:HG3 | 1:7:A:PHE:HB2 | 14       | 0.53          |
| (1,100) | 1:6:A:LYS:HG3 | 1:7:A:PHE:HB3 | 14       | 0.53          |
| (1,120) | 1:8:A:PHE:HA  | 1:8:A:PHE:HE1 | 1        | 0.52          |
| (1,120) | 1:8:A:PHE:HA  | 1:8:A:PHE:HE2 | 1        | 0.52          |
| (1,120) | 1:8:A:PHE:HA  | 1:8:A:PHE:HE1 | 5        | 0.52          |
| (1,120) | 1:8:A:PHE:HA  | 1:8:A:PHE:HE2 | 5        | 0.52          |
| (1,120) | 1:8:A:PHE:HA  | 1:8:A:PHE:HE1 | 8        | 0.52          |
| (1,120) | 1:8:A:PHE:HA  | 1:8:A:PHE:HE2 | 8        | 0.52          |
| (1,100) | 1:6:A:LYS:HG2 | 1:7:A:PHE:HB2 | 18       | 0.52          |
| (1,100) | 1:6:A:LYS:HG2 | 1:7:A:PHE:HB3 | 18       | 0.52          |
| (1,100) | 1:6:A:LYS:HG3 | 1:7:A:PHE:HB2 | 18       | 0.52          |
| (1,100) | 1:6:A:LYS:HG3 | 1:7:A:PHE:HB3 | 18       | 0.52          |
| (1,99)  | 1:6:A:LYS:HD2 | 1:7:A:PHE:HB2 | 20       | 0.52          |
| (1,99)  | 1:6:A:LYS:HD2 | 1:7:A:PHE:HB3 | 20       | 0.52          |
| (1,99)  | 1:6:A:LYS:HD3 | 1:7:A:PHE:HB2 | 20       | 0.52          |
| (1,99)  | 1:6:A:LYS:HD3 | 1:7:A:PHE:HB3 | 20       | 0.52          |
| (1,120) | 1:8:A:PHE:HA  | 1:8:A:PHE:HE1 | 10       | 0.51          |
| (1,120) | 1:8:A:PHE:HA  | 1:8:A:PHE:HE2 | 10       | 0.51          |
| (1,120) | 1:8:A:PHE:HA  | 1:8:A:PHE:HE1 | 9        | 0.5           |
| (1,120) | 1:8:A:PHE:HA  | 1:8:A:PHE:HE2 | 9        | 0.5           |

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| Key     | Atom-1         | Atom-2        | Model ID | Violation (Å) |
|---------|----------------|---------------|----------|---------------|
| (1,99)  | 1:6:A:LYS:HD2  | 1:7:A:PHE:HB2 | 6        | 0.5           |
| (1,99)  | 1:6:A:LYS:HD2  | 1:7:A:PHE:HB3 | 6        | 0.5           |
| (1,99)  | 1:6:A:LYS:HD3  | 1:7:A:PHE:HB2 | 6        | 0.5           |
| (1,99)  | 1:6:A:LYS:HD3  | 1:7:A:PHE:HB3 | 6        | 0.5           |
| (1,53)  | 1:4:A:LEU:HD11 | 1:6:A:LYS:HB2 | 6        | 0.5           |
| (1,53)  | 1:4:A:LEU:HD11 | 1:6:A:LYS:HB3 | 6        | 0.5           |
| (1,53)  | 1:4:A:LEU:HD12 | 1:6:A:LYS:HB2 | 6        | 0.5           |
| (1,53)  | 1:4:A:LEU:HD12 | 1:6:A:LYS:HB3 | 6        | 0.5           |
| (1,53)  | 1:4:A:LEU:HD13 | 1:6:A:LYS:HB2 | 6        | 0.5           |
| (1,53)  | 1:4:A:LEU:HD13 | 1:6:A:LYS:HB3 | 6        | 0.5           |
| (1,53)  | 1:4:A:LEU:HD21 | 1:6:A:LYS:HB2 | 6        | 0.5           |
| (1,53)  | 1:4:A:LEU:HD21 | 1:6:A:LYS:HB3 | 6        | 0.5           |
| (1,53)  | 1:4:A:LEU:HD22 | 1:6:A:LYS:HB2 | 6        | 0.5           |
| (1,53)  | 1:4:A:LEU:HD22 | 1:6:A:LYS:HB3 | 6        | 0.5           |
| (1,53)  | 1:4:A:LEU:HD23 | 1:6:A:LYS:HB2 | 6        | 0.5           |
| (1,53)  | 1:4:A:LEU:HD23 | 1:6:A:LYS:HB3 | 6        | 0.5           |
| (1,120) | 1:8:A:PHE:HA   | 1:8:A:PHE:HE1 | 14       | 0.49          |
| (1,120) | 1:8:A:PHE:HA   | 1:8:A:PHE:HE2 | 14       | 0.49          |
| (1,100) | 1:6:A:LYS:HG2  | 1:7:A:PHE:HB2 | 12       | 0.49          |
| (1,100) | 1:6:A:LYS:HG2  | 1:7:A:PHE:HB3 | 12       | 0.49          |
| (1,100) | 1:6:A:LYS:HG3  | 1:7:A:PHE:HB2 | 12       | 0.49          |
| (1,100) | 1:6:A:LYS:HG3  | 1:7:A:PHE:HB3 | 12       | 0.49          |
| (1,99)  | 1:6:A:LYS:HD2  | 1:7:A:PHE:HB2 | 8        | 0.48          |
| (1,99)  | 1:6:A:LYS:HD2  | 1:7:A:PHE:HB3 | 8        | 0.48          |
| (1,99)  | 1:6:A:LYS:HD3  | 1:7:A:PHE:HB2 | 8        | 0.48          |
| (1,99)  | 1:6:A:LYS:HD3  | 1:7:A:PHE:HB3 | 8        | 0.48          |
| (1,99)  | 1:6:A:LYS:HD2  | 1:7:A:PHE:HB2 | 17       | 0.48          |
| (1,99)  | 1:6:A:LYS:HD2  | 1:7:A:PHE:HB3 | 17       | 0.48          |
| (1,99)  | 1:6:A:LYS:HD3  | 1:7:A:PHE:HB2 | 17       | 0.48          |
| (1,99)  | 1:6:A:LYS:HD3  | 1:7:A:PHE:HB3 | 17       | 0.48          |
| (1,120) | 1:8:A:PHE:HA   | 1:8:A:PHE:HE1 | 11       | 0.47          |
| (1,120) | 1:8:A:PHE:HA   | 1:8:A:PHE:HE2 | 11       | 0.47          |
| (1,120) | 1:8:A:PHE:HA   | 1:8:A:PHE:HE1 | 16       | 0.47          |
| (1,120) | 1:8:A:PHE:HA   | 1:8:A:PHE:HE2 | 16       | 0.47          |
| (1,99)  | 1:6:A:LYS:HD2  | 1:7:A:PHE:HB2 | 1        | 0.47          |
| (1,99)  | 1:6:A:LYS:HD2  | 1:7:A:PHE:HB3 | 1        | 0.47          |
| (1,99)  | 1:6:A:LYS:HD3  | 1:7:A:PHE:HB2 | 1        | 0.47          |
| (1,99)  | 1:6:A:LYS:HD3  | 1:7:A:PHE:HB3 | 1        | 0.47          |
| (1,99)  | 1:6:A:LYS:HD2  | 1:7:A:PHE:HB2 | 2        | 0.47          |
| (1,99)  | 1:6:A:LYS:HD2  | 1:7:A:PHE:HB3 | 2        | 0.47          |
| (1,99)  | 1:6:A:LYS:HD3  | 1:7:A:PHE:HB2 | 2        | 0.47          |
| (1,99)  | 1:6:A:LYS:HD3  | 1:7:A:PHE:HB3 | 2        | 0.47          |

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| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,99)  | 1:6:A:LYS:HD2 | 1:7:A:PHE:HB2 | 13       | 0.47          |
| (1,99)  | 1:6:A:LYS:HD2 | 1:7:A:PHE:HB3 | 13       | 0.47          |
| (1,99)  | 1:6:A:LYS:HD3 | 1:7:A:PHE:HB2 | 13       | 0.47          |
| (1,99)  | 1:6:A:LYS:HD3 | 1:7:A:PHE:HB3 | 13       | 0.47          |
| (1,99)  | 1:6:A:LYS:HD2 | 1:7:A:PHE:HB2 | 4        | 0.46          |
| (1,99)  | 1:6:A:LYS:HD2 | 1:7:A:PHE:HB3 | 4        | 0.46          |
| (1,99)  | 1:6:A:LYS:HD3 | 1:7:A:PHE:HB2 | 4        | 0.46          |
| (1,99)  | 1:6:A:LYS:HD3 | 1:7:A:PHE:HB3 | 4        | 0.46          |
| (1,99)  | 1:6:A:LYS:HD2 | 1:7:A:PHE:HB2 | 5        | 0.46          |
| (1,99)  | 1:6:A:LYS:HD2 | 1:7:A:PHE:HB3 | 5        | 0.46          |
| (1,99)  | 1:6:A:LYS:HD3 | 1:7:A:PHE:HB2 | 5        | 0.46          |
| (1,99)  | 1:6:A:LYS:HD3 | 1:7:A:PHE:HB3 | 5        | 0.46          |
| (1,99)  | 1:6:A:LYS:HD2 | 1:7:A:PHE:HB2 | 15       | 0.46          |
| (1,99)  | 1:6:A:LYS:HD2 | 1:7:A:PHE:HB3 | 15       | 0.46          |
| (1,99)  | 1:6:A:LYS:HD3 | 1:7:A:PHE:HB2 | 15       | 0.46          |
| (1,99)  | 1:6:A:LYS:HD3 | 1:7:A:PHE:HB3 | 15       | 0.46          |
| (1,99)  | 1:6:A:LYS:HD2 | 1:7:A:PHE:HB2 | 19       | 0.46          |
| (1,99)  | 1:6:A:LYS:HD2 | 1:7:A:PHE:HB3 | 19       | 0.46          |
| (1,99)  | 1:6:A:LYS:HD3 | 1:7:A:PHE:HB2 | 19       | 0.46          |
| (1,99)  | 1:6:A:LYS:HD3 | 1:7:A:PHE:HB3 | 19       | 0.46          |
| (1,120) | 1:8:A:PHE:HA  | 1:8:A:PHE:HE1 | 7        | 0.45          |
| (1,120) | 1:8:A:PHE:HA  | 1:8:A:PHE:HE2 | 7        | 0.45          |
| (1,120) | 1:8:A:PHE:HA  | 1:8:A:PHE:HE1 | 19       | 0.45          |
| (1,120) | 1:8:A:PHE:HA  | 1:8:A:PHE:HE2 | 19       | 0.45          |
| (1,26)  | 1:3:A:ARG:HB2 | 1:4:A:LEU:H   | 6        | 0.45          |
| (1,26)  | 1:3:A:ARG:HB3 | 1:4:A:LEU:H   | 6        | 0.45          |
| (1,115) | 1:7:A:PHE:HB2 | 1:7:A:PHE:HZ  | 1        | 0.44          |
| (1,115) | 1:7:A:PHE:HB3 | 1:7:A:PHE:HZ  | 1        | 0.44          |
| (1,115) | 1:7:A:PHE:HB2 | 1:7:A:PHE:HZ  | 2        | 0.44          |
| (1,115) | 1:7:A:PHE:HB3 | 1:7:A:PHE:HZ  | 2        | 0.44          |
| (1,115) | 1:7:A:PHE:HB2 | 1:7:A:PHE:HZ  | 3        | 0.44          |
| (1,115) | 1:7:A:PHE:HB3 | 1:7:A:PHE:HZ  | 3        | 0.44          |
| (1,115) | 1:7:A:PHE:HB2 | 1:7:A:PHE:HZ  | 4        | 0.44          |
| (1,115) | 1:7:A:PHE:HB3 | 1:7:A:PHE:HZ  | 4        | 0.44          |
| (1,115) | 1:7:A:PHE:HB2 | 1:7:A:PHE:HZ  | 5        | 0.44          |
| (1,115) | 1:7:A:PHE:HB3 | 1:7:A:PHE:HZ  | 5        | 0.44          |
| (1,115) | 1:7:A:PHE:HB2 | 1:7:A:PHE:HZ  | 6        | 0.44          |
| (1,115) | 1:7:A:PHE:HB3 | 1:7:A:PHE:HZ  | 6        | 0.44          |
| (1,115) | 1:7:A:PHE:HB2 | 1:7:A:PHE:HZ  | 7        | 0.44          |
| (1,115) | 1:7:A:PHE:HB3 | 1:7:A:PHE:HZ  | 7        | 0.44          |
| (1,115) | 1:7:A:PHE:HB2 | 1:7:A:PHE:HZ  | 8        | 0.44          |
| (1,115) | 1:7:A:PHE:HB3 | 1:7:A:PHE:HZ  | 8        | 0.44          |

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| Key     | Atom-1        | Atom-2       | Model ID | Violation (Å) |
|---------|---------------|--------------|----------|---------------|
| (1,115) | 1:7:A:PHE:HB2 | 1:7:A:PHE:HZ | 9        | 0.44          |
| (1,115) | 1:7:A:PHE:HB3 | 1:7:A:PHE:HZ | 9        | 0.44          |
| (1,115) | 1:7:A:PHE:HB2 | 1:7:A:PHE:HZ | 10       | 0.44          |
| (1,115) | 1:7:A:PHE:HB3 | 1:7:A:PHE:HZ | 10       | 0.44          |
| (1,115) | 1:7:A:PHE:HB2 | 1:7:A:PHE:HZ | 11       | 0.44          |
| (1,115) | 1:7:A:PHE:HB3 | 1:7:A:PHE:HZ | 11       | 0.44          |
| (1,115) | 1:7:A:PHE:HB2 | 1:7:A:PHE:HZ | 12       | 0.44          |
| (1,115) | 1:7:A:PHE:HB3 | 1:7:A:PHE:HZ | 12       | 0.44          |
| (1,115) | 1:7:A:PHE:HB2 | 1:7:A:PHE:HZ | 13       | 0.44          |
| (1,115) | 1:7:A:PHE:HB3 | 1:7:A:PHE:HZ | 13       | 0.44          |
| (1,115) | 1:7:A:PHE:HB2 | 1:7:A:PHE:HZ | 14       | 0.44          |
| (1,115) | 1:7:A:PHE:HB3 | 1:7:A:PHE:HZ | 14       | 0.44          |
| (1,115) | 1:7:A:PHE:HB2 | 1:7:A:PHE:HZ | 15       | 0.44          |
| (1,115) | 1:7:A:PHE:HB3 | 1:7:A:PHE:HZ | 15       | 0.44          |
| (1,115) | 1:7:A:PHE:HB2 | 1:7:A:PHE:HZ | 16       | 0.44          |
| (1,115) | 1:7:A:PHE:HB3 | 1:7:A:PHE:HZ | 16       | 0.44          |
| (1,115) | 1:7:A:PHE:HB2 | 1:7:A:PHE:HZ | 17       | 0.44          |
| (1,115) | 1:7:A:PHE:HB3 | 1:7:A:PHE:HZ | 17       | 0.44          |
| (1,115) | 1:7:A:PHE:HB2 | 1:7:A:PHE:HZ | 18       | 0.44          |
| (1,115) | 1:7:A:PHE:HB3 | 1:7:A:PHE:HZ | 18       | 0.44          |
| (1,115) | 1:7:A:PHE:HB2 | 1:7:A:PHE:HZ | 19       | 0.44          |
| (1,115) | 1:7:A:PHE:HB3 | 1:7:A:PHE:HZ | 19       | 0.44          |
| (1,115) | 1:7:A:PHE:HB2 | 1:7:A:PHE:HZ | 20       | 0.44          |
| (1,115) | 1:7:A:PHE:HB3 | 1:7:A:PHE:HZ | 20       | 0.44          |
| (1,112) | 1:7:A:PHE:HB2 | 1:7:A:PHE:HZ | 1        | 0.44          |
| (1,112) | 1:7:A:PHE:HB3 | 1:7:A:PHE:HZ | 1        | 0.44          |
| (1,112) | 1:7:A:PHE:HB2 | 1:7:A:PHE:HZ | 2        | 0.44          |
| (1,112) | 1:7:A:PHE:HB3 | 1:7:A:PHE:HZ | 2        | 0.44          |
| (1,112) | 1:7:A:PHE:HB2 | 1:7:A:PHE:HZ | 3        | 0.44          |
| (1,112) | 1:7:A:PHE:HB3 | 1:7:A:PHE:HZ | 3        | 0.44          |
| (1,112) | 1:7:A:PHE:HB2 | 1:7:A:PHE:HZ | 4        | 0.44          |
| (1,112) | 1:7:A:PHE:HB3 | 1:7:A:PHE:HZ | 4        | 0.44          |
| (1,112) | 1:7:A:PHE:HB2 | 1:7:A:PHE:HZ | 5        | 0.44          |
| (1,112) | 1:7:A:PHE:HB3 | 1:7:A:PHE:HZ | 5        | 0.44          |
| (1,112) | 1:7:A:PHE:HB2 | 1:7:A:PHE:HZ | 6        | 0.44          |
| (1,112) | 1:7:A:PHE:HB3 | 1:7:A:PHE:HZ | 6        | 0.44          |
| (1,112) | 1:7:A:PHE:HB2 | 1:7:A:PHE:HZ | 7        | 0.44          |
| (1,112) | 1:7:A:PHE:HB3 | 1:7:A:PHE:HZ | 7        | 0.44          |
| (1,112) | 1:7:A:PHE:HB2 | 1:7:A:PHE:HZ | 8        | 0.44          |
| (1,112) | 1:7:A:PHE:HB3 | 1:7:A:PHE:HZ | 8        | 0.44          |
| (1,112) | 1:7:A:PHE:HB2 | 1:7:A:PHE:HZ | 9        | 0.44          |
| (1,112) | 1:7:A:PHE:HB3 | 1:7:A:PHE:HZ | 9        | 0.44          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,112) | 1:7:A:PHE:HB2  | 1:7:A:PHE:HZ   | 10       | 0.44          |
| (1,112) | 1:7:A:PHE:HB3  | 1:7:A:PHE:HZ   | 10       | 0.44          |
| (1,112) | 1:7:A:PHE:HB2  | 1:7:A:PHE:HZ   | 11       | 0.44          |
| (1,112) | 1:7:A:PHE:HB3  | 1:7:A:PHE:HZ   | 11       | 0.44          |
| (1,112) | 1:7:A:PHE:HB2  | 1:7:A:PHE:HZ   | 12       | 0.44          |
| (1,112) | 1:7:A:PHE:HB3  | 1:7:A:PHE:HZ   | 12       | 0.44          |
| (1,112) | 1:7:A:PHE:HB2  | 1:7:A:PHE:HZ   | 13       | 0.44          |
| (1,112) | 1:7:A:PHE:HB3  | 1:7:A:PHE:HZ   | 13       | 0.44          |
| (1,112) | 1:7:A:PHE:HB2  | 1:7:A:PHE:HZ   | 14       | 0.44          |
| (1,112) | 1:7:A:PHE:HB3  | 1:7:A:PHE:HZ   | 14       | 0.44          |
| (1,112) | 1:7:A:PHE:HB2  | 1:7:A:PHE:HZ   | 15       | 0.44          |
| (1,112) | 1:7:A:PHE:HB3  | 1:7:A:PHE:HZ   | 15       | 0.44          |
| (1,112) | 1:7:A:PHE:HB2  | 1:7:A:PHE:HZ   | 16       | 0.44          |
| (1,112) | 1:7:A:PHE:HB3  | 1:7:A:PHE:HZ   | 16       | 0.44          |
| (1,112) | 1:7:A:PHE:HB2  | 1:7:A:PHE:HZ   | 17       | 0.44          |
| (1,112) | 1:7:A:PHE:HB3  | 1:7:A:PHE:HZ   | 17       | 0.44          |
| (1,112) | 1:7:A:PHE:HB2  | 1:7:A:PHE:HZ   | 18       | 0.44          |
| (1,112) | 1:7:A:PHE:HB3  | 1:7:A:PHE:HZ   | 18       | 0.44          |
| (1,112) | 1:7:A:PHE:HB2  | 1:7:A:PHE:HZ   | 19       | 0.44          |
| (1,112) | 1:7:A:PHE:HB3  | 1:7:A:PHE:HZ   | 19       | 0.44          |
| (1,112) | 1:7:A:PHE:HB2  | 1:7:A:PHE:HZ   | 20       | 0.44          |
| (1,112) | 1:7:A:PHE:HB3  | 1:7:A:PHE:HZ   | 20       | 0.44          |
| (1,53)  | 1:4:A:LEU:HD11 | 1:6:A:LYS:HB2  | 11       | 0.44          |
| (1,53)  | 1:4:A:LEU:HD11 | 1:6:A:LYS:HB3  | 11       | 0.44          |
| (1,53)  | 1:4:A:LEU:HD12 | 1:6:A:LYS:HB2  | 11       | 0.44          |
| (1,53)  | 1:4:A:LEU:HD12 | 1:6:A:LYS:HB3  | 11       | 0.44          |
| (1,53)  | 1:4:A:LEU:HD13 | 1:6:A:LYS:HB2  | 11       | 0.44          |
| (1,53)  | 1:4:A:LEU:HD13 | 1:6:A:LYS:HB3  | 11       | 0.44          |
| (1,53)  | 1:4:A:LEU:HD21 | 1:6:A:LYS:HB2  | 11       | 0.44          |
| (1,53)  | 1:4:A:LEU:HD21 | 1:6:A:LYS:HB3  | 11       | 0.44          |
| (1,53)  | 1:4:A:LEU:HD22 | 1:6:A:LYS:HB2  | 11       | 0.44          |
| (1,53)  | 1:4:A:LEU:HD22 | 1:6:A:LYS:HB3  | 11       | 0.44          |
| (1,53)  | 1:4:A:LEU:HD23 | 1:6:A:LYS:HB2  | 11       | 0.44          |
| (1,53)  | 1:4:A:LEU:HD23 | 1:6:A:LYS:HB3  | 11       | 0.44          |
| (1,215) | 1:14:A:GLN:H   | 1:15:A:ARG:HA  | 4        | 0.43          |
| (1,132) | 1:8:A:PHE:HB2  | 1:11:A:PHE:HB2 | 12       | 0.43          |
| (1,132) | 1:8:A:PHE:HB2  | 1:11:A:PHE:HB3 | 12       | 0.43          |
| (1,132) | 1:8:A:PHE:HB3  | 1:11:A:PHE:HB2 | 12       | 0.43          |
| (1,132) | 1:8:A:PHE:HB3  | 1:11:A:PHE:HB3 | 12       | 0.43          |
| (1,120) | 1:8:A:PHE:HA   | 1:8:A:PHE:HE1  | 6        | 0.43          |
| (1,120) | 1:8:A:PHE:HA   | 1:8:A:PHE:HE2  | 6        | 0.43          |
| (1,53)  | 1:4:A:LEU:HD11 | 1:6:A:LYS:HB2  | 18       | 0.43          |

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| Key     | Atom-1         | Atom-2        | Model ID | Violation (Å) |
|---------|----------------|---------------|----------|---------------|
| (1,53)  | 1:4:A:LEU:HD11 | 1:6:A:LYS:HB3 | 18       | 0.43          |
| (1,53)  | 1:4:A:LEU:HD12 | 1:6:A:LYS:HB2 | 18       | 0.43          |
| (1,53)  | 1:4:A:LEU:HD12 | 1:6:A:LYS:HB3 | 18       | 0.43          |
| (1,53)  | 1:4:A:LEU:HD13 | 1:6:A:LYS:HB2 | 18       | 0.43          |
| (1,53)  | 1:4:A:LEU:HD13 | 1:6:A:LYS:HB3 | 18       | 0.43          |
| (1,53)  | 1:4:A:LEU:HD21 | 1:6:A:LYS:HB2 | 18       | 0.43          |
| (1,53)  | 1:4:A:LEU:HD21 | 1:6:A:LYS:HB3 | 18       | 0.43          |
| (1,53)  | 1:4:A:LEU:HD22 | 1:6:A:LYS:HB2 | 18       | 0.43          |
| (1,53)  | 1:4:A:LEU:HD22 | 1:6:A:LYS:HB3 | 18       | 0.43          |
| (1,53)  | 1:4:A:LEU:HD23 | 1:6:A:LYS:HB2 | 18       | 0.43          |
| (1,53)  | 1:4:A:LEU:HD23 | 1:6:A:LYS:HB3 | 18       | 0.43          |
| (1,53)  | 1:4:A:LEU:HD11 | 1:6:A:LYS:HB2 | 12       | 0.42          |
| (1,53)  | 1:4:A:LEU:HD11 | 1:6:A:LYS:HB3 | 12       | 0.42          |
| (1,53)  | 1:4:A:LEU:HD12 | 1:6:A:LYS:HB2 | 12       | 0.42          |
| (1,53)  | 1:4:A:LEU:HD12 | 1:6:A:LYS:HB3 | 12       | 0.42          |
| (1,53)  | 1:4:A:LEU:HD13 | 1:6:A:LYS:HB2 | 12       | 0.42          |
| (1,53)  | 1:4:A:LEU:HD13 | 1:6:A:LYS:HB3 | 12       | 0.42          |
| (1,53)  | 1:4:A:LEU:HD21 | 1:6:A:LYS:HB2 | 12       | 0.42          |
| (1,53)  | 1:4:A:LEU:HD21 | 1:6:A:LYS:HB3 | 12       | 0.42          |
| (1,53)  | 1:4:A:LEU:HD22 | 1:6:A:LYS:HB2 | 12       | 0.42          |
| (1,53)  | 1:4:A:LEU:HD22 | 1:6:A:LYS:HB3 | 12       | 0.42          |
| (1,53)  | 1:4:A:LEU:HD23 | 1:6:A:LYS:HB2 | 12       | 0.42          |
| (1,53)  | 1:4:A:LEU:HD23 | 1:6:A:LYS:HB3 | 12       | 0.42          |
| (1,26)  | 1:3:A:ARG:HB2  | 1:4:A:LEU:H   | 3        | 0.42          |
| (1,26)  | 1:3:A:ARG:HB3  | 1:4:A:LEU:H   | 3        | 0.42          |
| (1,53)  | 1:4:A:LEU:HD11 | 1:6:A:LYS:HB2 | 16       | 0.41          |
| (1,53)  | 1:4:A:LEU:HD11 | 1:6:A:LYS:HB3 | 16       | 0.41          |
| (1,53)  | 1:4:A:LEU:HD12 | 1:6:A:LYS:HB2 | 16       | 0.41          |
| (1,53)  | 1:4:A:LEU:HD12 | 1:6:A:LYS:HB3 | 16       | 0.41          |
| (1,53)  | 1:4:A:LEU:HD13 | 1:6:A:LYS:HB2 | 16       | 0.41          |
| (1,53)  | 1:4:A:LEU:HD13 | 1:6:A:LYS:HB3 | 16       | 0.41          |
| (1,53)  | 1:4:A:LEU:HD21 | 1:6:A:LYS:HB2 | 16       | 0.41          |
| (1,53)  | 1:4:A:LEU:HD21 | 1:6:A:LYS:HB3 | 16       | 0.41          |
| (1,53)  | 1:4:A:LEU:HD22 | 1:6:A:LYS:HB2 | 16       | 0.41          |
| (1,53)  | 1:4:A:LEU:HD22 | 1:6:A:LYS:HB3 | 16       | 0.41          |
| (1,53)  | 1:4:A:LEU:HD23 | 1:6:A:LYS:HB2 | 16       | 0.41          |
| (1,53)  | 1:4:A:LEU:HD23 | 1:6:A:LYS:HB3 | 16       | 0.41          |
| (1,139) | 1:9:A:ARG:HA   | 1:9:A:ARG:HD2 | 1        | 0.4           |
| (1,139) | 1:9:A:ARG:HA   | 1:9:A:ARG:HD3 | 1        | 0.4           |
| (1,120) | 1:8:A:PHE:HA   | 1:8:A:PHE:HE1 | 18       | 0.4           |
| (1,120) | 1:8:A:PHE:HA   | 1:8:A:PHE:HE2 | 18       | 0.4           |
| (1,53)  | 1:4:A:LEU:HD11 | 1:6:A:LYS:HB2 | 3        | 0.4           |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,53)  | 1:4:A:LEU:HD11 | 1:6:A:LYS:HB3  | 3        | 0.4           |
| (1,53)  | 1:4:A:LEU:HD12 | 1:6:A:LYS:HB2  | 3        | 0.4           |
| (1,53)  | 1:4:A:LEU:HD12 | 1:6:A:LYS:HB3  | 3        | 0.4           |
| (1,53)  | 1:4:A:LEU:HD13 | 1:6:A:LYS:HB2  | 3        | 0.4           |
| (1,53)  | 1:4:A:LEU:HD13 | 1:6:A:LYS:HB3  | 3        | 0.4           |
| (1,53)  | 1:4:A:LEU:HD21 | 1:6:A:LYS:HB2  | 3        | 0.4           |
| (1,53)  | 1:4:A:LEU:HD21 | 1:6:A:LYS:HB3  | 3        | 0.4           |
| (1,53)  | 1:4:A:LEU:HD22 | 1:6:A:LYS:HB2  | 3        | 0.4           |
| (1,53)  | 1:4:A:LEU:HD22 | 1:6:A:LYS:HB3  | 3        | 0.4           |
| (1,53)  | 1:4:A:LEU:HD23 | 1:6:A:LYS:HB2  | 3        | 0.4           |
| (1,53)  | 1:4:A:LEU:HD23 | 1:6:A:LYS:HB3  | 3        | 0.4           |
| (1,139) | 1:9:A:ARG:HA   | 1:9:A:ARG:HD2  | 2        | 0.39          |
| (1,139) | 1:9:A:ARG:HA   | 1:9:A:ARG:HD3  | 2        | 0.39          |
| (1,139) | 1:9:A:ARG:HA   | 1:9:A:ARG:HD2  | 13       | 0.39          |
| (1,139) | 1:9:A:ARG:HA   | 1:9:A:ARG:HD3  | 13       | 0.39          |
| (1,139) | 1:9:A:ARG:HA   | 1:9:A:ARG:HD2  | 15       | 0.39          |
| (1,139) | 1:9:A:ARG:HA   | 1:9:A:ARG:HD3  | 15       | 0.39          |
| (1,95)  | 1:6:A:LYS:HB2  | 1:7:A:PHE:HB2  | 10       | 0.39          |
| (1,95)  | 1:6:A:LYS:HB2  | 1:7:A:PHE:HB3  | 10       | 0.39          |
| (1,95)  | 1:6:A:LYS:HB3  | 1:7:A:PHE:HB2  | 10       | 0.39          |
| (1,95)  | 1:6:A:LYS:HB3  | 1:7:A:PHE:HB3  | 10       | 0.39          |
| (1,95)  | 1:6:A:LYS:HB2  | 1:7:A:PHE:HB2  | 14       | 0.39          |
| (1,95)  | 1:6:A:LYS:HB2  | 1:7:A:PHE:HB3  | 14       | 0.39          |
| (1,95)  | 1:6:A:LYS:HB3  | 1:7:A:PHE:HB2  | 14       | 0.39          |
| (1,95)  | 1:6:A:LYS:HB3  | 1:7:A:PHE:HB3  | 14       | 0.39          |
| (1,139) | 1:9:A:ARG:HA   | 1:9:A:ARG:HD2  | 5        | 0.38          |
| (1,139) | 1:9:A:ARG:HA   | 1:9:A:ARG:HD3  | 5        | 0.38          |
| (1,132) | 1:8:A:PHE:HB2  | 1:11:A:PHE:HB2 | 6        | 0.38          |
| (1,132) | 1:8:A:PHE:HB2  | 1:11:A:PHE:HB3 | 6        | 0.38          |
| (1,132) | 1:8:A:PHE:HB3  | 1:11:A:PHE:HB2 | 6        | 0.38          |
| (1,132) | 1:8:A:PHE:HB3  | 1:11:A:PHE:HB3 | 6        | 0.38          |
| (1,132) | 1:8:A:PHE:HB2  | 1:11:A:PHE:HB2 | 16       | 0.38          |
| (1,132) | 1:8:A:PHE:HB2  | 1:11:A:PHE:HB3 | 16       | 0.38          |
| (1,132) | 1:8:A:PHE:HB3  | 1:11:A:PHE:HB2 | 16       | 0.38          |
| (1,132) | 1:8:A:PHE:HB3  | 1:11:A:PHE:HB3 | 16       | 0.38          |
| (1,132) | 1:8:A:PHE:HB2  | 1:11:A:PHE:HB2 | 18       | 0.38          |
| (1,132) | 1:8:A:PHE:HB2  | 1:11:A:PHE:HB3 | 18       | 0.38          |
| (1,132) | 1:8:A:PHE:HB3  | 1:11:A:PHE:HB2 | 18       | 0.38          |
| (1,132) | 1:8:A:PHE:HB3  | 1:11:A:PHE:HB3 | 18       | 0.38          |
| (1,93)  | 1:6:A:LYS:HA   | 1:7:A:PHE:HB2  | 1        | 0.38          |
| (1,93)  | 1:6:A:LYS:HA   | 1:7:A:PHE:HB3  | 1        | 0.38          |
| (1,93)  | 1:6:A:LYS:HA   | 1:7:A:PHE:HB2  | 4        | 0.38          |

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| Key     | Atom-1          | Atom-2        | Model ID | Violation (Å) |
|---------|-----------------|---------------|----------|---------------|
| (1,93)  | 1:6:A:LYS:HA    | 1:7:A:PHE:HB3 | 4        | 0.38          |
| (1,93)  | 1:6:A:LYS:HA    | 1:7:A:PHE:HB2 | 5        | 0.38          |
| (1,93)  | 1:6:A:LYS:HA    | 1:7:A:PHE:HB3 | 5        | 0.38          |
| (1,93)  | 1:6:A:LYS:HA    | 1:7:A:PHE:HB2 | 6        | 0.38          |
| (1,93)  | 1:6:A:LYS:HA    | 1:7:A:PHE:HB3 | 6        | 0.38          |
| (1,93)  | 1:6:A:LYS:HA    | 1:7:A:PHE:HB2 | 8        | 0.38          |
| (1,93)  | 1:6:A:LYS:HA    | 1:7:A:PHE:HB3 | 8        | 0.38          |
| (1,139) | 1:9:A:ARG:HA    | 1:9:A:ARG:HD2 | 4        | 0.37          |
| (1,139) | 1:9:A:ARG:HA    | 1:9:A:ARG:HD3 | 4        | 0.37          |
| (1,93)  | 1:6:A:LYS:HA    | 1:7:A:PHE:HB2 | 2        | 0.37          |
| (1,93)  | 1:6:A:LYS:HA    | 1:7:A:PHE:HB3 | 2        | 0.37          |
| (1,93)  | 1:6:A:LYS:HA    | 1:7:A:PHE:HB2 | 11       | 0.37          |
| (1,93)  | 1:6:A:LYS:HA    | 1:7:A:PHE:HB3 | 11       | 0.37          |
| (1,93)  | 1:6:A:LYS:HA    | 1:7:A:PHE:HB2 | 13       | 0.37          |
| (1,93)  | 1:6:A:LYS:HA    | 1:7:A:PHE:HB3 | 13       | 0.37          |
| (1,93)  | 1:6:A:LYS:HA    | 1:7:A:PHE:HB2 | 15       | 0.37          |
| (1,93)  | 1:6:A:LYS:HA    | 1:7:A:PHE:HB3 | 15       | 0.37          |
| (1,93)  | 1:6:A:LYS:HA    | 1:7:A:PHE:HB2 | 19       | 0.37          |
| (1,93)  | 1:6:A:LYS:HA    | 1:7:A:PHE:HB3 | 19       | 0.37          |
| (1,53)  | 1:4:A:LEU:HD11  | 1:6:A:LYS:HB2 | 14       | 0.37          |
| (1,53)  | 1:4:A:LEU:HD11  | 1:6:A:LYS:HB3 | 14       | 0.37          |
| (1,53)  | 1:4:A:LEU:HD12  | 1:6:A:LYS:HB2 | 14       | 0.37          |
| (1,53)  | 1:4:A:LEU:HD12  | 1:6:A:LYS:HB3 | 14       | 0.37          |
| (1,53)  | 1:4:A:LEU:HD13  | 1:6:A:LYS:HB2 | 14       | 0.37          |
| (1,53)  | 1:4:A:LEU:HD13  | 1:6:A:LYS:HB3 | 14       | 0.37          |
| (1,53)  | 1:4:A:LEU:HD21  | 1:6:A:LYS:HB2 | 14       | 0.37          |
| (1,53)  | 1:4:A:LEU:HD21  | 1:6:A:LYS:HB3 | 14       | 0.37          |
| (1,53)  | 1:4:A:LEU:HD22  | 1:6:A:LYS:HB2 | 14       | 0.37          |
| (1,53)  | 1:4:A:LEU:HD22  | 1:6:A:LYS:HB3 | 14       | 0.37          |
| (1,53)  | 1:4:A:LEU:HD23  | 1:6:A:LYS:HB2 | 14       | 0.37          |
| (1,53)  | 1:4:A:LEU:HD23  | 1:6:A:LYS:HB3 | 14       | 0.37          |
| (1,215) | 1:14:A:GLN:H    | 1:15:A:ARG:HA | 15       | 0.36          |
| (1,179) | 1:12:A:ILE:HG12 | 1:12:A:ILE:H  | 19       | 0.36          |
| (1,179) | 1:12:A:ILE:HG13 | 1:12:A:ILE:H  | 19       | 0.36          |
| (1,177) | 1:12:A:ILE:HD11 | 1:12:A:ILE:H  | 8        | 0.36          |
| (1,177) | 1:12:A:ILE:HD12 | 1:12:A:ILE:H  | 8        | 0.36          |
| (1,177) | 1:12:A:ILE:HD13 | 1:12:A:ILE:H  | 8        | 0.36          |
| (1,150) | 1:9:A:ARG:HG2   | 1:12:A:ILE:HA | 12       | 0.36          |
| (1,150) | 1:9:A:ARG:HG3   | 1:12:A:ILE:HA | 12       | 0.36          |
| (1,95)  | 1:6:A:LYS:HB2   | 1:7:A:PHE:HB2 | 19       | 0.36          |
| (1,95)  | 1:6:A:LYS:HB2   | 1:7:A:PHE:HB3 | 19       | 0.36          |
| (1,95)  | 1:6:A:LYS:HB3   | 1:7:A:PHE:HB2 | 19       | 0.36          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,95)  | 1:6:A:LYS:HB3   | 1:7:A:PHE:HB3  | 19       | 0.36          |
| (1,93)  | 1:6:A:LYS:HA    | 1:7:A:PHE:HB2  | 12       | 0.36          |
| (1,93)  | 1:6:A:LYS:HA    | 1:7:A:PHE:HB3  | 12       | 0.36          |
| (1,93)  | 1:6:A:LYS:HA    | 1:7:A:PHE:HB2  | 17       | 0.36          |
| (1,93)  | 1:6:A:LYS:HA    | 1:7:A:PHE:HB3  | 17       | 0.36          |
| (1,93)  | 1:6:A:LYS:HA    | 1:7:A:PHE:HB2  | 18       | 0.36          |
| (1,93)  | 1:6:A:LYS:HA    | 1:7:A:PHE:HB3  | 18       | 0.36          |
| (1,93)  | 1:6:A:LYS:HA    | 1:7:A:PHE:HB2  | 20       | 0.36          |
| (1,93)  | 1:6:A:LYS:HA    | 1:7:A:PHE:HB3  | 20       | 0.36          |
| (1,53)  | 1:4:A:LEU:HD11  | 1:6:A:LYS:HB2  | 4        | 0.36          |
| (1,53)  | 1:4:A:LEU:HD11  | 1:6:A:LYS:HB3  | 4        | 0.36          |
| (1,53)  | 1:4:A:LEU:HD12  | 1:6:A:LYS:HB2  | 4        | 0.36          |
| (1,53)  | 1:4:A:LEU:HD12  | 1:6:A:LYS:HB3  | 4        | 0.36          |
| (1,53)  | 1:4:A:LEU:HD13  | 1:6:A:LYS:HB2  | 4        | 0.36          |
| (1,53)  | 1:4:A:LEU:HD13  | 1:6:A:LYS:HB3  | 4        | 0.36          |
| (1,53)  | 1:4:A:LEU:HD21  | 1:6:A:LYS:HB2  | 4        | 0.36          |
| (1,53)  | 1:4:A:LEU:HD21  | 1:6:A:LYS:HB3  | 4        | 0.36          |
| (1,53)  | 1:4:A:LEU:HD22  | 1:6:A:LYS:HB2  | 4        | 0.36          |
| (1,53)  | 1:4:A:LEU:HD22  | 1:6:A:LYS:HB3  | 4        | 0.36          |
| (1,53)  | 1:4:A:LEU:HD23  | 1:6:A:LYS:HB2  | 4        | 0.36          |
| (1,53)  | 1:4:A:LEU:HD23  | 1:6:A:LYS:HB3  | 4        | 0.36          |
| (1,31)  | 1:3:A:ARG:HG2   | 1:6:A:LYS:HA   | 5        | 0.36          |
| (1,31)  | 1:3:A:ARG:HG3   | 1:6:A:LYS:HA   | 5        | 0.36          |
| (1,215) | 1:14:A:GLN:H    | 1:15:A:ARG:HA  | 8        | 0.35          |
| (1,177) | 1:12:A:ILE:HD11 | 1:12:A:ILE:H   | 2        | 0.35          |
| (1,177) | 1:12:A:ILE:HD12 | 1:12:A:ILE:H   | 2        | 0.35          |
| (1,177) | 1:12:A:ILE:HD13 | 1:12:A:ILE:H   | 2        | 0.35          |
| (1,177) | 1:12:A:ILE:HD11 | 1:12:A:ILE:H   | 6        | 0.35          |
| (1,177) | 1:12:A:ILE:HD12 | 1:12:A:ILE:H   | 6        | 0.35          |
| (1,177) | 1:12:A:ILE:HD13 | 1:12:A:ILE:H   | 6        | 0.35          |
| (1,177) | 1:12:A:ILE:HD11 | 1:12:A:ILE:H   | 13       | 0.35          |
| (1,177) | 1:12:A:ILE:HD12 | 1:12:A:ILE:H   | 13       | 0.35          |
| (1,177) | 1:12:A:ILE:HD13 | 1:12:A:ILE:H   | 13       | 0.35          |
| (1,177) | 1:12:A:ILE:HD11 | 1:12:A:ILE:H   | 15       | 0.35          |
| (1,177) | 1:12:A:ILE:HD12 | 1:12:A:ILE:H   | 15       | 0.35          |
| (1,177) | 1:12:A:ILE:HD13 | 1:12:A:ILE:H   | 15       | 0.35          |
| (1,139) | 1:9:A:ARG:HA    | 1:9:A:ARG:HD2  | 10       | 0.35          |
| (1,139) | 1:9:A:ARG:HA    | 1:9:A:ARG:HD3  | 10       | 0.35          |
| (1,132) | 1:8:A:PHE:HB2   | 1:11:A:PHE:HB2 | 9        | 0.35          |
| (1,132) | 1:8:A:PHE:HB2   | 1:11:A:PHE:HB3 | 9        | 0.35          |
| (1,132) | 1:8:A:PHE:HB3   | 1:11:A:PHE:HB2 | 9        | 0.35          |
| (1,132) | 1:8:A:PHE:HB3   | 1:11:A:PHE:HB3 | 9        | 0.35          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,132) | 1:8:A:PHE:HB2  | 1:11:A:PHE:HB2 | 11       | 0.35          |
| (1,132) | 1:8:A:PHE:HB2  | 1:11:A:PHE:HB3 | 11       | 0.35          |
| (1,132) | 1:8:A:PHE:HB3  | 1:11:A:PHE:HB2 | 11       | 0.35          |
| (1,132) | 1:8:A:PHE:HB3  | 1:11:A:PHE:HB3 | 11       | 0.35          |
| (1,95)  | 1:6:A:LYS:HB2  | 1:7:A:PHE:HB2  | 3        | 0.35          |
| (1,95)  | 1:6:A:LYS:HB2  | 1:7:A:PHE:HB3  | 3        | 0.35          |
| (1,95)  | 1:6:A:LYS:HB3  | 1:7:A:PHE:HB2  | 3        | 0.35          |
| (1,95)  | 1:6:A:LYS:HB3  | 1:7:A:PHE:HB3  | 3        | 0.35          |
| (1,95)  | 1:6:A:LYS:HB2  | 1:7:A:PHE:HB2  | 7        | 0.35          |
| (1,95)  | 1:6:A:LYS:HB2  | 1:7:A:PHE:HB3  | 7        | 0.35          |
| (1,95)  | 1:6:A:LYS:HB3  | 1:7:A:PHE:HB2  | 7        | 0.35          |
| (1,95)  | 1:6:A:LYS:HB3  | 1:7:A:PHE:HB3  | 7        | 0.35          |
| (1,95)  | 1:6:A:LYS:HB2  | 1:7:A:PHE:HB2  | 9        | 0.35          |
| (1,95)  | 1:6:A:LYS:HB2  | 1:7:A:PHE:HB3  | 9        | 0.35          |
| (1,95)  | 1:6:A:LYS:HB3  | 1:7:A:PHE:HB2  | 9        | 0.35          |
| (1,95)  | 1:6:A:LYS:HB3  | 1:7:A:PHE:HB3  | 9        | 0.35          |
| (1,95)  | 1:6:A:LYS:HB2  | 1:7:A:PHE:HB2  | 13       | 0.35          |
| (1,95)  | 1:6:A:LYS:HB2  | 1:7:A:PHE:HB3  | 13       | 0.35          |
| (1,95)  | 1:6:A:LYS:HB3  | 1:7:A:PHE:HB2  | 13       | 0.35          |
| (1,95)  | 1:6:A:LYS:HB3  | 1:7:A:PHE:HB3  | 13       | 0.35          |
| (1,93)  | 1:6:A:LYS:HA   | 1:7:A:PHE:HB2  | 7        | 0.35          |
| (1,93)  | 1:6:A:LYS:HA   | 1:7:A:PHE:HB3  | 7        | 0.35          |
| (1,93)  | 1:6:A:LYS:HA   | 1:7:A:PHE:HB2  | 14       | 0.35          |
| (1,93)  | 1:6:A:LYS:HA   | 1:7:A:PHE:HB3  | 14       | 0.35          |
| (1,93)  | 1:6:A:LYS:HA   | 1:7:A:PHE:HB2  | 16       | 0.35          |
| (1,93)  | 1:6:A:LYS:HA   | 1:7:A:PHE:HB3  | 16       | 0.35          |
| (1,53)  | 1:4:A:LEU:HD11 | 1:6:A:LYS:HB2  | 1        | 0.35          |
| (1,53)  | 1:4:A:LEU:HD11 | 1:6:A:LYS:HB3  | 1        | 0.35          |
| (1,53)  | 1:4:A:LEU:HD12 | 1:6:A:LYS:HB2  | 1        | 0.35          |
| (1,53)  | 1:4:A:LEU:HD12 | 1:6:A:LYS:HB3  | 1        | 0.35          |
| (1,53)  | 1:4:A:LEU:HD13 | 1:6:A:LYS:HB2  | 1        | 0.35          |
| (1,53)  | 1:4:A:LEU:HD13 | 1:6:A:LYS:HB3  | 1        | 0.35          |
| (1,53)  | 1:4:A:LEU:HD21 | 1:6:A:LYS:HB2  | 1        | 0.35          |
| (1,53)  | 1:4:A:LEU:HD21 | 1:6:A:LYS:HB3  | 1        | 0.35          |
| (1,53)  | 1:4:A:LEU:HD22 | 1:6:A:LYS:HB2  | 1        | 0.35          |
| (1,53)  | 1:4:A:LEU:HD22 | 1:6:A:LYS:HB3  | 1        | 0.35          |
| (1,53)  | 1:4:A:LEU:HD23 | 1:6:A:LYS:HB2  | 1        | 0.35          |
| (1,53)  | 1:4:A:LEU:HD23 | 1:6:A:LYS:HB3  | 1        | 0.35          |
| (1,31)  | 1:3:A:ARG:HG2  | 1:6:A:LYS:HA   | 4        | 0.35          |
| (1,31)  | 1:3:A:ARG:HG3  | 1:6:A:LYS:HA   | 4        | 0.35          |
| (1,18)  | 1:3:A:ARG:HB2  | 1:3:A:ARG:H    | 8        | 0.35          |
| (1,18)  | 1:3:A:ARG:HB3  | 1:3:A:ARG:H    | 8        | 0.35          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,215) | 1:14:A:GLN:H   | 1:15:A:ARG:HA  | 18       | 0.34          |
| (1,139) | 1:9:A:ARG:HA   | 1:9:A:ARG:HD2  | 14       | 0.34          |
| (1,139) | 1:9:A:ARG:HA   | 1:9:A:ARG:HD3  | 14       | 0.34          |
| (1,132) | 1:8:A:PHE:HB2  | 1:11:A:PHE:HB2 | 3        | 0.34          |
| (1,132) | 1:8:A:PHE:HB2  | 1:11:A:PHE:HB3 | 3        | 0.34          |
| (1,132) | 1:8:A:PHE:HB3  | 1:11:A:PHE:HB2 | 3        | 0.34          |
| (1,132) | 1:8:A:PHE:HB3  | 1:11:A:PHE:HB3 | 3        | 0.34          |
| (1,132) | 1:8:A:PHE:HB2  | 1:11:A:PHE:HB2 | 7        | 0.34          |
| (1,132) | 1:8:A:PHE:HB2  | 1:11:A:PHE:HB3 | 7        | 0.34          |
| (1,132) | 1:8:A:PHE:HB3  | 1:11:A:PHE:HB2 | 7        | 0.34          |
| (1,132) | 1:8:A:PHE:HB3  | 1:11:A:PHE:HB3 | 7        | 0.34          |
| (1,120) | 1:8:A:PHE:HA   | 1:8:A:PHE:HE1  | 17       | 0.34          |
| (1,120) | 1:8:A:PHE:HA   | 1:8:A:PHE:HE2  | 17       | 0.34          |
| (1,95)  | 1:6:A:LYS:HB2  | 1:7:A:PHE:HB2  | 2        | 0.34          |
| (1,95)  | 1:6:A:LYS:HB2  | 1:7:A:PHE:HB3  | 2        | 0.34          |
| (1,95)  | 1:6:A:LYS:HB3  | 1:7:A:PHE:HB2  | 2        | 0.34          |
| (1,95)  | 1:6:A:LYS:HB3  | 1:7:A:PHE:HB3  | 2        | 0.34          |
| (1,95)  | 1:6:A:LYS:HB2  | 1:7:A:PHE:HB2  | 16       | 0.34          |
| (1,95)  | 1:6:A:LYS:HB2  | 1:7:A:PHE:HB3  | 16       | 0.34          |
| (1,95)  | 1:6:A:LYS:HB3  | 1:7:A:PHE:HB2  | 16       | 0.34          |
| (1,95)  | 1:6:A:LYS:HB3  | 1:7:A:PHE:HB3  | 16       | 0.34          |
| (1,93)  | 1:6:A:LYS:HA   | 1:7:A:PHE:HB2  | 9        | 0.34          |
| (1,93)  | 1:6:A:LYS:HA   | 1:7:A:PHE:HB3  | 9        | 0.34          |
| (1,53)  | 1:4:A:LEU:HD11 | 1:6:A:LYS:HB2  | 5        | 0.34          |
| (1,53)  | 1:4:A:LEU:HD11 | 1:6:A:LYS:HB3  | 5        | 0.34          |
| (1,53)  | 1:4:A:LEU:HD12 | 1:6:A:LYS:HB2  | 5        | 0.34          |
| (1,53)  | 1:4:A:LEU:HD12 | 1:6:A:LYS:HB3  | 5        | 0.34          |
| (1,53)  | 1:4:A:LEU:HD13 | 1:6:A:LYS:HB2  | 5        | 0.34          |
| (1,53)  | 1:4:A:LEU:HD13 | 1:6:A:LYS:HB3  | 5        | 0.34          |
| (1,53)  | 1:4:A:LEU:HD21 | 1:6:A:LYS:HB2  | 5        | 0.34          |
| (1,53)  | 1:4:A:LEU:HD21 | 1:6:A:LYS:HB3  | 5        | 0.34          |
| (1,53)  | 1:4:A:LEU:HD22 | 1:6:A:LYS:HB2  | 5        | 0.34          |
| (1,53)  | 1:4:A:LEU:HD22 | 1:6:A:LYS:HB3  | 5        | 0.34          |
| (1,53)  | 1:4:A:LEU:HD23 | 1:6:A:LYS:HB2  | 5        | 0.34          |
| (1,53)  | 1:4:A:LEU:HD23 | 1:6:A:LYS:HB3  | 5        | 0.34          |
| (1,53)  | 1:4:A:LEU:HD11 | 1:6:A:LYS:HB2  | 7        | 0.34          |
| (1,53)  | 1:4:A:LEU:HD11 | 1:6:A:LYS:HB3  | 7        | 0.34          |
| (1,53)  | 1:4:A:LEU:HD12 | 1:6:A:LYS:HB2  | 7        | 0.34          |
| (1,53)  | 1:4:A:LEU:HD12 | 1:6:A:LYS:HB3  | 7        | 0.34          |
| (1,53)  | 1:4:A:LEU:HD13 | 1:6:A:LYS:HB2  | 7        | 0.34          |
| (1,53)  | 1:4:A:LEU:HD13 | 1:6:A:LYS:HB3  | 7        | 0.34          |
| (1,53)  | 1:4:A:LEU:HD21 | 1:6:A:LYS:HB2  | 7        | 0.34          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,53)  | 1:4:A:LEU:HD21  | 1:6:A:LYS:HB3  | 7        | 0.34          |
| (1,53)  | 1:4:A:LEU:HD22  | 1:6:A:LYS:HB2  | 7        | 0.34          |
| (1,53)  | 1:4:A:LEU:HD22  | 1:6:A:LYS:HB3  | 7        | 0.34          |
| (1,53)  | 1:4:A:LEU:HD23  | 1:6:A:LYS:HB2  | 7        | 0.34          |
| (1,53)  | 1:4:A:LEU:HD23  | 1:6:A:LYS:HB3  | 7        | 0.34          |
| (1,53)  | 1:4:A:LEU:HD11  | 1:6:A:LYS:HB2  | 8        | 0.34          |
| (1,53)  | 1:4:A:LEU:HD11  | 1:6:A:LYS:HB3  | 8        | 0.34          |
| (1,53)  | 1:4:A:LEU:HD12  | 1:6:A:LYS:HB2  | 8        | 0.34          |
| (1,53)  | 1:4:A:LEU:HD12  | 1:6:A:LYS:HB3  | 8        | 0.34          |
| (1,53)  | 1:4:A:LEU:HD13  | 1:6:A:LYS:HB2  | 8        | 0.34          |
| (1,53)  | 1:4:A:LEU:HD13  | 1:6:A:LYS:HB3  | 8        | 0.34          |
| (1,53)  | 1:4:A:LEU:HD21  | 1:6:A:LYS:HB2  | 8        | 0.34          |
| (1,53)  | 1:4:A:LEU:HD21  | 1:6:A:LYS:HB3  | 8        | 0.34          |
| (1,53)  | 1:4:A:LEU:HD22  | 1:6:A:LYS:HB2  | 8        | 0.34          |
| (1,53)  | 1:4:A:LEU:HD22  | 1:6:A:LYS:HB3  | 8        | 0.34          |
| (1,53)  | 1:4:A:LEU:HD23  | 1:6:A:LYS:HB2  | 8        | 0.34          |
| (1,53)  | 1:4:A:LEU:HD23  | 1:6:A:LYS:HB3  | 8        | 0.34          |
| (1,31)  | 1:3:A:ARG:HG2   | 1:6:A:LYS:HA   | 8        | 0.34          |
| (1,31)  | 1:3:A:ARG:HG3   | 1:6:A:LYS:HA   | 8        | 0.34          |
| (1,18)  | 1:3:A:ARG:HB2   | 1:3:A:ARG:H    | 1        | 0.34          |
| (1,18)  | 1:3:A:ARG:HB3   | 1:3:A:ARG:H    | 1        | 0.34          |
| (1,18)  | 1:3:A:ARG:HB2   | 1:3:A:ARG:H    | 9        | 0.34          |
| (1,18)  | 1:3:A:ARG:HB3   | 1:3:A:ARG:H    | 9        | 0.34          |
| (1,18)  | 1:3:A:ARG:HB2   | 1:3:A:ARG:H    | 12       | 0.34          |
| (1,18)  | 1:3:A:ARG:HB3   | 1:3:A:ARG:H    | 12       | 0.34          |
| (1,18)  | 1:3:A:ARG:HB2   | 1:3:A:ARG:H    | 15       | 0.34          |
| (1,18)  | 1:3:A:ARG:HB3   | 1:3:A:ARG:H    | 15       | 0.34          |
| (1,179) | 1:12:A:ILE:HG12 | 1:12:A:ILE:H   | 1        | 0.33          |
| (1,179) | 1:12:A:ILE:HG13 | 1:12:A:ILE:H   | 1        | 0.33          |
| (1,179) | 1:12:A:ILE:HG12 | 1:12:A:ILE:H   | 17       | 0.33          |
| (1,179) | 1:12:A:ILE:HG13 | 1:12:A:ILE:H   | 17       | 0.33          |
| (1,139) | 1:9:A:ARG:HA    | 1:9:A:ARG:HD2  | 19       | 0.33          |
| (1,139) | 1:9:A:ARG:HA    | 1:9:A:ARG:HD3  | 19       | 0.33          |
| (1,132) | 1:8:A:PHE:HB2   | 1:11:A:PHE:HB2 | 10       | 0.33          |
| (1,132) | 1:8:A:PHE:HB2   | 1:11:A:PHE:HB3 | 10       | 0.33          |
| (1,132) | 1:8:A:PHE:HB3   | 1:11:A:PHE:HB2 | 10       | 0.33          |
| (1,132) | 1:8:A:PHE:HB3   | 1:11:A:PHE:HB3 | 10       | 0.33          |
| (1,95)  | 1:6:A:LYS:HB2   | 1:7:A:PHE:HB2  | 12       | 0.33          |
| (1,95)  | 1:6:A:LYS:HB2   | 1:7:A:PHE:HB3  | 12       | 0.33          |
| (1,95)  | 1:6:A:LYS:HB3   | 1:7:A:PHE:HB2  | 12       | 0.33          |
| (1,95)  | 1:6:A:LYS:HB3   | 1:7:A:PHE:HB3  | 12       | 0.33          |
| (1,95)  | 1:6:A:LYS:HB2   | 1:7:A:PHE:HB2  | 15       | 0.33          |

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| Key    | Atom-1         | Atom-2        | Model ID | Violation (Å) |
|--------|----------------|---------------|----------|---------------|
| (1,95) | 1:6:A:LYS:HB2  | 1:7:A:PHE:HB3 | 15       | 0.33          |
| (1,95) | 1:6:A:LYS:HB3  | 1:7:A:PHE:HB2 | 15       | 0.33          |
| (1,95) | 1:6:A:LYS:HB3  | 1:7:A:PHE:HB3 | 15       | 0.33          |
| (1,95) | 1:6:A:LYS:HB2  | 1:7:A:PHE:HB2 | 17       | 0.33          |
| (1,95) | 1:6:A:LYS:HB2  | 1:7:A:PHE:HB3 | 17       | 0.33          |
| (1,95) | 1:6:A:LYS:HB3  | 1:7:A:PHE:HB2 | 17       | 0.33          |
| (1,95) | 1:6:A:LYS:HB3  | 1:7:A:PHE:HB3 | 17       | 0.33          |
| (1,93) | 1:6:A:LYS:HA   | 1:7:A:PHE:HB2 | 3        | 0.33          |
| (1,93) | 1:6:A:LYS:HA   | 1:7:A:PHE:HB3 | 3        | 0.33          |
| (1,93) | 1:6:A:LYS:HA   | 1:7:A:PHE:HB2 | 10       | 0.33          |
| (1,93) | 1:6:A:LYS:HA   | 1:7:A:PHE:HB3 | 10       | 0.33          |
| (1,53) | 1:4:A:LEU:HD11 | 1:6:A:LYS:HB2 | 9        | 0.33          |
| (1,53) | 1:4:A:LEU:HD11 | 1:6:A:LYS:HB3 | 9        | 0.33          |
| (1,53) | 1:4:A:LEU:HD12 | 1:6:A:LYS:HB2 | 9        | 0.33          |
| (1,53) | 1:4:A:LEU:HD12 | 1:6:A:LYS:HB3 | 9        | 0.33          |
| (1,53) | 1:4:A:LEU:HD13 | 1:6:A:LYS:HB2 | 9        | 0.33          |
| (1,53) | 1:4:A:LEU:HD13 | 1:6:A:LYS:HB3 | 9        | 0.33          |
| (1,53) | 1:4:A:LEU:HD21 | 1:6:A:LYS:HB2 | 9        | 0.33          |
| (1,53) | 1:4:A:LEU:HD21 | 1:6:A:LYS:HB3 | 9        | 0.33          |
| (1,53) | 1:4:A:LEU:HD22 | 1:6:A:LYS:HB2 | 9        | 0.33          |
| (1,53) | 1:4:A:LEU:HD22 | 1:6:A:LYS:HB3 | 9        | 0.33          |
| (1,53) | 1:4:A:LEU:HD23 | 1:6:A:LYS:HB2 | 9        | 0.33          |
| (1,53) | 1:4:A:LEU:HD23 | 1:6:A:LYS:HB3 | 9        | 0.33          |
| (1,53) | 1:4:A:LEU:HD11 | 1:6:A:LYS:HB2 | 10       | 0.33          |
| (1,53) | 1:4:A:LEU:HD11 | 1:6:A:LYS:HB3 | 10       | 0.33          |
| (1,53) | 1:4:A:LEU:HD12 | 1:6:A:LYS:HB2 | 10       | 0.33          |
| (1,53) | 1:4:A:LEU:HD12 | 1:6:A:LYS:HB3 | 10       | 0.33          |
| (1,53) | 1:4:A:LEU:HD13 | 1:6:A:LYS:HB2 | 10       | 0.33          |
| (1,53) | 1:4:A:LEU:HD13 | 1:6:A:LYS:HB3 | 10       | 0.33          |
| (1,53) | 1:4:A:LEU:HD21 | 1:6:A:LYS:HB2 | 10       | 0.33          |
| (1,53) | 1:4:A:LEU:HD21 | 1:6:A:LYS:HB3 | 10       | 0.33          |
| (1,53) | 1:4:A:LEU:HD22 | 1:6:A:LYS:HB2 | 10       | 0.33          |
| (1,53) | 1:4:A:LEU:HD22 | 1:6:A:LYS:HB3 | 10       | 0.33          |
| (1,53) | 1:4:A:LEU:HD23 | 1:6:A:LYS:HB2 | 10       | 0.33          |
| (1,53) | 1:4:A:LEU:HD23 | 1:6:A:LYS:HB3 | 10       | 0.33          |
| (1,18) | 1:3:A:ARG:HB2  | 1:3:A:ARG:H   | 4        | 0.33          |
| (1,18) | 1:3:A:ARG:HB3  | 1:3:A:ARG:H   | 4        | 0.33          |
| (1,18) | 1:3:A:ARG:HB2  | 1:3:A:ARG:H   | 5        | 0.33          |
| (1,18) | 1:3:A:ARG:HB3  | 1:3:A:ARG:H   | 5        | 0.33          |
| (1,18) | 1:3:A:ARG:HB2  | 1:3:A:ARG:H   | 7        | 0.33          |
| (1,18) | 1:3:A:ARG:HB3  | 1:3:A:ARG:H   | 7        | 0.33          |
| (1,18) | 1:3:A:ARG:HB2  | 1:3:A:ARG:H   | 10       | 0.33          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,18)  | 1:3:A:ARG:HB3   | 1:3:A:ARG:H    | 10       | 0.33          |
| (1,18)  | 1:3:A:ARG:HB2   | 1:3:A:ARG:H    | 13       | 0.33          |
| (1,18)  | 1:3:A:ARG:HB3   | 1:3:A:ARG:H    | 13       | 0.33          |
| (1,18)  | 1:3:A:ARG:HB2   | 1:3:A:ARG:H    | 16       | 0.33          |
| (1,18)  | 1:3:A:ARG:HB3   | 1:3:A:ARG:H    | 16       | 0.33          |
| (1,18)  | 1:3:A:ARG:HB2   | 1:3:A:ARG:H    | 18       | 0.33          |
| (1,18)  | 1:3:A:ARG:HB3   | 1:3:A:ARG:H    | 18       | 0.33          |
| (1,18)  | 1:3:A:ARG:HB2   | 1:3:A:ARG:H    | 19       | 0.33          |
| (1,18)  | 1:3:A:ARG:HB3   | 1:3:A:ARG:H    | 19       | 0.33          |
| (1,179) | 1:12:A:ILE:HG12 | 1:12:A:ILE:H   | 5        | 0.32          |
| (1,179) | 1:12:A:ILE:HG13 | 1:12:A:ILE:H   | 5        | 0.32          |
| (1,179) | 1:12:A:ILE:HG12 | 1:12:A:ILE:H   | 14       | 0.32          |
| (1,179) | 1:12:A:ILE:HG13 | 1:12:A:ILE:H   | 14       | 0.32          |
| (1,177) | 1:12:A:ILE:HD11 | 1:12:A:ILE:H   | 11       | 0.32          |
| (1,177) | 1:12:A:ILE:HD12 | 1:12:A:ILE:H   | 11       | 0.32          |
| (1,177) | 1:12:A:ILE:HD13 | 1:12:A:ILE:H   | 11       | 0.32          |
| (1,116) | 1:7:A:PHE:H     | 1:7:A:PHE:HZ   | 18       | 0.32          |
| (1,106) | 1:6:A:LYS:HA    | 1:9:A:ARG:HG2  | 12       | 0.32          |
| (1,106) | 1:6:A:LYS:HA    | 1:9:A:ARG:HG3  | 12       | 0.32          |
| (1,31)  | 1:3:A:ARG:HG2   | 1:6:A:LYS:HA   | 1        | 0.32          |
| (1,31)  | 1:3:A:ARG:HG3   | 1:6:A:LYS:HA   | 1        | 0.32          |
| (1,31)  | 1:3:A:ARG:HG2   | 1:6:A:LYS:HA   | 16       | 0.32          |
| (1,31)  | 1:3:A:ARG:HG3   | 1:6:A:LYS:HA   | 16       | 0.32          |
| (1,18)  | 1:3:A:ARG:HB2   | 1:3:A:ARG:H    | 2        | 0.32          |
| (1,18)  | 1:3:A:ARG:HB3   | 1:3:A:ARG:H    | 2        | 0.32          |
| (1,18)  | 1:3:A:ARG:HB2   | 1:3:A:ARG:H    | 11       | 0.32          |
| (1,18)  | 1:3:A:ARG:HB3   | 1:3:A:ARG:H    | 11       | 0.32          |
| (1,18)  | 1:3:A:ARG:HB2   | 1:3:A:ARG:H    | 17       | 0.32          |
| (1,18)  | 1:3:A:ARG:HB3   | 1:3:A:ARG:H    | 17       | 0.32          |
| (1,215) | 1:14:A:GLN:H    | 1:15:A:ARG:HA  | 1        | 0.31          |
| (1,179) | 1:12:A:ILE:HG12 | 1:12:A:ILE:H   | 7        | 0.31          |
| (1,179) | 1:12:A:ILE:HG13 | 1:12:A:ILE:H   | 7        | 0.31          |
| (1,132) | 1:8:A:PHE:HB2   | 1:11:A:PHE:HB2 | 8        | 0.31          |
| (1,132) | 1:8:A:PHE:HB2   | 1:11:A:PHE:HB3 | 8        | 0.31          |
| (1,132) | 1:8:A:PHE:HB3   | 1:11:A:PHE:HB2 | 8        | 0.31          |
| (1,132) | 1:8:A:PHE:HB3   | 1:11:A:PHE:HB3 | 8        | 0.31          |
| (1,132) | 1:8:A:PHE:HB2   | 1:11:A:PHE:HB2 | 17       | 0.31          |
| (1,132) | 1:8:A:PHE:HB2   | 1:11:A:PHE:HB3 | 17       | 0.31          |
| (1,132) | 1:8:A:PHE:HB3   | 1:11:A:PHE:HB2 | 17       | 0.31          |
| (1,132) | 1:8:A:PHE:HB3   | 1:11:A:PHE:HB3 | 17       | 0.31          |
| (1,116) | 1:7:A:PHE:H     | 1:7:A:PHE:HZ   | 12       | 0.31          |
| (1,95)  | 1:6:A:LYS:HB2   | 1:7:A:PHE:HB2  | 1        | 0.31          |

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| Key     | Atom-1        | Atom-2         | Model ID | Violation (Å) |
|---------|---------------|----------------|----------|---------------|
| (1,95)  | 1:6:A:LYS:HB2 | 1:7:A:PHE:HB3  | 1        | 0.31          |
| (1,95)  | 1:6:A:LYS:HB3 | 1:7:A:PHE:HB2  | 1        | 0.31          |
| (1,95)  | 1:6:A:LYS:HB3 | 1:7:A:PHE:HB3  | 1        | 0.31          |
| (1,95)  | 1:6:A:LYS:HB2 | 1:7:A:PHE:HB2  | 5        | 0.31          |
| (1,95)  | 1:6:A:LYS:HB2 | 1:7:A:PHE:HB3  | 5        | 0.31          |
| (1,95)  | 1:6:A:LYS:HB3 | 1:7:A:PHE:HB2  | 5        | 0.31          |
| (1,95)  | 1:6:A:LYS:HB3 | 1:7:A:PHE:HB3  | 5        | 0.31          |
| (1,95)  | 1:6:A:LYS:HB2 | 1:7:A:PHE:HB2  | 20       | 0.31          |
| (1,95)  | 1:6:A:LYS:HB2 | 1:7:A:PHE:HB3  | 20       | 0.31          |
| (1,95)  | 1:6:A:LYS:HB3 | 1:7:A:PHE:HB2  | 20       | 0.31          |
| (1,95)  | 1:6:A:LYS:HB3 | 1:7:A:PHE:HB3  | 20       | 0.31          |
| (1,31)  | 1:3:A:ARG:HG2 | 1:6:A:LYS:HA   | 11       | 0.31          |
| (1,31)  | 1:3:A:ARG:HG3 | 1:6:A:LYS:HA   | 11       | 0.31          |
| (1,31)  | 1:3:A:ARG:HG2 | 1:6:A:LYS:HA   | 15       | 0.31          |
| (1,31)  | 1:3:A:ARG:HG3 | 1:6:A:LYS:HA   | 15       | 0.31          |
| (1,31)  | 1:3:A:ARG:HG2 | 1:6:A:LYS:HA   | 18       | 0.31          |
| (1,31)  | 1:3:A:ARG:HG3 | 1:6:A:LYS:HA   | 18       | 0.31          |
| (1,18)  | 1:3:A:ARG:HB2 | 1:3:A:ARG:H    | 14       | 0.31          |
| (1,18)  | 1:3:A:ARG:HB3 | 1:3:A:ARG:H    | 14       | 0.31          |
| (1,18)  | 1:3:A:ARG:HB2 | 1:3:A:ARG:H    | 20       | 0.31          |
| (1,18)  | 1:3:A:ARG:HB3 | 1:3:A:ARG:H    | 20       | 0.31          |
| (1,150) | 1:9:A:ARG:HG2 | 1:12:A:ILE:HA  | 2        | 0.3           |
| (1,150) | 1:9:A:ARG:HG3 | 1:12:A:ILE:HA  | 2        | 0.3           |
| (1,150) | 1:9:A:ARG:HG2 | 1:12:A:ILE:HA  | 13       | 0.3           |
| (1,150) | 1:9:A:ARG:HG3 | 1:12:A:ILE:HA  | 13       | 0.3           |
| (1,132) | 1:8:A:PHE:HB2 | 1:11:A:PHE:HB2 | 14       | 0.3           |
| (1,132) | 1:8:A:PHE:HB2 | 1:11:A:PHE:HB3 | 14       | 0.3           |
| (1,132) | 1:8:A:PHE:HB3 | 1:11:A:PHE:HB2 | 14       | 0.3           |
| (1,132) | 1:8:A:PHE:HB3 | 1:11:A:PHE:HB3 | 14       | 0.3           |
| (1,116) | 1:7:A:PHE:H   | 1:7:A:PHE:HZ   | 11       | 0.3           |
| (1,116) | 1:7:A:PHE:H   | 1:7:A:PHE:HZ   | 14       | 0.3           |
| (1,103) | 1:6:A:LYS:HA  | 1:8:A:PHE:HA   | 8        | 0.3           |
| (1,103) | 1:6:A:LYS:HA  | 1:8:A:PHE:HA   | 12       | 0.3           |
| (1,95)  | 1:6:A:LYS:HB2 | 1:7:A:PHE:HB2  | 4        | 0.3           |
| (1,95)  | 1:6:A:LYS:HB2 | 1:7:A:PHE:HB3  | 4        | 0.3           |
| (1,95)  | 1:6:A:LYS:HB3 | 1:7:A:PHE:HB2  | 4        | 0.3           |
| (1,95)  | 1:6:A:LYS:HB3 | 1:7:A:PHE:HB3  | 4        | 0.3           |
| (1,95)  | 1:6:A:LYS:HB2 | 1:7:A:PHE:HB2  | 8        | 0.3           |
| (1,95)  | 1:6:A:LYS:HB2 | 1:7:A:PHE:HB3  | 8        | 0.3           |
| (1,95)  | 1:6:A:LYS:HB3 | 1:7:A:PHE:HB2  | 8        | 0.3           |
| (1,95)  | 1:6:A:LYS:HB3 | 1:7:A:PHE:HB3  | 8        | 0.3           |
| (1,95)  | 1:6:A:LYS:HB2 | 1:7:A:PHE:HB2  | 18       | 0.3           |

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| Key     | Atom-1          | Atom-2        | Model ID | Violation (Å) |
|---------|-----------------|---------------|----------|---------------|
| (1,95)  | 1:6:A:LYS:HB2   | 1:7:A:PHE:HB3 | 18       | 0.3           |
| (1,95)  | 1:6:A:LYS:HB3   | 1:7:A:PHE:HB2 | 18       | 0.3           |
| (1,95)  | 1:6:A:LYS:HB3   | 1:7:A:PHE:HB3 | 18       | 0.3           |
| (1,26)  | 1:3:A:ARG:HB2   | 1:4:A:LEU:H   | 20       | 0.3           |
| (1,26)  | 1:3:A:ARG:HB3   | 1:4:A:LEU:H   | 20       | 0.3           |
| (1,215) | 1:14:A:GLN:H    | 1:15:A:ARG:HA | 2        | 0.29          |
| (1,215) | 1:14:A:GLN:H    | 1:15:A:ARG:HA | 6        | 0.29          |
| (1,215) | 1:14:A:GLN:H    | 1:15:A:ARG:HA | 11       | 0.29          |
| (1,188) | 1:12:A:ILE:H    | 1:13:A:LEU:H  | 3        | 0.29          |
| (1,177) | 1:12:A:ILE:HD11 | 1:12:A:ILE:H  | 10       | 0.29          |
| (1,177) | 1:12:A:ILE:HD12 | 1:12:A:ILE:H  | 10       | 0.29          |
| (1,177) | 1:12:A:ILE:HD13 | 1:12:A:ILE:H  | 10       | 0.29          |
| (1,150) | 1:9:A:ARG:HG2   | 1:12:A:ILE:HA | 1        | 0.29          |
| (1,150) | 1:9:A:ARG:HG3   | 1:12:A:ILE:HA | 1        | 0.29          |
| (1,150) | 1:9:A:ARG:HG2   | 1:12:A:ILE:HA | 5        | 0.29          |
| (1,150) | 1:9:A:ARG:HG3   | 1:12:A:ILE:HA | 5        | 0.29          |
| (1,150) | 1:9:A:ARG:HG2   | 1:12:A:ILE:HA | 15       | 0.29          |
| (1,150) | 1:9:A:ARG:HG3   | 1:12:A:ILE:HA | 15       | 0.29          |
| (1,139) | 1:9:A:ARG:HA    | 1:9:A:ARG:HD2 | 11       | 0.29          |
| (1,139) | 1:9:A:ARG:HA    | 1:9:A:ARG:HD3 | 11       | 0.29          |
| (1,116) | 1:7:A:PHE:H     | 1:7:A:PHE:HZ  | 3        | 0.29          |
| (1,116) | 1:7:A:PHE:H     | 1:7:A:PHE:HZ  | 7        | 0.29          |
| (1,116) | 1:7:A:PHE:H     | 1:7:A:PHE:HZ  | 16       | 0.29          |
| (1,106) | 1:6:A:LYS:HA    | 1:9:A:ARG:HG2 | 2        | 0.29          |
| (1,106) | 1:6:A:LYS:HA    | 1:9:A:ARG:HG3 | 2        | 0.29          |
| (1,106) | 1:6:A:LYS:HA    | 1:9:A:ARG:HG2 | 4        | 0.29          |
| (1,106) | 1:6:A:LYS:HA    | 1:9:A:ARG:HG3 | 4        | 0.29          |
| (1,106) | 1:6:A:LYS:HA    | 1:9:A:ARG:HG2 | 5        | 0.29          |
| (1,106) | 1:6:A:LYS:HA    | 1:9:A:ARG:HG3 | 5        | 0.29          |
| (1,106) | 1:6:A:LYS:HA    | 1:9:A:ARG:HG2 | 13       | 0.29          |
| (1,106) | 1:6:A:LYS:HA    | 1:9:A:ARG:HG3 | 13       | 0.29          |
| (1,106) | 1:6:A:LYS:HA    | 1:9:A:ARG:HG2 | 15       | 0.29          |
| (1,106) | 1:6:A:LYS:HA    | 1:9:A:ARG:HG3 | 15       | 0.29          |
| (1,103) | 1:6:A:LYS:HA    | 1:8:A:PHE:HA  | 5        | 0.29          |
| (1,103) | 1:6:A:LYS:HA    | 1:8:A:PHE:HA  | 6        | 0.29          |
| (1,53)  | 1:4:A:LEU:HD11  | 1:6:A:LYS:HB2 | 17       | 0.29          |
| (1,53)  | 1:4:A:LEU:HD11  | 1:6:A:LYS:HB3 | 17       | 0.29          |
| (1,53)  | 1:4:A:LEU:HD12  | 1:6:A:LYS:HB2 | 17       | 0.29          |
| (1,53)  | 1:4:A:LEU:HD12  | 1:6:A:LYS:HB3 | 17       | 0.29          |
| (1,53)  | 1:4:A:LEU:HD13  | 1:6:A:LYS:HB2 | 17       | 0.29          |
| (1,53)  | 1:4:A:LEU:HD13  | 1:6:A:LYS:HB3 | 17       | 0.29          |
| (1,53)  | 1:4:A:LEU:HD21  | 1:6:A:LYS:HB2 | 17       | 0.29          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,53)  | 1:4:A:LEU:HD21  | 1:6:A:LYS:HB3  | 17       | 0.29          |
| (1,53)  | 1:4:A:LEU:HD22  | 1:6:A:LYS:HB2  | 17       | 0.29          |
| (1,53)  | 1:4:A:LEU:HD22  | 1:6:A:LYS:HB3  | 17       | 0.29          |
| (1,53)  | 1:4:A:LEU:HD23  | 1:6:A:LYS:HB2  | 17       | 0.29          |
| (1,53)  | 1:4:A:LEU:HD23  | 1:6:A:LYS:HB3  | 17       | 0.29          |
| (1,53)  | 1:4:A:LEU:HD11  | 1:6:A:LYS:HB2  | 20       | 0.29          |
| (1,53)  | 1:4:A:LEU:HD11  | 1:6:A:LYS:HB3  | 20       | 0.29          |
| (1,53)  | 1:4:A:LEU:HD12  | 1:6:A:LYS:HB2  | 20       | 0.29          |
| (1,53)  | 1:4:A:LEU:HD12  | 1:6:A:LYS:HB3  | 20       | 0.29          |
| (1,53)  | 1:4:A:LEU:HD13  | 1:6:A:LYS:HB2  | 20       | 0.29          |
| (1,53)  | 1:4:A:LEU:HD13  | 1:6:A:LYS:HB3  | 20       | 0.29          |
| (1,53)  | 1:4:A:LEU:HD21  | 1:6:A:LYS:HB2  | 20       | 0.29          |
| (1,53)  | 1:4:A:LEU:HD21  | 1:6:A:LYS:HB3  | 20       | 0.29          |
| (1,53)  | 1:4:A:LEU:HD22  | 1:6:A:LYS:HB2  | 20       | 0.29          |
| (1,53)  | 1:4:A:LEU:HD22  | 1:6:A:LYS:HB3  | 20       | 0.29          |
| (1,53)  | 1:4:A:LEU:HD23  | 1:6:A:LYS:HB2  | 20       | 0.29          |
| (1,53)  | 1:4:A:LEU:HD23  | 1:6:A:LYS:HB3  | 20       | 0.29          |
| (1,31)  | 1:3:A:ARG:HG2   | 1:6:A:LYS:HA   | 9        | 0.29          |
| (1,31)  | 1:3:A:ARG:HG3   | 1:6:A:LYS:HA   | 9        | 0.29          |
| (1,215) | 1:14:A:GLN:H    | 1:15:A:ARG:HA  | 13       | 0.28          |
| (1,177) | 1:12:A:ILE:HD11 | 1:12:A:ILE:H   | 9        | 0.28          |
| (1,177) | 1:12:A:ILE:HD12 | 1:12:A:ILE:H   | 9        | 0.28          |
| (1,177) | 1:12:A:ILE:HD13 | 1:12:A:ILE:H   | 9        | 0.28          |
| (1,139) | 1:9:A:ARG:HA    | 1:9:A:ARG:HD2  | 16       | 0.28          |
| (1,139) | 1:9:A:ARG:HA    | 1:9:A:ARG:HD3  | 16       | 0.28          |
| (1,132) | 1:8:A:PHE:HB2   | 1:11:A:PHE:HB2 | 1        | 0.28          |
| (1,132) | 1:8:A:PHE:HB2   | 1:11:A:PHE:HB3 | 1        | 0.28          |
| (1,132) | 1:8:A:PHE:HB3   | 1:11:A:PHE:HB2 | 1        | 0.28          |
| (1,132) | 1:8:A:PHE:HB3   | 1:11:A:PHE:HB3 | 1        | 0.28          |
| (1,132) | 1:8:A:PHE:HB2   | 1:11:A:PHE:HB2 | 5        | 0.28          |
| (1,132) | 1:8:A:PHE:HB2   | 1:11:A:PHE:HB3 | 5        | 0.28          |
| (1,132) | 1:8:A:PHE:HB3   | 1:11:A:PHE:HB2 | 5        | 0.28          |
| (1,132) | 1:8:A:PHE:HB3   | 1:11:A:PHE:HB3 | 5        | 0.28          |
| (1,116) | 1:7:A:PHE:H     | 1:7:A:PHE:HZ   | 6        | 0.28          |
| (1,116) | 1:7:A:PHE:H     | 1:7:A:PHE:HZ   | 9        | 0.28          |
| (1,116) | 1:7:A:PHE:H     | 1:7:A:PHE:HZ   | 20       | 0.28          |
| (1,106) | 1:6:A:LYS:HA    | 1:9:A:ARG:HG2  | 1        | 0.28          |
| (1,106) | 1:6:A:LYS:HA    | 1:9:A:ARG:HG3  | 1        | 0.28          |
| (1,103) | 1:6:A:LYS:HA    | 1:8:A:PHE:HA   | 1        | 0.28          |
| (1,103) | 1:6:A:LYS:HA    | 1:8:A:PHE:HA   | 2        | 0.28          |
| (1,103) | 1:6:A:LYS:HA    | 1:8:A:PHE:HA   | 4        | 0.28          |
| (1,103) | 1:6:A:LYS:HA    | 1:8:A:PHE:HA   | 11       | 0.28          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,103) | 1:6:A:LYS:HA   | 1:8:A:PHE:HA   | 15       | 0.28          |
| (1,103) | 1:6:A:LYS:HA   | 1:8:A:PHE:HA   | 17       | 0.28          |
| (1,103) | 1:6:A:LYS:HA   | 1:8:A:PHE:HA   | 18       | 0.28          |
| (1,95)  | 1:6:A:LYS:HB2  | 1:7:A:PHE:HB2  | 11       | 0.28          |
| (1,95)  | 1:6:A:LYS:HB2  | 1:7:A:PHE:HB3  | 11       | 0.28          |
| (1,95)  | 1:6:A:LYS:HB3  | 1:7:A:PHE:HB2  | 11       | 0.28          |
| (1,95)  | 1:6:A:LYS:HB3  | 1:7:A:PHE:HB3  | 11       | 0.28          |
| (1,53)  | 1:4:A:LEU:HD11 | 1:6:A:LYS:HB2  | 2        | 0.28          |
| (1,53)  | 1:4:A:LEU:HD11 | 1:6:A:LYS:HB3  | 2        | 0.28          |
| (1,53)  | 1:4:A:LEU:HD12 | 1:6:A:LYS:HB2  | 2        | 0.28          |
| (1,53)  | 1:4:A:LEU:HD12 | 1:6:A:LYS:HB3  | 2        | 0.28          |
| (1,53)  | 1:4:A:LEU:HD13 | 1:6:A:LYS:HB2  | 2        | 0.28          |
| (1,53)  | 1:4:A:LEU:HD13 | 1:6:A:LYS:HB3  | 2        | 0.28          |
| (1,53)  | 1:4:A:LEU:HD21 | 1:6:A:LYS:HB2  | 2        | 0.28          |
| (1,53)  | 1:4:A:LEU:HD21 | 1:6:A:LYS:HB3  | 2        | 0.28          |
| (1,53)  | 1:4:A:LEU:HD22 | 1:6:A:LYS:HB2  | 2        | 0.28          |
| (1,53)  | 1:4:A:LEU:HD22 | 1:6:A:LYS:HB3  | 2        | 0.28          |
| (1,53)  | 1:4:A:LEU:HD23 | 1:6:A:LYS:HB2  | 2        | 0.28          |
| (1,53)  | 1:4:A:LEU:HD23 | 1:6:A:LYS:HB3  | 2        | 0.28          |
| (1,31)  | 1:3:A:ARG:HG2  | 1:6:A:LYS:HA   | 12       | 0.28          |
| (1,31)  | 1:3:A:ARG:HG3  | 1:6:A:LYS:HA   | 12       | 0.28          |
| (1,31)  | 1:3:A:ARG:HG2  | 1:6:A:LYS:HA   | 13       | 0.28          |
| (1,31)  | 1:3:A:ARG:HG3  | 1:6:A:LYS:HA   | 13       | 0.28          |
| (1,215) | 1:14:A:GLN:H   | 1:15:A:ARG:HA  | 14       | 0.27          |
| (1,215) | 1:14:A:GLN:H   | 1:15:A:ARG:HA  | 19       | 0.27          |
| (1,215) | 1:14:A:GLN:H   | 1:15:A:ARG:HA  | 20       | 0.27          |
| (1,150) | 1:9:A:ARG:HG2  | 1:12:A:ILE:HA  | 19       | 0.27          |
| (1,150) | 1:9:A:ARG:HG3  | 1:12:A:ILE:HA  | 19       | 0.27          |
| (1,132) | 1:8:A:PHE:HB2  | 1:11:A:PHE:HB2 | 4        | 0.27          |
| (1,132) | 1:8:A:PHE:HB2  | 1:11:A:PHE:HB3 | 4        | 0.27          |
| (1,132) | 1:8:A:PHE:HB3  | 1:11:A:PHE:HB2 | 4        | 0.27          |
| (1,132) | 1:8:A:PHE:HB3  | 1:11:A:PHE:HB3 | 4        | 0.27          |
| (1,132) | 1:8:A:PHE:HB2  | 1:11:A:PHE:HB2 | 19       | 0.27          |
| (1,132) | 1:8:A:PHE:HB2  | 1:11:A:PHE:HB3 | 19       | 0.27          |
| (1,132) | 1:8:A:PHE:HB3  | 1:11:A:PHE:HB2 | 19       | 0.27          |
| (1,132) | 1:8:A:PHE:HB3  | 1:11:A:PHE:HB3 | 19       | 0.27          |
| (1,116) | 1:7:A:PHE:H    | 1:7:A:PHE:HZ   | 10       | 0.27          |
| (1,116) | 1:7:A:PHE:H    | 1:7:A:PHE:HZ   | 17       | 0.27          |
| (1,116) | 1:7:A:PHE:H    | 1:7:A:PHE:HZ   | 19       | 0.27          |
| (1,103) | 1:6:A:LYS:HA   | 1:8:A:PHE:HA   | 13       | 0.27          |
| (1,103) | 1:6:A:LYS:HA   | 1:8:A:PHE:HA   | 14       | 0.27          |
| (1,103) | 1:6:A:LYS:HA   | 1:8:A:PHE:HA   | 19       | 0.27          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,103) | 1:6:A:LYS:HA   | 1:8:A:PHE:HA   | 20       | 0.27          |
| (1,53)  | 1:4:A:LEU:HD11 | 1:6:A:LYS:HB2  | 15       | 0.27          |
| (1,53)  | 1:4:A:LEU:HD11 | 1:6:A:LYS:HB3  | 15       | 0.27          |
| (1,53)  | 1:4:A:LEU:HD12 | 1:6:A:LYS:HB2  | 15       | 0.27          |
| (1,53)  | 1:4:A:LEU:HD12 | 1:6:A:LYS:HB3  | 15       | 0.27          |
| (1,53)  | 1:4:A:LEU:HD13 | 1:6:A:LYS:HB2  | 15       | 0.27          |
| (1,53)  | 1:4:A:LEU:HD13 | 1:6:A:LYS:HB3  | 15       | 0.27          |
| (1,53)  | 1:4:A:LEU:HD21 | 1:6:A:LYS:HB2  | 15       | 0.27          |
| (1,53)  | 1:4:A:LEU:HD21 | 1:6:A:LYS:HB3  | 15       | 0.27          |
| (1,53)  | 1:4:A:LEU:HD22 | 1:6:A:LYS:HB2  | 15       | 0.27          |
| (1,53)  | 1:4:A:LEU:HD22 | 1:6:A:LYS:HB3  | 15       | 0.27          |
| (1,53)  | 1:4:A:LEU:HD23 | 1:6:A:LYS:HB2  | 15       | 0.27          |
| (1,53)  | 1:4:A:LEU:HD23 | 1:6:A:LYS:HB3  | 15       | 0.27          |
| (1,53)  | 1:4:A:LEU:HD11 | 1:6:A:LYS:HB2  | 19       | 0.27          |
| (1,53)  | 1:4:A:LEU:HD11 | 1:6:A:LYS:HB3  | 19       | 0.27          |
| (1,53)  | 1:4:A:LEU:HD12 | 1:6:A:LYS:HB2  | 19       | 0.27          |
| (1,53)  | 1:4:A:LEU:HD12 | 1:6:A:LYS:HB3  | 19       | 0.27          |
| (1,53)  | 1:4:A:LEU:HD13 | 1:6:A:LYS:HB2  | 19       | 0.27          |
| (1,53)  | 1:4:A:LEU:HD13 | 1:6:A:LYS:HB3  | 19       | 0.27          |
| (1,53)  | 1:4:A:LEU:HD21 | 1:6:A:LYS:HB2  | 19       | 0.27          |
| (1,53)  | 1:4:A:LEU:HD21 | 1:6:A:LYS:HB3  | 19       | 0.27          |
| (1,53)  | 1:4:A:LEU:HD22 | 1:6:A:LYS:HB2  | 19       | 0.27          |
| (1,53)  | 1:4:A:LEU:HD22 | 1:6:A:LYS:HB3  | 19       | 0.27          |
| (1,53)  | 1:4:A:LEU:HD23 | 1:6:A:LYS:HB2  | 19       | 0.27          |
| (1,53)  | 1:4:A:LEU:HD23 | 1:6:A:LYS:HB3  | 19       | 0.27          |
| (1,215) | 1:14:A:GLN:H   | 1:15:A:ARG:HA  | 17       | 0.26          |
| (1,157) | 1:11:A:PHE:HA  | 1:11:A:PHE:HE1 | 14       | 0.26          |
| (1,157) | 1:11:A:PHE:HA  | 1:11:A:PHE:HE2 | 14       | 0.26          |
| (1,157) | 1:11:A:PHE:HA  | 1:11:A:PHE:HE1 | 20       | 0.26          |
| (1,157) | 1:11:A:PHE:HA  | 1:11:A:PHE:HE2 | 20       | 0.26          |
| (1,139) | 1:9:A:ARG:HA   | 1:9:A:ARG:HD2  | 3        | 0.26          |
| (1,139) | 1:9:A:ARG:HA   | 1:9:A:ARG:HD3  | 3        | 0.26          |
| (1,139) | 1:9:A:ARG:HA   | 1:9:A:ARG:HD2  | 9        | 0.26          |
| (1,139) | 1:9:A:ARG:HA   | 1:9:A:ARG:HD3  | 9        | 0.26          |
| (1,132) | 1:8:A:PHE:HB2  | 1:11:A:PHE:HB2 | 2        | 0.26          |
| (1,132) | 1:8:A:PHE:HB2  | 1:11:A:PHE:HB3 | 2        | 0.26          |
| (1,132) | 1:8:A:PHE:HB3  | 1:11:A:PHE:HB2 | 2        | 0.26          |
| (1,132) | 1:8:A:PHE:HB3  | 1:11:A:PHE:HB3 | 2        | 0.26          |
| (1,132) | 1:8:A:PHE:HB2  | 1:11:A:PHE:HB2 | 13       | 0.26          |
| (1,132) | 1:8:A:PHE:HB2  | 1:11:A:PHE:HB3 | 13       | 0.26          |
| (1,132) | 1:8:A:PHE:HB3  | 1:11:A:PHE:HB2 | 13       | 0.26          |
| (1,132) | 1:8:A:PHE:HB3  | 1:11:A:PHE:HB3 | 13       | 0.26          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,132) | 1:8:A:PHE:HB2   | 1:11:A:PHE:HB2 | 15       | 0.26          |
| (1,132) | 1:8:A:PHE:HB2   | 1:11:A:PHE:HB3 | 15       | 0.26          |
| (1,132) | 1:8:A:PHE:HB3   | 1:11:A:PHE:HB2 | 15       | 0.26          |
| (1,132) | 1:8:A:PHE:HB3   | 1:11:A:PHE:HB3 | 15       | 0.26          |
| (1,116) | 1:7:A:PHE:H     | 1:7:A:PHE:HZ   | 2        | 0.26          |
| (1,106) | 1:6:A:LYS:HA    | 1:9:A:ARG:HG2  | 19       | 0.26          |
| (1,106) | 1:6:A:LYS:HA    | 1:9:A:ARG:HG3  | 19       | 0.26          |
| (1,103) | 1:6:A:LYS:HA    | 1:8:A:PHE:HA   | 7        | 0.26          |
| (1,103) | 1:6:A:LYS:HA    | 1:8:A:PHE:HA   | 9        | 0.26          |
| (1,103) | 1:6:A:LYS:HA    | 1:8:A:PHE:HA   | 16       | 0.26          |
| (1,53)  | 1:4:A:LEU:HD11  | 1:6:A:LYS:HB2  | 13       | 0.26          |
| (1,53)  | 1:4:A:LEU:HD11  | 1:6:A:LYS:HB3  | 13       | 0.26          |
| (1,53)  | 1:4:A:LEU:HD12  | 1:6:A:LYS:HB2  | 13       | 0.26          |
| (1,53)  | 1:4:A:LEU:HD12  | 1:6:A:LYS:HB3  | 13       | 0.26          |
| (1,53)  | 1:4:A:LEU:HD13  | 1:6:A:LYS:HB2  | 13       | 0.26          |
| (1,53)  | 1:4:A:LEU:HD13  | 1:6:A:LYS:HB3  | 13       | 0.26          |
| (1,53)  | 1:4:A:LEU:HD21  | 1:6:A:LYS:HB2  | 13       | 0.26          |
| (1,53)  | 1:4:A:LEU:HD21  | 1:6:A:LYS:HB3  | 13       | 0.26          |
| (1,53)  | 1:4:A:LEU:HD22  | 1:6:A:LYS:HB2  | 13       | 0.26          |
| (1,53)  | 1:4:A:LEU:HD22  | 1:6:A:LYS:HB3  | 13       | 0.26          |
| (1,53)  | 1:4:A:LEU:HD23  | 1:6:A:LYS:HB2  | 13       | 0.26          |
| (1,53)  | 1:4:A:LEU:HD23  | 1:6:A:LYS:HB3  | 13       | 0.26          |
| (1,31)  | 1:3:A:ARG:HG2   | 1:6:A:LYS:HA   | 7        | 0.26          |
| (1,31)  | 1:3:A:ARG:HG3   | 1:6:A:LYS:HA   | 7        | 0.26          |
| (1,31)  | 1:3:A:ARG:HG2   | 1:6:A:LYS:HA   | 10       | 0.26          |
| (1,31)  | 1:3:A:ARG:HG3   | 1:6:A:LYS:HA   | 10       | 0.26          |
| (1,215) | 1:14:A:GLN:H    | 1:15:A:ARG:HA  | 12       | 0.25          |
| (1,185) | 1:12:A:ILE:HD11 | 1:13:A:LEU:H   | 16       | 0.25          |
| (1,185) | 1:12:A:ILE:HD12 | 1:13:A:LEU:H   | 16       | 0.25          |
| (1,185) | 1:12:A:ILE:HD13 | 1:13:A:LEU:H   | 16       | 0.25          |
| (1,184) | 1:12:A:ILE:HB   | 1:13:A:LEU:H   | 6        | 0.25          |
| (1,184) | 1:12:A:ILE:HB   | 1:13:A:LEU:H   | 12       | 0.25          |
| (1,184) | 1:12:A:ILE:HB   | 1:13:A:LEU:H   | 20       | 0.25          |
| (1,150) | 1:9:A:ARG:HG2   | 1:12:A:ILE:HA  | 14       | 0.25          |
| (1,150) | 1:9:A:ARG:HG3   | 1:12:A:ILE:HA  | 14       | 0.25          |
| (1,139) | 1:9:A:ARG:HA    | 1:9:A:ARG:HD2  | 8        | 0.25          |
| (1,139) | 1:9:A:ARG:HA    | 1:9:A:ARG:HD3  | 8        | 0.25          |
| (1,120) | 1:8:A:PHE:HA    | 1:8:A:PHE:HE1  | 12       | 0.25          |
| (1,120) | 1:8:A:PHE:HA    | 1:8:A:PHE:HE2  | 12       | 0.25          |
| (1,116) | 1:7:A:PHE:H     | 1:7:A:PHE:HZ   | 1        | 0.25          |
| (1,116) | 1:7:A:PHE:H     | 1:7:A:PHE:HZ   | 4        | 0.25          |
| (1,116) | 1:7:A:PHE:H     | 1:7:A:PHE:HZ   | 13       | 0.25          |

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| Key     | Atom-1          | Atom-2        | Model ID | Violation (Å) |
|---------|-----------------|---------------|----------|---------------|
| (1,116) | 1:7:A:PHE:H     | 1:7:A:PHE:HZ  | 15       | 0.25          |
| (1,106) | 1:6:A:LYS:HA    | 1:9:A:ARG:HG2 | 11       | 0.25          |
| (1,106) | 1:6:A:LYS:HA    | 1:9:A:ARG:HG3 | 11       | 0.25          |
| (1,103) | 1:6:A:LYS:HA    | 1:8:A:PHE:HA  | 10       | 0.25          |
| (1,95)  | 1:6:A:LYS:HB2   | 1:7:A:PHE:HB2 | 6        | 0.25          |
| (1,95)  | 1:6:A:LYS:HB2   | 1:7:A:PHE:HB3 | 6        | 0.25          |
| (1,95)  | 1:6:A:LYS:HB3   | 1:7:A:PHE:HB2 | 6        | 0.25          |
| (1,95)  | 1:6:A:LYS:HB3   | 1:7:A:PHE:HB3 | 6        | 0.25          |
| (1,31)  | 1:3:A:ARG:HG2   | 1:6:A:LYS:HA  | 2        | 0.25          |
| (1,31)  | 1:3:A:ARG:HG3   | 1:6:A:LYS:HA  | 2        | 0.25          |
| (1,31)  | 1:3:A:ARG:HG2   | 1:6:A:LYS:HA  | 6        | 0.25          |
| (1,31)  | 1:3:A:ARG:HG3   | 1:6:A:LYS:HA  | 6        | 0.25          |
| (1,31)  | 1:3:A:ARG:HG2   | 1:6:A:LYS:HA  | 17       | 0.25          |
| (1,31)  | 1:3:A:ARG:HG3   | 1:6:A:LYS:HA  | 17       | 0.25          |
| (1,31)  | 1:3:A:ARG:HG2   | 1:6:A:LYS:HA  | 19       | 0.25          |
| (1,31)  | 1:3:A:ARG:HG3   | 1:6:A:LYS:HA  | 19       | 0.25          |
| (1,18)  | 1:3:A:ARG:HB2   | 1:3:A:ARG:H   | 6        | 0.25          |
| (1,18)  | 1:3:A:ARG:HB3   | 1:3:A:ARG:H   | 6        | 0.25          |
| (1,214) | 1:14:A:GLN:HG2  | 1:15:A:ARG:H  | 17       | 0.24          |
| (1,214) | 1:14:A:GLN:HG3  | 1:15:A:ARG:H  | 17       | 0.24          |
| (1,188) | 1:12:A:ILE:H    | 1:13:A:LEU:H  | 16       | 0.24          |
| (1,185) | 1:12:A:ILE:HD11 | 1:13:A:LEU:H  | 4        | 0.24          |
| (1,185) | 1:12:A:ILE:HD12 | 1:13:A:LEU:H  | 4        | 0.24          |
| (1,185) | 1:12:A:ILE:HD13 | 1:13:A:LEU:H  | 4        | 0.24          |
| (1,184) | 1:12:A:ILE:HB   | 1:13:A:LEU:H  | 8        | 0.24          |
| (1,184) | 1:12:A:ILE:HB   | 1:13:A:LEU:H  | 11       | 0.24          |
| (1,179) | 1:12:A:ILE:HG12 | 1:12:A:ILE:H  | 2        | 0.24          |
| (1,179) | 1:12:A:ILE:HG13 | 1:12:A:ILE:H  | 2        | 0.24          |
| (1,179) | 1:12:A:ILE:HG12 | 1:12:A:ILE:H  | 13       | 0.24          |
| (1,179) | 1:12:A:ILE:HG13 | 1:12:A:ILE:H  | 13       | 0.24          |
| (1,150) | 1:9:A:ARG:HG2   | 1:12:A:ILE:HA | 11       | 0.24          |
| (1,150) | 1:9:A:ARG:HG3   | 1:12:A:ILE:HA | 11       | 0.24          |
| (1,146) | 1:9:A:ARG:HD2   | 1:9:A:ARG:H   | 3        | 0.24          |
| (1,146) | 1:9:A:ARG:HD3   | 1:9:A:ARG:H   | 3        | 0.24          |
| (1,106) | 1:6:A:LYS:HA    | 1:9:A:ARG:HG2 | 14       | 0.24          |
| (1,106) | 1:6:A:LYS:HA    | 1:9:A:ARG:HG3 | 14       | 0.24          |
| (1,31)  | 1:3:A:ARG:HG2   | 1:6:A:LYS:HA  | 20       | 0.24          |
| (1,31)  | 1:3:A:ARG:HG3   | 1:6:A:LYS:HA  | 20       | 0.24          |
| (1,26)  | 1:3:A:ARG:HB2   | 1:4:A:LEU:H   | 17       | 0.24          |
| (1,26)  | 1:3:A:ARG:HB3   | 1:4:A:LEU:H   | 17       | 0.24          |
| (1,214) | 1:14:A:GLN:HG2  | 1:15:A:ARG:H  | 18       | 0.23          |
| (1,214) | 1:14:A:GLN:HG3  | 1:15:A:ARG:H  | 18       | 0.23          |

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| Key     | Atom-1          | Atom-2        | Model ID | Violation (Å) |
|---------|-----------------|---------------|----------|---------------|
| (1,214) | 1:14:A:GLN:HG2  | 1:15:A:ARG:H  | 19       | 0.23          |
| (1,214) | 1:14:A:GLN:HG3  | 1:15:A:ARG:H  | 19       | 0.23          |
| (1,211) | 1:14:A:GLN:HG2  | 1:14:A:GLN:H  | 9        | 0.23          |
| (1,211) | 1:14:A:GLN:HG3  | 1:14:A:GLN:H  | 9        | 0.23          |
| (1,184) | 1:12:A:ILE:HB   | 1:13:A:LEU:H  | 2        | 0.23          |
| (1,184) | 1:12:A:ILE:HB   | 1:13:A:LEU:H  | 9        | 0.23          |
| (1,184) | 1:12:A:ILE:HB   | 1:13:A:LEU:H  | 10       | 0.23          |
| (1,184) | 1:12:A:ILE:HB   | 1:13:A:LEU:H  | 13       | 0.23          |
| (1,184) | 1:12:A:ILE:HB   | 1:13:A:LEU:H  | 15       | 0.23          |
| (1,179) | 1:12:A:ILE:HG12 | 1:12:A:ILE:H  | 8        | 0.23          |
| (1,179) | 1:12:A:ILE:HG13 | 1:12:A:ILE:H  | 8        | 0.23          |
| (1,179) | 1:12:A:ILE:HG12 | 1:12:A:ILE:H  | 11       | 0.23          |
| (1,179) | 1:12:A:ILE:HG13 | 1:12:A:ILE:H  | 11       | 0.23          |
| (1,179) | 1:12:A:ILE:HG12 | 1:12:A:ILE:H  | 15       | 0.23          |
| (1,179) | 1:12:A:ILE:HG13 | 1:12:A:ILE:H  | 15       | 0.23          |
| (1,139) | 1:9:A:ARG:HA    | 1:9:A:ARG:HD2 | 6        | 0.23          |
| (1,139) | 1:9:A:ARG:HA    | 1:9:A:ARG:HD3 | 6        | 0.23          |
| (1,116) | 1:7:A:PHE:H     | 1:7:A:PHE:HZ  | 5        | 0.23          |
| (1,116) | 1:7:A:PHE:H     | 1:7:A:PHE:HZ  | 8        | 0.23          |
| (1,103) | 1:6:A:LYS:HA    | 1:8:A:PHE:HA  | 3        | 0.23          |
| (1,31)  | 1:3:A:ARG:HG2   | 1:6:A:LYS:HA  | 14       | 0.23          |
| (1,31)  | 1:3:A:ARG:HG3   | 1:6:A:LYS:HA  | 14       | 0.23          |
| (1,214) | 1:14:A:GLN:HG2  | 1:15:A:ARG:H  | 2        | 0.22          |
| (1,214) | 1:14:A:GLN:HG3  | 1:15:A:ARG:H  | 2        | 0.22          |
| (1,214) | 1:14:A:GLN:HG2  | 1:15:A:ARG:H  | 6        | 0.22          |
| (1,214) | 1:14:A:GLN:HG3  | 1:15:A:ARG:H  | 6        | 0.22          |
| (1,214) | 1:14:A:GLN:HG2  | 1:15:A:ARG:H  | 11       | 0.22          |
| (1,214) | 1:14:A:GLN:HG3  | 1:15:A:ARG:H  | 11       | 0.22          |
| (1,214) | 1:14:A:GLN:HG2  | 1:15:A:ARG:H  | 15       | 0.22          |
| (1,214) | 1:14:A:GLN:HG3  | 1:15:A:ARG:H  | 15       | 0.22          |
| (1,184) | 1:12:A:ILE:HB   | 1:13:A:LEU:H  | 17       | 0.22          |
| (1,154) | 1:9:A:ARG:HG2   | 1:13:A:LEU:H  | 3        | 0.22          |
| (1,154) | 1:9:A:ARG:HG3   | 1:13:A:LEU:H  | 3        | 0.22          |
| (1,150) | 1:9:A:ARG:HG2   | 1:12:A:ILE:HA | 10       | 0.22          |
| (1,150) | 1:9:A:ARG:HG3   | 1:12:A:ILE:HA | 10       | 0.22          |
| (1,124) | 1:8:A:PHE:HB2   | 1:8:A:PHE:HZ  | 6        | 0.22          |
| (1,124) | 1:8:A:PHE:HB3   | 1:8:A:PHE:HZ  | 6        | 0.22          |
| (1,106) | 1:6:A:LYS:HA    | 1:9:A:ARG:HG2 | 6        | 0.22          |
| (1,106) | 1:6:A:LYS:HA    | 1:9:A:ARG:HG3 | 6        | 0.22          |
| (1,106) | 1:6:A:LYS:HA    | 1:9:A:ARG:HG2 | 16       | 0.22          |
| (1,106) | 1:6:A:LYS:HA    | 1:9:A:ARG:HG3 | 16       | 0.22          |
| (1,26)  | 1:3:A:ARG:HB2   | 1:4:A:LEU:H   | 2        | 0.22          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,26)  | 1:3:A:ARG:HB3   | 1:4:A:LEU:H    | 2        | 0.22          |
| (1,26)  | 1:3:A:ARG:HB2   | 1:4:A:LEU:H    | 14       | 0.22          |
| (1,26)  | 1:3:A:ARG:HB3   | 1:4:A:LEU:H    | 14       | 0.22          |
| (2,1)   | 1:12:A:ILE:HG22 | 1:13:A:LEU:H   | 6        | 0.21          |
| (1,215) | 1:14:A:GLN:H    | 1:15:A:ARG:HA  | 3        | 0.21          |
| (1,215) | 1:14:A:GLN:H    | 1:15:A:ARG:HA  | 5        | 0.21          |
| (1,215) | 1:14:A:GLN:H    | 1:15:A:ARG:HA  | 7        | 0.21          |
| (1,214) | 1:14:A:GLN:HG2  | 1:15:A:ARG:H   | 13       | 0.21          |
| (1,214) | 1:14:A:GLN:HG3  | 1:15:A:ARG:H   | 13       | 0.21          |
| (1,214) | 1:14:A:GLN:HG2  | 1:15:A:ARG:H   | 14       | 0.21          |
| (1,214) | 1:14:A:GLN:HG3  | 1:15:A:ARG:H   | 14       | 0.21          |
| (1,201) | 1:13:A:LEU:H    | 1:14:A:GLN:H   | 19       | 0.21          |
| (1,179) | 1:12:A:ILE:HG12 | 1:12:A:ILE:H   | 6        | 0.21          |
| (1,179) | 1:12:A:ILE:HG13 | 1:12:A:ILE:H   | 6        | 0.21          |
| (1,179) | 1:12:A:ILE:HG12 | 1:12:A:ILE:H   | 10       | 0.21          |
| (1,179) | 1:12:A:ILE:HG13 | 1:12:A:ILE:H   | 10       | 0.21          |
| (1,154) | 1:9:A:ARG:HG2   | 1:13:A:LEU:H   | 16       | 0.21          |
| (1,154) | 1:9:A:ARG:HG3   | 1:13:A:LEU:H   | 16       | 0.21          |
| (1,150) | 1:9:A:ARG:HG2   | 1:12:A:ILE:HA  | 4        | 0.21          |
| (1,150) | 1:9:A:ARG:HG3   | 1:12:A:ILE:HA  | 4        | 0.21          |
| (1,146) | 1:9:A:ARG:HD2   | 1:9:A:ARG:H    | 16       | 0.21          |
| (1,146) | 1:9:A:ARG:HD3   | 1:9:A:ARG:H    | 16       | 0.21          |
| (1,132) | 1:8:A:PHE:HB2   | 1:11:A:PHE:HB2 | 20       | 0.21          |
| (1,132) | 1:8:A:PHE:HB2   | 1:11:A:PHE:HB3 | 20       | 0.21          |
| (1,132) | 1:8:A:PHE:HB3   | 1:11:A:PHE:HB2 | 20       | 0.21          |
| (1,132) | 1:8:A:PHE:HB3   | 1:11:A:PHE:HB3 | 20       | 0.21          |
| (1,124) | 1:8:A:PHE:HB2   | 1:8:A:PHE:HZ   | 1        | 0.21          |
| (1,124) | 1:8:A:PHE:HB3   | 1:8:A:PHE:HZ   | 1        | 0.21          |
| (1,124) | 1:8:A:PHE:HB2   | 1:8:A:PHE:HZ   | 2        | 0.21          |
| (1,124) | 1:8:A:PHE:HB3   | 1:8:A:PHE:HZ   | 2        | 0.21          |
| (1,124) | 1:8:A:PHE:HB2   | 1:8:A:PHE:HZ   | 3        | 0.21          |
| (1,124) | 1:8:A:PHE:HB3   | 1:8:A:PHE:HZ   | 3        | 0.21          |
| (1,124) | 1:8:A:PHE:HB2   | 1:8:A:PHE:HZ   | 4        | 0.21          |
| (1,124) | 1:8:A:PHE:HB3   | 1:8:A:PHE:HZ   | 4        | 0.21          |
| (1,124) | 1:8:A:PHE:HB2   | 1:8:A:PHE:HZ   | 5        | 0.21          |
| (1,124) | 1:8:A:PHE:HB3   | 1:8:A:PHE:HZ   | 5        | 0.21          |
| (1,124) | 1:8:A:PHE:HB2   | 1:8:A:PHE:HZ   | 7        | 0.21          |
| (1,124) | 1:8:A:PHE:HB3   | 1:8:A:PHE:HZ   | 7        | 0.21          |
| (1,124) | 1:8:A:PHE:HB2   | 1:8:A:PHE:HZ   | 8        | 0.21          |
| (1,124) | 1:8:A:PHE:HB3   | 1:8:A:PHE:HZ   | 8        | 0.21          |
| (1,124) | 1:8:A:PHE:HB2   | 1:8:A:PHE:HZ   | 9        | 0.21          |
| (1,124) | 1:8:A:PHE:HB3   | 1:8:A:PHE:HZ   | 9        | 0.21          |

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| Key     | Atom-1        | Atom-2         | Model ID | Violation (Å) |
|---------|---------------|----------------|----------|---------------|
| (1,124) | 1:8:A:PHE:HB2 | 1:8:A:PHE:HZ   | 10       | 0.21          |
| (1,124) | 1:8:A:PHE:HB3 | 1:8:A:PHE:HZ   | 10       | 0.21          |
| (1,124) | 1:8:A:PHE:HB2 | 1:8:A:PHE:HZ   | 11       | 0.21          |
| (1,124) | 1:8:A:PHE:HB3 | 1:8:A:PHE:HZ   | 11       | 0.21          |
| (1,124) | 1:8:A:PHE:HB2 | 1:8:A:PHE:HZ   | 12       | 0.21          |
| (1,124) | 1:8:A:PHE:HB3 | 1:8:A:PHE:HZ   | 12       | 0.21          |
| (1,124) | 1:8:A:PHE:HB2 | 1:8:A:PHE:HZ   | 13       | 0.21          |
| (1,124) | 1:8:A:PHE:HB3 | 1:8:A:PHE:HZ   | 13       | 0.21          |
| (1,124) | 1:8:A:PHE:HB2 | 1:8:A:PHE:HZ   | 14       | 0.21          |
| (1,124) | 1:8:A:PHE:HB3 | 1:8:A:PHE:HZ   | 14       | 0.21          |
| (1,124) | 1:8:A:PHE:HB2 | 1:8:A:PHE:HZ   | 15       | 0.21          |
| (1,124) | 1:8:A:PHE:HB3 | 1:8:A:PHE:HZ   | 15       | 0.21          |
| (1,124) | 1:8:A:PHE:HB2 | 1:8:A:PHE:HZ   | 16       | 0.21          |
| (1,124) | 1:8:A:PHE:HB3 | 1:8:A:PHE:HZ   | 16       | 0.21          |
| (1,124) | 1:8:A:PHE:HB2 | 1:8:A:PHE:HZ   | 17       | 0.21          |
| (1,124) | 1:8:A:PHE:HB3 | 1:8:A:PHE:HZ   | 17       | 0.21          |
| (1,124) | 1:8:A:PHE:HB2 | 1:8:A:PHE:HZ   | 18       | 0.21          |
| (1,124) | 1:8:A:PHE:HB3 | 1:8:A:PHE:HZ   | 18       | 0.21          |
| (1,124) | 1:8:A:PHE:HB2 | 1:8:A:PHE:HZ   | 19       | 0.21          |
| (1,124) | 1:8:A:PHE:HB3 | 1:8:A:PHE:HZ   | 19       | 0.21          |
| (1,124) | 1:8:A:PHE:HB2 | 1:8:A:PHE:HZ   | 20       | 0.21          |
| (1,124) | 1:8:A:PHE:HB3 | 1:8:A:PHE:HZ   | 20       | 0.21          |
| (1,106) | 1:6:A:LYS:HA  | 1:9:A:ARG:HG2  | 8        | 0.21          |
| (1,106) | 1:6:A:LYS:HA  | 1:9:A:ARG:HG3  | 8        | 0.21          |
| (1,31)  | 1:3:A:ARG:HG2 | 1:6:A:LYS:HA   | 3        | 0.21          |
| (1,31)  | 1:3:A:ARG:HG3 | 1:6:A:LYS:HA   | 3        | 0.21          |
| (1,27)  | 1:3:A:ARG:HG2 | 1:4:A:LEU:HD11 | 3        | 0.21          |
| (1,27)  | 1:3:A:ARG:HG2 | 1:4:A:LEU:HD12 | 3        | 0.21          |
| (1,27)  | 1:3:A:ARG:HG2 | 1:4:A:LEU:HD13 | 3        | 0.21          |
| (1,27)  | 1:3:A:ARG:HG2 | 1:4:A:LEU:HD21 | 3        | 0.21          |
| (1,27)  | 1:3:A:ARG:HG2 | 1:4:A:LEU:HD22 | 3        | 0.21          |
| (1,27)  | 1:3:A:ARG:HG2 | 1:4:A:LEU:HD23 | 3        | 0.21          |
| (1,27)  | 1:3:A:ARG:HG3 | 1:4:A:LEU:HD11 | 3        | 0.21          |
| (1,27)  | 1:3:A:ARG:HG3 | 1:4:A:LEU:HD12 | 3        | 0.21          |
| (1,27)  | 1:3:A:ARG:HG3 | 1:4:A:LEU:HD13 | 3        | 0.21          |
| (1,27)  | 1:3:A:ARG:HG3 | 1:4:A:LEU:HD21 | 3        | 0.21          |
| (1,27)  | 1:3:A:ARG:HG3 | 1:4:A:LEU:HD22 | 3        | 0.21          |
| (1,27)  | 1:3:A:ARG:HG3 | 1:4:A:LEU:HD23 | 3        | 0.21          |
| (1,26)  | 1:3:A:ARG:HB2 | 1:4:A:LEU:H    | 1        | 0.21          |
| (1,26)  | 1:3:A:ARG:HB3 | 1:4:A:LEU:H    | 1        | 0.21          |
| (1,26)  | 1:3:A:ARG:HB2 | 1:4:A:LEU:H    | 19       | 0.21          |
| (1,26)  | 1:3:A:ARG:HB3 | 1:4:A:LEU:H    | 19       | 0.21          |

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| Key     | Atom-1          | Atom-2        | Model ID | Violation (Å) |
|---------|-----------------|---------------|----------|---------------|
| (2,1)   | 1:12:A:ILE:HG23 | 1:13:A:LEU:H  | 8        | 0.2           |
| (1,217) | 1:14:A:GLN:HA   | 1:16:A:LYS:H  | 9        | 0.2           |
| (1,217) | 1:14:A:GLN:HA   | 1:16:A:LYS:H  | 12       | 0.2           |
| (1,215) | 1:14:A:GLN:H    | 1:15:A:ARG:HA | 16       | 0.2           |
| (1,214) | 1:14:A:GLN:HG2  | 1:15:A:ARG:H  | 8        | 0.2           |
| (1,214) | 1:14:A:GLN:HG3  | 1:15:A:ARG:H  | 8        | 0.2           |
| (1,214) | 1:14:A:GLN:HG2  | 1:15:A:ARG:H  | 20       | 0.2           |
| (1,214) | 1:14:A:GLN:HG3  | 1:15:A:ARG:H  | 20       | 0.2           |
| (1,201) | 1:13:A:LEU:H    | 1:14:A:GLN:H  | 3        | 0.2           |
| (1,185) | 1:12:A:ILE:HD11 | 1:13:A:LEU:H  | 3        | 0.2           |
| (1,185) | 1:12:A:ILE:HD12 | 1:13:A:LEU:H  | 3        | 0.2           |
| (1,185) | 1:12:A:ILE:HD13 | 1:13:A:LEU:H  | 3        | 0.2           |
| (1,184) | 1:12:A:ILE:HB   | 1:13:A:LEU:H  | 1        | 0.2           |
| (1,184) | 1:12:A:ILE:HB   | 1:13:A:LEU:H  | 19       | 0.2           |
| (1,179) | 1:12:A:ILE:HG12 | 1:12:A:ILE:H  | 9        | 0.2           |
| (1,179) | 1:12:A:ILE:HG13 | 1:12:A:ILE:H  | 9        | 0.2           |
| (1,146) | 1:9:A:ARG:HD2   | 1:9:A:ARG:H   | 8        | 0.2           |
| (1,146) | 1:9:A:ARG:HD3   | 1:9:A:ARG:H   | 8        | 0.2           |
| (1,106) | 1:6:A:LYS:HA    | 1:9:A:ARG:HG2 | 3        | 0.2           |
| (1,106) | 1:6:A:LYS:HA    | 1:9:A:ARG:HG3 | 3        | 0.2           |
| (1,106) | 1:6:A:LYS:HA    | 1:9:A:ARG:HG2 | 18       | 0.2           |
| (1,106) | 1:6:A:LYS:HA    | 1:9:A:ARG:HG3 | 18       | 0.2           |
| (1,26)  | 1:3:A:ARG:HB2   | 1:4:A:LEU:H   | 11       | 0.2           |
| (1,26)  | 1:3:A:ARG:HB3   | 1:4:A:LEU:H   | 11       | 0.2           |
| (1,250) | 1:17:A:LYS:HG2  | 1:17:A:LYS:H  | 11       | 0.19          |
| (1,250) | 1:17:A:LYS:HG3  | 1:17:A:LYS:H  | 11       | 0.19          |
| (1,215) | 1:14:A:GLN:H    | 1:15:A:ARG:HA | 9        | 0.19          |
| (1,214) | 1:14:A:GLN:HG2  | 1:15:A:ARG:H  | 1        | 0.19          |
| (1,214) | 1:14:A:GLN:HG3  | 1:15:A:ARG:H  | 1        | 0.19          |
| (1,203) | 1:13:A:LEU:HD11 | 1:15:A:ARG:HA | 14       | 0.19          |
| (1,203) | 1:13:A:LEU:HD12 | 1:15:A:ARG:HA | 14       | 0.19          |
| (1,203) | 1:13:A:LEU:HD13 | 1:15:A:ARG:HA | 14       | 0.19          |
| (1,203) | 1:13:A:LEU:HD21 | 1:15:A:ARG:HA | 14       | 0.19          |
| (1,203) | 1:13:A:LEU:HD22 | 1:15:A:ARG:HA | 14       | 0.19          |
| (1,203) | 1:13:A:LEU:HD23 | 1:15:A:ARG:HA | 14       | 0.19          |
| (1,203) | 1:13:A:LEU:HD11 | 1:15:A:ARG:HA | 15       | 0.19          |
| (1,203) | 1:13:A:LEU:HD12 | 1:15:A:ARG:HA | 15       | 0.19          |
| (1,203) | 1:13:A:LEU:HD13 | 1:15:A:ARG:HA | 15       | 0.19          |
| (1,203) | 1:13:A:LEU:HD21 | 1:15:A:ARG:HA | 15       | 0.19          |
| (1,203) | 1:13:A:LEU:HD22 | 1:15:A:ARG:HA | 15       | 0.19          |
| (1,203) | 1:13:A:LEU:HD23 | 1:15:A:ARG:HA | 15       | 0.19          |
| (1,196) | 1:13:A:LEU:HD11 | 1:13:A:LEU:H  | 17       | 0.19          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,196) | 1:13:A:LEU:HD12 | 1:13:A:LEU:H   | 17       | 0.19          |
| (1,196) | 1:13:A:LEU:HD13 | 1:13:A:LEU:H   | 17       | 0.19          |
| (1,196) | 1:13:A:LEU:HD21 | 1:13:A:LEU:H   | 17       | 0.19          |
| (1,196) | 1:13:A:LEU:HD22 | 1:13:A:LEU:H   | 17       | 0.19          |
| (1,196) | 1:13:A:LEU:HD23 | 1:13:A:LEU:H   | 17       | 0.19          |
| (1,196) | 1:13:A:LEU:HD11 | 1:13:A:LEU:H   | 18       | 0.19          |
| (1,196) | 1:13:A:LEU:HD12 | 1:13:A:LEU:H   | 18       | 0.19          |
| (1,196) | 1:13:A:LEU:HD13 | 1:13:A:LEU:H   | 18       | 0.19          |
| (1,196) | 1:13:A:LEU:HD21 | 1:13:A:LEU:H   | 18       | 0.19          |
| (1,196) | 1:13:A:LEU:HD22 | 1:13:A:LEU:H   | 18       | 0.19          |
| (1,196) | 1:13:A:LEU:HD23 | 1:13:A:LEU:H   | 18       | 0.19          |
| (1,184) | 1:12:A:ILE:HB   | 1:13:A:LEU:H   | 7        | 0.19          |
| (1,184) | 1:12:A:ILE:HB   | 1:13:A:LEU:H   | 14       | 0.19          |
| (1,164) | 1:11:A:PHE:HB2  | 1:12:A:ILE:H   | 12       | 0.19          |
| (1,164) | 1:11:A:PHE:HB3  | 1:12:A:ILE:H   | 12       | 0.19          |
| (1,106) | 1:6:A:LYS:HA    | 1:9:A:ARG:HG2  | 7        | 0.19          |
| (1,106) | 1:6:A:LYS:HA    | 1:9:A:ARG:HG3  | 7        | 0.19          |
| (1,106) | 1:6:A:LYS:HA    | 1:9:A:ARG:HG2  | 10       | 0.19          |
| (1,106) | 1:6:A:LYS:HA    | 1:9:A:ARG:HG3  | 10       | 0.19          |
| (1,27)  | 1:3:A:ARG:HG2   | 1:4:A:LEU:HD11 | 9        | 0.19          |
| (1,27)  | 1:3:A:ARG:HG2   | 1:4:A:LEU:HD12 | 9        | 0.19          |
| (1,27)  | 1:3:A:ARG:HG2   | 1:4:A:LEU:HD13 | 9        | 0.19          |
| (1,27)  | 1:3:A:ARG:HG2   | 1:4:A:LEU:HD21 | 9        | 0.19          |
| (1,27)  | 1:3:A:ARG:HG2   | 1:4:A:LEU:HD22 | 9        | 0.19          |
| (1,27)  | 1:3:A:ARG:HG2   | 1:4:A:LEU:HD23 | 9        | 0.19          |
| (1,27)  | 1:3:A:ARG:HG3   | 1:4:A:LEU:HD11 | 9        | 0.19          |
| (1,27)  | 1:3:A:ARG:HG3   | 1:4:A:LEU:HD12 | 9        | 0.19          |
| (1,27)  | 1:3:A:ARG:HG3   | 1:4:A:LEU:HD13 | 9        | 0.19          |
| (1,27)  | 1:3:A:ARG:HG3   | 1:4:A:LEU:HD21 | 9        | 0.19          |
| (1,27)  | 1:3:A:ARG:HG3   | 1:4:A:LEU:HD22 | 9        | 0.19          |
| (1,27)  | 1:3:A:ARG:HG3   | 1:4:A:LEU:HD23 | 9        | 0.19          |
| (1,217) | 1:14:A:GLN:HA   | 1:16:A:LYS:H   | 3        | 0.18          |
| (1,217) | 1:14:A:GLN:HA   | 1:16:A:LYS:H   | 5        | 0.18          |
| (1,217) | 1:14:A:GLN:HA   | 1:16:A:LYS:H   | 16       | 0.18          |
| (1,215) | 1:14:A:GLN:H    | 1:15:A:ARG:HA  | 10       | 0.18          |
| (1,203) | 1:13:A:LEU:HD11 | 1:15:A:ARG:HA  | 2        | 0.18          |
| (1,203) | 1:13:A:LEU:HD12 | 1:15:A:ARG:HA  | 2        | 0.18          |
| (1,203) | 1:13:A:LEU:HD13 | 1:15:A:ARG:HA  | 2        | 0.18          |
| (1,203) | 1:13:A:LEU:HD21 | 1:15:A:ARG:HA  | 2        | 0.18          |
| (1,203) | 1:13:A:LEU:HD22 | 1:15:A:ARG:HA  | 2        | 0.18          |
| (1,203) | 1:13:A:LEU:HD23 | 1:15:A:ARG:HA  | 2        | 0.18          |
| (1,203) | 1:13:A:LEU:HD11 | 1:15:A:ARG:HA  | 7        | 0.18          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,203) | 1:13:A:LEU:HD12 | 1:15:A:ARG:HA  | 7        | 0.18          |
| (1,203) | 1:13:A:LEU:HD13 | 1:15:A:ARG:HA  | 7        | 0.18          |
| (1,203) | 1:13:A:LEU:HD21 | 1:15:A:ARG:HA  | 7        | 0.18          |
| (1,203) | 1:13:A:LEU:HD22 | 1:15:A:ARG:HA  | 7        | 0.18          |
| (1,203) | 1:13:A:LEU:HD23 | 1:15:A:ARG:HA  | 7        | 0.18          |
| (1,203) | 1:13:A:LEU:HD11 | 1:15:A:ARG:HA  | 8        | 0.18          |
| (1,203) | 1:13:A:LEU:HD12 | 1:15:A:ARG:HA  | 8        | 0.18          |
| (1,203) | 1:13:A:LEU:HD13 | 1:15:A:ARG:HA  | 8        | 0.18          |
| (1,203) | 1:13:A:LEU:HD21 | 1:15:A:ARG:HA  | 8        | 0.18          |
| (1,203) | 1:13:A:LEU:HD22 | 1:15:A:ARG:HA  | 8        | 0.18          |
| (1,203) | 1:13:A:LEU:HD23 | 1:15:A:ARG:HA  | 8        | 0.18          |
| (1,203) | 1:13:A:LEU:HD11 | 1:15:A:ARG:HA  | 13       | 0.18          |
| (1,203) | 1:13:A:LEU:HD12 | 1:15:A:ARG:HA  | 13       | 0.18          |
| (1,203) | 1:13:A:LEU:HD13 | 1:15:A:ARG:HA  | 13       | 0.18          |
| (1,203) | 1:13:A:LEU:HD21 | 1:15:A:ARG:HA  | 13       | 0.18          |
| (1,203) | 1:13:A:LEU:HD22 | 1:15:A:ARG:HA  | 13       | 0.18          |
| (1,203) | 1:13:A:LEU:HD23 | 1:15:A:ARG:HA  | 13       | 0.18          |
| (1,184) | 1:12:A:ILE:HB   | 1:13:A:LEU:H   | 5        | 0.18          |
| (1,181) | 1:12:A:ILE:HD11 | 1:12:A:ILE:H   | 12       | 0.18          |
| (1,154) | 1:9:A:ARG:HG2   | 1:13:A:LEU:H   | 4        | 0.18          |
| (1,154) | 1:9:A:ARG:HG3   | 1:13:A:LEU:H   | 4        | 0.18          |
| (1,146) | 1:9:A:ARG:HD2   | 1:9:A:ARG:H    | 11       | 0.18          |
| (1,146) | 1:9:A:ARG:HD3   | 1:9:A:ARG:H    | 11       | 0.18          |
| (1,139) | 1:9:A:ARG:HA    | 1:9:A:ARG:HD2  | 18       | 0.18          |
| (1,139) | 1:9:A:ARG:HA    | 1:9:A:ARG:HD3  | 18       | 0.18          |
| (1,106) | 1:6:A:LYS:HA    | 1:9:A:ARG:HG2  | 9        | 0.18          |
| (1,106) | 1:6:A:LYS:HA    | 1:9:A:ARG:HG3  | 9        | 0.18          |
| (1,57)  | 1:4:A:LEU:HA    | 1:7:A:PHE:HZ   | 12       | 0.18          |
| (1,27)  | 1:3:A:ARG:HG2   | 1:4:A:LEU:HD11 | 1        | 0.18          |
| (1,27)  | 1:3:A:ARG:HG2   | 1:4:A:LEU:HD12 | 1        | 0.18          |
| (1,27)  | 1:3:A:ARG:HG2   | 1:4:A:LEU:HD13 | 1        | 0.18          |
| (1,27)  | 1:3:A:ARG:HG2   | 1:4:A:LEU:HD21 | 1        | 0.18          |
| (1,27)  | 1:3:A:ARG:HG2   | 1:4:A:LEU:HD22 | 1        | 0.18          |
| (1,27)  | 1:3:A:ARG:HG2   | 1:4:A:LEU:HD23 | 1        | 0.18          |
| (1,27)  | 1:3:A:ARG:HG3   | 1:4:A:LEU:HD11 | 1        | 0.18          |
| (1,27)  | 1:3:A:ARG:HG3   | 1:4:A:LEU:HD12 | 1        | 0.18          |
| (1,27)  | 1:3:A:ARG:HG3   | 1:4:A:LEU:HD13 | 1        | 0.18          |
| (1,27)  | 1:3:A:ARG:HG3   | 1:4:A:LEU:HD21 | 1        | 0.18          |
| (1,27)  | 1:3:A:ARG:HG3   | 1:4:A:LEU:HD22 | 1        | 0.18          |
| (1,27)  | 1:3:A:ARG:HG3   | 1:4:A:LEU:HD23 | 1        | 0.18          |
| (1,27)  | 1:3:A:ARG:HG2   | 1:4:A:LEU:HD11 | 16       | 0.18          |
| (1,27)  | 1:3:A:ARG:HG2   | 1:4:A:LEU:HD12 | 16       | 0.18          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,27)  | 1:3:A:ARG:HG2   | 1:4:A:LEU:HD13 | 16       | 0.18          |
| (1,27)  | 1:3:A:ARG:HG2   | 1:4:A:LEU:HD21 | 16       | 0.18          |
| (1,27)  | 1:3:A:ARG:HG2   | 1:4:A:LEU:HD22 | 16       | 0.18          |
| (1,27)  | 1:3:A:ARG:HG2   | 1:4:A:LEU:HD23 | 16       | 0.18          |
| (1,27)  | 1:3:A:ARG:HG3   | 1:4:A:LEU:HD11 | 16       | 0.18          |
| (1,27)  | 1:3:A:ARG:HG3   | 1:4:A:LEU:HD12 | 16       | 0.18          |
| (1,27)  | 1:3:A:ARG:HG3   | 1:4:A:LEU:HD13 | 16       | 0.18          |
| (1,27)  | 1:3:A:ARG:HG3   | 1:4:A:LEU:HD21 | 16       | 0.18          |
| (1,27)  | 1:3:A:ARG:HG3   | 1:4:A:LEU:HD22 | 16       | 0.18          |
| (1,27)  | 1:3:A:ARG:HG3   | 1:4:A:LEU:HD23 | 16       | 0.18          |
| (1,26)  | 1:3:A:ARG:HB2   | 1:4:A:LEU:H    | 4        | 0.18          |
| (1,26)  | 1:3:A:ARG:HB3   | 1:4:A:LEU:H    | 4        | 0.18          |
| (1,26)  | 1:3:A:ARG:HB2   | 1:4:A:LEU:H    | 10       | 0.18          |
| (1,26)  | 1:3:A:ARG:HB3   | 1:4:A:LEU:H    | 10       | 0.18          |
| (1,26)  | 1:3:A:ARG:HB2   | 1:4:A:LEU:H    | 16       | 0.18          |
| (1,26)  | 1:3:A:ARG:HB3   | 1:4:A:LEU:H    | 16       | 0.18          |
| (1,217) | 1:14:A:GLN:HA   | 1:16:A:LYS:H   | 10       | 0.17          |
| (1,214) | 1:14:A:GLN:HG2  | 1:15:A:ARG:H   | 4        | 0.17          |
| (1,214) | 1:14:A:GLN:HG3  | 1:15:A:ARG:H   | 4        | 0.17          |
| (1,203) | 1:13:A:LEU:HD11 | 1:15:A:ARG:HA  | 20       | 0.17          |
| (1,203) | 1:13:A:LEU:HD12 | 1:15:A:ARG:HA  | 20       | 0.17          |
| (1,203) | 1:13:A:LEU:HD13 | 1:15:A:ARG:HA  | 20       | 0.17          |
| (1,203) | 1:13:A:LEU:HD21 | 1:15:A:ARG:HA  | 20       | 0.17          |
| (1,203) | 1:13:A:LEU:HD22 | 1:15:A:ARG:HA  | 20       | 0.17          |
| (1,203) | 1:13:A:LEU:HD23 | 1:15:A:ARG:HA  | 20       | 0.17          |
| (1,196) | 1:13:A:LEU:HD11 | 1:13:A:LEU:H   | 6        | 0.17          |
| (1,196) | 1:13:A:LEU:HD12 | 1:13:A:LEU:H   | 6        | 0.17          |
| (1,196) | 1:13:A:LEU:HD13 | 1:13:A:LEU:H   | 6        | 0.17          |
| (1,196) | 1:13:A:LEU:HD21 | 1:13:A:LEU:H   | 6        | 0.17          |
| (1,196) | 1:13:A:LEU:HD22 | 1:13:A:LEU:H   | 6        | 0.17          |
| (1,196) | 1:13:A:LEU:HD23 | 1:13:A:LEU:H   | 6        | 0.17          |
| (1,196) | 1:13:A:LEU:HD11 | 1:13:A:LEU:H   | 12       | 0.17          |
| (1,196) | 1:13:A:LEU:HD12 | 1:13:A:LEU:H   | 12       | 0.17          |
| (1,196) | 1:13:A:LEU:HD13 | 1:13:A:LEU:H   | 12       | 0.17          |
| (1,196) | 1:13:A:LEU:HD21 | 1:13:A:LEU:H   | 12       | 0.17          |
| (1,196) | 1:13:A:LEU:HD22 | 1:13:A:LEU:H   | 12       | 0.17          |
| (1,196) | 1:13:A:LEU:HD23 | 1:13:A:LEU:H   | 12       | 0.17          |
| (1,185) | 1:12:A:ILE:HD11 | 1:13:A:LEU:H   | 18       | 0.17          |
| (1,185) | 1:12:A:ILE:HD12 | 1:13:A:LEU:H   | 18       | 0.17          |
| (1,185) | 1:12:A:ILE:HD13 | 1:13:A:LEU:H   | 18       | 0.17          |
| (1,157) | 1:11:A:PHE:HA   | 1:11:A:PHE:HE1 | 3        | 0.17          |
| (1,157) | 1:11:A:PHE:HA   | 1:11:A:PHE:HE2 | 3        | 0.17          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,150) | 1:9:A:ARG:HG2   | 1:12:A:ILE:HA  | 7        | 0.17          |
| (1,150) | 1:9:A:ARG:HG3   | 1:12:A:ILE:HA  | 7        | 0.17          |
| (1,146) | 1:9:A:ARG:HD2   | 1:9:A:ARG:H    | 14       | 0.17          |
| (1,146) | 1:9:A:ARG:HD3   | 1:9:A:ARG:H    | 14       | 0.17          |
| (1,146) | 1:9:A:ARG:HD2   | 1:9:A:ARG:H    | 17       | 0.17          |
| (1,146) | 1:9:A:ARG:HD3   | 1:9:A:ARG:H    | 17       | 0.17          |
| (1,106) | 1:6:A:LYS:HA    | 1:9:A:ARG:HG2  | 17       | 0.17          |
| (1,106) | 1:6:A:LYS:HA    | 1:9:A:ARG:HG3  | 17       | 0.17          |
| (1,106) | 1:6:A:LYS:HA    | 1:9:A:ARG:HG2  | 20       | 0.17          |
| (1,106) | 1:6:A:LYS:HA    | 1:9:A:ARG:HG3  | 20       | 0.17          |
| (1,27)  | 1:3:A:ARG:HG2   | 1:4:A:LEU:HD11 | 8        | 0.17          |
| (1,27)  | 1:3:A:ARG:HG2   | 1:4:A:LEU:HD12 | 8        | 0.17          |
| (1,27)  | 1:3:A:ARG:HG2   | 1:4:A:LEU:HD13 | 8        | 0.17          |
| (1,27)  | 1:3:A:ARG:HG2   | 1:4:A:LEU:HD21 | 8        | 0.17          |
| (1,27)  | 1:3:A:ARG:HG2   | 1:4:A:LEU:HD22 | 8        | 0.17          |
| (1,27)  | 1:3:A:ARG:HG2   | 1:4:A:LEU:HD23 | 8        | 0.17          |
| (1,27)  | 1:3:A:ARG:HG3   | 1:4:A:LEU:HD11 | 8        | 0.17          |
| (1,27)  | 1:3:A:ARG:HG3   | 1:4:A:LEU:HD12 | 8        | 0.17          |
| (1,27)  | 1:3:A:ARG:HG3   | 1:4:A:LEU:HD13 | 8        | 0.17          |
| (1,27)  | 1:3:A:ARG:HG3   | 1:4:A:LEU:HD21 | 8        | 0.17          |
| (1,27)  | 1:3:A:ARG:HG3   | 1:4:A:LEU:HD22 | 8        | 0.17          |
| (1,27)  | 1:3:A:ARG:HG3   | 1:4:A:LEU:HD23 | 8        | 0.17          |
| (1,27)  | 1:3:A:ARG:HG2   | 1:4:A:LEU:HD11 | 15       | 0.17          |
| (1,27)  | 1:3:A:ARG:HG2   | 1:4:A:LEU:HD12 | 15       | 0.17          |
| (1,27)  | 1:3:A:ARG:HG2   | 1:4:A:LEU:HD13 | 15       | 0.17          |
| (1,27)  | 1:3:A:ARG:HG2   | 1:4:A:LEU:HD21 | 15       | 0.17          |
| (1,27)  | 1:3:A:ARG:HG2   | 1:4:A:LEU:HD22 | 15       | 0.17          |
| (1,27)  | 1:3:A:ARG:HG2   | 1:4:A:LEU:HD23 | 15       | 0.17          |
| (1,27)  | 1:3:A:ARG:HG3   | 1:4:A:LEU:HD11 | 15       | 0.17          |
| (1,27)  | 1:3:A:ARG:HG3   | 1:4:A:LEU:HD12 | 15       | 0.17          |
| (1,27)  | 1:3:A:ARG:HG3   | 1:4:A:LEU:HD13 | 15       | 0.17          |
| (1,27)  | 1:3:A:ARG:HG3   | 1:4:A:LEU:HD21 | 15       | 0.17          |
| (1,27)  | 1:3:A:ARG:HG3   | 1:4:A:LEU:HD22 | 15       | 0.17          |
| (1,27)  | 1:3:A:ARG:HG3   | 1:4:A:LEU:HD23 | 15       | 0.17          |
| (2,1)   | 1:12:A:ILE:HG22 | 1:13:A:LEU:H   | 2        | 0.16          |
| (2,1)   | 1:12:A:ILE:HG21 | 1:13:A:LEU:H   | 13       | 0.16          |
| (2,1)   | 1:12:A:ILE:HG22 | 1:13:A:LEU:H   | 15       | 0.16          |
| (1,201) | 1:13:A:LEU:H    | 1:14:A:GLN:H   | 4        | 0.16          |
| (1,196) | 1:13:A:LEU:HD11 | 1:13:A:LEU:H   | 11       | 0.16          |
| (1,196) | 1:13:A:LEU:HD12 | 1:13:A:LEU:H   | 11       | 0.16          |
| (1,196) | 1:13:A:LEU:HD13 | 1:13:A:LEU:H   | 11       | 0.16          |
| (1,196) | 1:13:A:LEU:HD21 | 1:13:A:LEU:H   | 11       | 0.16          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,196) | 1:13:A:LEU:HD22 | 1:13:A:LEU:H   | 11       | 0.16          |
| (1,196) | 1:13:A:LEU:HD23 | 1:13:A:LEU:H   | 11       | 0.16          |
| (1,157) | 1:11:A:PHE:HA   | 1:11:A:PHE:HE1 | 9        | 0.16          |
| (1,157) | 1:11:A:PHE:HA   | 1:11:A:PHE:HE2 | 9        | 0.16          |
| (1,157) | 1:11:A:PHE:HA   | 1:11:A:PHE:HE1 | 10       | 0.16          |
| (1,157) | 1:11:A:PHE:HA   | 1:11:A:PHE:HE2 | 10       | 0.16          |
| (1,157) | 1:11:A:PHE:HA   | 1:11:A:PHE:HE1 | 16       | 0.16          |
| (1,157) | 1:11:A:PHE:HA   | 1:11:A:PHE:HE2 | 16       | 0.16          |
| (1,150) | 1:9:A:ARG:HG2   | 1:12:A:ILE:HA  | 8        | 0.16          |
| (1,150) | 1:9:A:ARG:HG3   | 1:12:A:ILE:HA  | 8        | 0.16          |
| (1,150) | 1:9:A:ARG:HG2   | 1:12:A:ILE:HA  | 17       | 0.16          |
| (1,150) | 1:9:A:ARG:HG3   | 1:12:A:ILE:HA  | 17       | 0.16          |
| (1,146) | 1:9:A:ARG:HD2   | 1:9:A:ARG:H    | 6        | 0.16          |
| (1,146) | 1:9:A:ARG:HD3   | 1:9:A:ARG:H    | 6        | 0.16          |
| (1,27)  | 1:3:A:ARG:HG2   | 1:4:A:LEU:HD11 | 4        | 0.16          |
| (1,27)  | 1:3:A:ARG:HG2   | 1:4:A:LEU:HD12 | 4        | 0.16          |
| (1,27)  | 1:3:A:ARG:HG2   | 1:4:A:LEU:HD13 | 4        | 0.16          |
| (1,27)  | 1:3:A:ARG:HG2   | 1:4:A:LEU:HD21 | 4        | 0.16          |
| (1,27)  | 1:3:A:ARG:HG2   | 1:4:A:LEU:HD22 | 4        | 0.16          |
| (1,27)  | 1:3:A:ARG:HG2   | 1:4:A:LEU:HD23 | 4        | 0.16          |
| (1,27)  | 1:3:A:ARG:HG3   | 1:4:A:LEU:HD11 | 4        | 0.16          |
| (1,27)  | 1:3:A:ARG:HG3   | 1:4:A:LEU:HD12 | 4        | 0.16          |
| (1,27)  | 1:3:A:ARG:HG3   | 1:4:A:LEU:HD13 | 4        | 0.16          |
| (1,27)  | 1:3:A:ARG:HG3   | 1:4:A:LEU:HD21 | 4        | 0.16          |
| (1,27)  | 1:3:A:ARG:HG3   | 1:4:A:LEU:HD22 | 4        | 0.16          |
| (1,27)  | 1:3:A:ARG:HG3   | 1:4:A:LEU:HD23 | 4        | 0.16          |
| (1,27)  | 1:3:A:ARG:HG2   | 1:4:A:LEU:HD11 | 11       | 0.16          |
| (1,27)  | 1:3:A:ARG:HG2   | 1:4:A:LEU:HD12 | 11       | 0.16          |
| (1,27)  | 1:3:A:ARG:HG2   | 1:4:A:LEU:HD13 | 11       | 0.16          |
| (1,27)  | 1:3:A:ARG:HG2   | 1:4:A:LEU:HD21 | 11       | 0.16          |
| (1,27)  | 1:3:A:ARG:HG2   | 1:4:A:LEU:HD22 | 11       | 0.16          |
| (1,27)  | 1:3:A:ARG:HG2   | 1:4:A:LEU:HD23 | 11       | 0.16          |
| (1,27)  | 1:3:A:ARG:HG3   | 1:4:A:LEU:HD11 | 11       | 0.16          |
| (1,27)  | 1:3:A:ARG:HG3   | 1:4:A:LEU:HD12 | 11       | 0.16          |
| (1,27)  | 1:3:A:ARG:HG3   | 1:4:A:LEU:HD13 | 11       | 0.16          |
| (1,27)  | 1:3:A:ARG:HG3   | 1:4:A:LEU:HD21 | 11       | 0.16          |
| (1,27)  | 1:3:A:ARG:HG3   | 1:4:A:LEU:HD22 | 11       | 0.16          |
| (1,27)  | 1:3:A:ARG:HG3   | 1:4:A:LEU:HD23 | 11       | 0.16          |
| (1,27)  | 1:3:A:ARG:HG2   | 1:4:A:LEU:HD11 | 18       | 0.16          |
| (1,27)  | 1:3:A:ARG:HG2   | 1:4:A:LEU:HD12 | 18       | 0.16          |
| (1,27)  | 1:3:A:ARG:HG2   | 1:4:A:LEU:HD13 | 18       | 0.16          |
| (1,27)  | 1:3:A:ARG:HG2   | 1:4:A:LEU:HD21 | 18       | 0.16          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,27)  | 1:3:A:ARG:HG2   | 1:4:A:LEU:HD22 | 18       | 0.16          |
| (1,27)  | 1:3:A:ARG:HG2   | 1:4:A:LEU:HD23 | 18       | 0.16          |
| (1,27)  | 1:3:A:ARG:HG3   | 1:4:A:LEU:HD11 | 18       | 0.16          |
| (1,27)  | 1:3:A:ARG:HG3   | 1:4:A:LEU:HD12 | 18       | 0.16          |
| (1,27)  | 1:3:A:ARG:HG3   | 1:4:A:LEU:HD13 | 18       | 0.16          |
| (1,27)  | 1:3:A:ARG:HG3   | 1:4:A:LEU:HD21 | 18       | 0.16          |
| (1,27)  | 1:3:A:ARG:HG3   | 1:4:A:LEU:HD22 | 18       | 0.16          |
| (1,27)  | 1:3:A:ARG:HG3   | 1:4:A:LEU:HD23 | 18       | 0.16          |
| (1,26)  | 1:3:A:ARG:HB2   | 1:4:A:LEU:H    | 7        | 0.16          |
| (1,26)  | 1:3:A:ARG:HB3   | 1:4:A:LEU:H    | 7        | 0.16          |
| (1,26)  | 1:3:A:ARG:HB2   | 1:4:A:LEU:H    | 13       | 0.16          |
| (1,26)  | 1:3:A:ARG:HB3   | 1:4:A:LEU:H    | 13       | 0.16          |
| (1,26)  | 1:3:A:ARG:HB2   | 1:4:A:LEU:H    | 18       | 0.16          |
| (1,26)  | 1:3:A:ARG:HB3   | 1:4:A:LEU:H    | 18       | 0.16          |
| (1,240) | 1:16:A:LYS:HG2  | 1:16:A:LYS:H   | 10       | 0.15          |
| (1,240) | 1:16:A:LYS:HG3  | 1:16:A:LYS:H   | 10       | 0.15          |
| (1,232) | 1:15:A:ARG:HA   | 1:17:A:LYS:H   | 7        | 0.15          |
| (1,201) | 1:13:A:LEU:H    | 1:14:A:GLN:H   | 1        | 0.15          |
| (1,201) | 1:13:A:LEU:H    | 1:14:A:GLN:H   | 17       | 0.15          |
| (1,201) | 1:13:A:LEU:H    | 1:14:A:GLN:H   | 20       | 0.15          |
| (1,196) | 1:13:A:LEU:HD11 | 1:13:A:LEU:H   | 5        | 0.15          |
| (1,196) | 1:13:A:LEU:HD12 | 1:13:A:LEU:H   | 5        | 0.15          |
| (1,196) | 1:13:A:LEU:HD13 | 1:13:A:LEU:H   | 5        | 0.15          |
| (1,196) | 1:13:A:LEU:HD21 | 1:13:A:LEU:H   | 5        | 0.15          |
| (1,196) | 1:13:A:LEU:HD22 | 1:13:A:LEU:H   | 5        | 0.15          |
| (1,196) | 1:13:A:LEU:HD23 | 1:13:A:LEU:H   | 5        | 0.15          |
| (1,196) | 1:13:A:LEU:HD11 | 1:13:A:LEU:H   | 15       | 0.15          |
| (1,196) | 1:13:A:LEU:HD12 | 1:13:A:LEU:H   | 15       | 0.15          |
| (1,196) | 1:13:A:LEU:HD13 | 1:13:A:LEU:H   | 15       | 0.15          |
| (1,196) | 1:13:A:LEU:HD21 | 1:13:A:LEU:H   | 15       | 0.15          |
| (1,196) | 1:13:A:LEU:HD22 | 1:13:A:LEU:H   | 15       | 0.15          |
| (1,196) | 1:13:A:LEU:HD23 | 1:13:A:LEU:H   | 15       | 0.15          |
| (1,196) | 1:13:A:LEU:HD11 | 1:13:A:LEU:H   | 19       | 0.15          |
| (1,196) | 1:13:A:LEU:HD12 | 1:13:A:LEU:H   | 19       | 0.15          |
| (1,196) | 1:13:A:LEU:HD13 | 1:13:A:LEU:H   | 19       | 0.15          |
| (1,196) | 1:13:A:LEU:HD21 | 1:13:A:LEU:H   | 19       | 0.15          |
| (1,196) | 1:13:A:LEU:HD22 | 1:13:A:LEU:H   | 19       | 0.15          |
| (1,196) | 1:13:A:LEU:HD23 | 1:13:A:LEU:H   | 19       | 0.15          |
| (1,185) | 1:12:A:ILE:HD11 | 1:13:A:LEU:H   | 6        | 0.15          |
| (1,185) | 1:12:A:ILE:HD12 | 1:13:A:LEU:H   | 6        | 0.15          |
| (1,185) | 1:12:A:ILE:HD13 | 1:13:A:LEU:H   | 6        | 0.15          |
| (1,157) | 1:11:A:PHE:HA   | 1:11:A:PHE:HE1 | 11       | 0.15          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,157) | 1:11:A:PHE:HA   | 1:11:A:PHE:HE2 | 11       | 0.15          |
| (1,157) | 1:11:A:PHE:HA   | 1:11:A:PHE:HE1 | 15       | 0.15          |
| (1,157) | 1:11:A:PHE:HA   | 1:11:A:PHE:HE2 | 15       | 0.15          |
| (1,146) | 1:9:A:ARG:HD2   | 1:9:A:ARG:H    | 10       | 0.15          |
| (1,146) | 1:9:A:ARG:HD3   | 1:9:A:ARG:H    | 10       | 0.15          |
| (1,146) | 1:9:A:ARG:HD2   | 1:9:A:ARG:H    | 19       | 0.15          |
| (1,146) | 1:9:A:ARG:HD3   | 1:9:A:ARG:H    | 19       | 0.15          |
| (1,65)  | 1:4:A:LEU:HD11  | 1:8:A:PHE:HZ   | 6        | 0.15          |
| (1,65)  | 1:4:A:LEU:HD12  | 1:8:A:PHE:HZ   | 6        | 0.15          |
| (1,65)  | 1:4:A:LEU:HD13  | 1:8:A:PHE:HZ   | 6        | 0.15          |
| (1,65)  | 1:4:A:LEU:HD21  | 1:8:A:PHE:HZ   | 6        | 0.15          |
| (1,65)  | 1:4:A:LEU:HD22  | 1:8:A:PHE:HZ   | 6        | 0.15          |
| (1,65)  | 1:4:A:LEU:HD23  | 1:8:A:PHE:HZ   | 6        | 0.15          |
| (1,57)  | 1:4:A:LEU:HA    | 1:7:A:PHE:HZ   | 8        | 0.15          |
| (1,57)  | 1:4:A:LEU:HA    | 1:7:A:PHE:HZ   | 18       | 0.15          |
| (1,27)  | 1:3:A:ARG:HG2   | 1:4:A:LEU:HD11 | 12       | 0.15          |
| (1,27)  | 1:3:A:ARG:HG2   | 1:4:A:LEU:HD12 | 12       | 0.15          |
| (1,27)  | 1:3:A:ARG:HG2   | 1:4:A:LEU:HD13 | 12       | 0.15          |
| (1,27)  | 1:3:A:ARG:HG2   | 1:4:A:LEU:HD21 | 12       | 0.15          |
| (1,27)  | 1:3:A:ARG:HG2   | 1:4:A:LEU:HD22 | 12       | 0.15          |
| (1,27)  | 1:3:A:ARG:HG2   | 1:4:A:LEU:HD23 | 12       | 0.15          |
| (1,27)  | 1:3:A:ARG:HG3   | 1:4:A:LEU:HD11 | 12       | 0.15          |
| (1,27)  | 1:3:A:ARG:HG3   | 1:4:A:LEU:HD12 | 12       | 0.15          |
| (1,27)  | 1:3:A:ARG:HG3   | 1:4:A:LEU:HD13 | 12       | 0.15          |
| (1,27)  | 1:3:A:ARG:HG3   | 1:4:A:LEU:HD21 | 12       | 0.15          |
| (1,27)  | 1:3:A:ARG:HG3   | 1:4:A:LEU:HD22 | 12       | 0.15          |
| (1,27)  | 1:3:A:ARG:HG3   | 1:4:A:LEU:HD23 | 12       | 0.15          |
| (1,26)  | 1:3:A:ARG:HB2   | 1:4:A:LEU:H    | 5        | 0.15          |
| (1,26)  | 1:3:A:ARG:HB3   | 1:4:A:LEU:H    | 5        | 0.15          |
| (1,26)  | 1:3:A:ARG:HB2   | 1:4:A:LEU:H    | 12       | 0.15          |
| (1,26)  | 1:3:A:ARG:HB3   | 1:4:A:LEU:H    | 12       | 0.15          |
| (2,1)   | 1:12:A:ILE:HG22 | 1:13:A:LEU:H   | 9        | 0.14          |
| (1,240) | 1:16:A:LYS:HG2  | 1:16:A:LYS:H   | 3        | 0.14          |
| (1,240) | 1:16:A:LYS:HG3  | 1:16:A:LYS:H   | 3        | 0.14          |
| (1,240) | 1:16:A:LYS:HG2  | 1:16:A:LYS:H   | 4        | 0.14          |
| (1,240) | 1:16:A:LYS:HG3  | 1:16:A:LYS:H   | 4        | 0.14          |
| (1,240) | 1:16:A:LYS:HG2  | 1:16:A:LYS:H   | 5        | 0.14          |
| (1,240) | 1:16:A:LYS:HG3  | 1:16:A:LYS:H   | 5        | 0.14          |
| (1,240) | 1:16:A:LYS:HG2  | 1:16:A:LYS:H   | 13       | 0.14          |
| (1,240) | 1:16:A:LYS:HG3  | 1:16:A:LYS:H   | 13       | 0.14          |
| (1,240) | 1:16:A:LYS:HG2  | 1:16:A:LYS:H   | 15       | 0.14          |
| (1,240) | 1:16:A:LYS:HG3  | 1:16:A:LYS:H   | 15       | 0.14          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,201) | 1:13:A:LEU:H    | 1:14:A:GLN:H   | 9        | 0.14          |
| (1,201) | 1:13:A:LEU:H    | 1:14:A:GLN:H   | 15       | 0.14          |
| (1,196) | 1:13:A:LEU:HD11 | 1:13:A:LEU:H   | 1        | 0.14          |
| (1,196) | 1:13:A:LEU:HD12 | 1:13:A:LEU:H   | 1        | 0.14          |
| (1,196) | 1:13:A:LEU:HD13 | 1:13:A:LEU:H   | 1        | 0.14          |
| (1,196) | 1:13:A:LEU:HD21 | 1:13:A:LEU:H   | 1        | 0.14          |
| (1,196) | 1:13:A:LEU:HD22 | 1:13:A:LEU:H   | 1        | 0.14          |
| (1,196) | 1:13:A:LEU:HD23 | 1:13:A:LEU:H   | 1        | 0.14          |
| (1,196) | 1:13:A:LEU:HD11 | 1:13:A:LEU:H   | 10       | 0.14          |
| (1,196) | 1:13:A:LEU:HD12 | 1:13:A:LEU:H   | 10       | 0.14          |
| (1,196) | 1:13:A:LEU:HD13 | 1:13:A:LEU:H   | 10       | 0.14          |
| (1,196) | 1:13:A:LEU:HD21 | 1:13:A:LEU:H   | 10       | 0.14          |
| (1,196) | 1:13:A:LEU:HD22 | 1:13:A:LEU:H   | 10       | 0.14          |
| (1,196) | 1:13:A:LEU:HD23 | 1:13:A:LEU:H   | 10       | 0.14          |
| (1,196) | 1:13:A:LEU:HD11 | 1:13:A:LEU:H   | 16       | 0.14          |
| (1,196) | 1:13:A:LEU:HD12 | 1:13:A:LEU:H   | 16       | 0.14          |
| (1,196) | 1:13:A:LEU:HD13 | 1:13:A:LEU:H   | 16       | 0.14          |
| (1,196) | 1:13:A:LEU:HD21 | 1:13:A:LEU:H   | 16       | 0.14          |
| (1,196) | 1:13:A:LEU:HD22 | 1:13:A:LEU:H   | 16       | 0.14          |
| (1,196) | 1:13:A:LEU:HD23 | 1:13:A:LEU:H   | 16       | 0.14          |
| (1,157) | 1:11:A:PHE:HA   | 1:11:A:PHE:HE1 | 12       | 0.14          |
| (1,157) | 1:11:A:PHE:HA   | 1:11:A:PHE:HE2 | 12       | 0.14          |
| (1,150) | 1:9:A:ARG:HG2   | 1:12:A:ILE:HA  | 3        | 0.14          |
| (1,150) | 1:9:A:ARG:HG3   | 1:12:A:ILE:HA  | 3        | 0.14          |
| (1,57)  | 1:4:A:LEU:HA    | 1:7:A:PHE:HZ   | 5        | 0.14          |
| (1,57)  | 1:4:A:LEU:HA    | 1:7:A:PHE:HZ   | 9        | 0.14          |
| (1,57)  | 1:4:A:LEU:HA    | 1:7:A:PHE:HZ   | 11       | 0.14          |
| (1,57)  | 1:4:A:LEU:HA    | 1:7:A:PHE:HZ   | 15       | 0.14          |
| (1,28)  | 1:3:A:ARG:H     | 1:4:A:LEU:H    | 6        | 0.14          |
| (1,27)  | 1:3:A:ARG:HG2   | 1:4:A:LEU:HD11 | 5        | 0.14          |
| (1,27)  | 1:3:A:ARG:HG2   | 1:4:A:LEU:HD12 | 5        | 0.14          |
| (1,27)  | 1:3:A:ARG:HG2   | 1:4:A:LEU:HD13 | 5        | 0.14          |
| (1,27)  | 1:3:A:ARG:HG2   | 1:4:A:LEU:HD21 | 5        | 0.14          |
| (1,27)  | 1:3:A:ARG:HG2   | 1:4:A:LEU:HD22 | 5        | 0.14          |
| (1,27)  | 1:3:A:ARG:HG2   | 1:4:A:LEU:HD23 | 5        | 0.14          |
| (1,27)  | 1:3:A:ARG:HG3   | 1:4:A:LEU:HD11 | 5        | 0.14          |
| (1,27)  | 1:3:A:ARG:HG3   | 1:4:A:LEU:HD12 | 5        | 0.14          |
| (1,27)  | 1:3:A:ARG:HG3   | 1:4:A:LEU:HD13 | 5        | 0.14          |
| (1,27)  | 1:3:A:ARG:HG3   | 1:4:A:LEU:HD21 | 5        | 0.14          |
| (1,27)  | 1:3:A:ARG:HG3   | 1:4:A:LEU:HD22 | 5        | 0.14          |
| (1,27)  | 1:3:A:ARG:HG3   | 1:4:A:LEU:HD23 | 5        | 0.14          |
| (1,26)  | 1:3:A:ARG:HB2   | 1:4:A:LEU:H    | 8        | 0.14          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,26)  | 1:3:A:ARG:HB3   | 1:4:A:LEU:H    | 8        | 0.14          |
| (2,1)   | 1:12:A:ILE:HG22 | 1:13:A:LEU:H   | 11       | 0.13          |
| (1,240) | 1:16:A:LYS:HG2  | 1:16:A:LYS:H   | 6        | 0.13          |
| (1,240) | 1:16:A:LYS:HG3  | 1:16:A:LYS:H   | 6        | 0.13          |
| (1,240) | 1:16:A:LYS:HG2  | 1:16:A:LYS:H   | 7        | 0.13          |
| (1,240) | 1:16:A:LYS:HG3  | 1:16:A:LYS:H   | 7        | 0.13          |
| (1,240) | 1:16:A:LYS:HG2  | 1:16:A:LYS:H   | 8        | 0.13          |
| (1,240) | 1:16:A:LYS:HG3  | 1:16:A:LYS:H   | 8        | 0.13          |
| (1,240) | 1:16:A:LYS:HG2  | 1:16:A:LYS:H   | 9        | 0.13          |
| (1,240) | 1:16:A:LYS:HG3  | 1:16:A:LYS:H   | 9        | 0.13          |
| (1,240) | 1:16:A:LYS:HG2  | 1:16:A:LYS:H   | 12       | 0.13          |
| (1,240) | 1:16:A:LYS:HG3  | 1:16:A:LYS:H   | 12       | 0.13          |
| (1,232) | 1:15:A:ARG:HA   | 1:17:A:LYS:H   | 12       | 0.13          |
| (1,203) | 1:13:A:LEU:HD11 | 1:15:A:ARG:HA  | 4        | 0.13          |
| (1,203) | 1:13:A:LEU:HD12 | 1:15:A:ARG:HA  | 4        | 0.13          |
| (1,203) | 1:13:A:LEU:HD13 | 1:15:A:ARG:HA  | 4        | 0.13          |
| (1,203) | 1:13:A:LEU:HD21 | 1:15:A:ARG:HA  | 4        | 0.13          |
| (1,203) | 1:13:A:LEU:HD22 | 1:15:A:ARG:HA  | 4        | 0.13          |
| (1,203) | 1:13:A:LEU:HD23 | 1:15:A:ARG:HA  | 4        | 0.13          |
| (1,203) | 1:13:A:LEU:HD11 | 1:15:A:ARG:HA  | 18       | 0.13          |
| (1,203) | 1:13:A:LEU:HD12 | 1:15:A:ARG:HA  | 18       | 0.13          |
| (1,203) | 1:13:A:LEU:HD13 | 1:15:A:ARG:HA  | 18       | 0.13          |
| (1,203) | 1:13:A:LEU:HD21 | 1:15:A:ARG:HA  | 18       | 0.13          |
| (1,203) | 1:13:A:LEU:HD22 | 1:15:A:ARG:HA  | 18       | 0.13          |
| (1,203) | 1:13:A:LEU:HD23 | 1:15:A:ARG:HA  | 18       | 0.13          |
| (1,201) | 1:13:A:LEU:H    | 1:14:A:GLN:H   | 5        | 0.13          |
| (1,201) | 1:13:A:LEU:H    | 1:14:A:GLN:H   | 10       | 0.13          |
| (1,201) | 1:13:A:LEU:H    | 1:14:A:GLN:H   | 13       | 0.13          |
| (1,187) | 1:12:A:ILE:HG12 | 1:13:A:LEU:H   | 2        | 0.13          |
| (1,187) | 1:12:A:ILE:HG13 | 1:13:A:LEU:H   | 2        | 0.13          |
| (1,187) | 1:12:A:ILE:HG12 | 1:13:A:LEU:H   | 10       | 0.13          |
| (1,187) | 1:12:A:ILE:HG13 | 1:13:A:LEU:H   | 10       | 0.13          |
| (1,187) | 1:12:A:ILE:HG12 | 1:13:A:LEU:H   | 13       | 0.13          |
| (1,187) | 1:12:A:ILE:HG13 | 1:13:A:LEU:H   | 13       | 0.13          |
| (1,185) | 1:12:A:ILE:HD11 | 1:13:A:LEU:H   | 8        | 0.13          |
| (1,185) | 1:12:A:ILE:HD12 | 1:13:A:LEU:H   | 8        | 0.13          |
| (1,185) | 1:12:A:ILE:HD13 | 1:13:A:LEU:H   | 8        | 0.13          |
| (1,185) | 1:12:A:ILE:HD11 | 1:13:A:LEU:H   | 9        | 0.13          |
| (1,185) | 1:12:A:ILE:HD12 | 1:13:A:LEU:H   | 9        | 0.13          |
| (1,185) | 1:12:A:ILE:HD13 | 1:13:A:LEU:H   | 9        | 0.13          |
| (1,157) | 1:11:A:PHE:HA   | 1:11:A:PHE:HE1 | 1        | 0.13          |
| (1,157) | 1:11:A:PHE:HA   | 1:11:A:PHE:HE2 | 1        | 0.13          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,157) | 1:11:A:PHE:HA   | 1:11:A:PHE:HE1 | 4        | 0.13          |
| (1,157) | 1:11:A:PHE:HA   | 1:11:A:PHE:HE2 | 4        | 0.13          |
| (1,157) | 1:11:A:PHE:HA   | 1:11:A:PHE:HE1 | 5        | 0.13          |
| (1,157) | 1:11:A:PHE:HA   | 1:11:A:PHE:HE2 | 5        | 0.13          |
| (1,157) | 1:11:A:PHE:HA   | 1:11:A:PHE:HE1 | 18       | 0.13          |
| (1,157) | 1:11:A:PHE:HA   | 1:11:A:PHE:HE2 | 18       | 0.13          |
| (1,154) | 1:9:A:ARG:HG2   | 1:13:A:LEU:H   | 8        | 0.13          |
| (1,154) | 1:9:A:ARG:HG3   | 1:13:A:LEU:H   | 8        | 0.13          |
| (1,150) | 1:9:A:ARG:HG2   | 1:12:A:ILE:HA  | 16       | 0.13          |
| (1,150) | 1:9:A:ARG:HG3   | 1:12:A:ILE:HA  | 16       | 0.13          |
| (1,150) | 1:9:A:ARG:HG2   | 1:12:A:ILE:HA  | 18       | 0.13          |
| (1,150) | 1:9:A:ARG:HG3   | 1:12:A:ILE:HA  | 18       | 0.13          |
| (1,146) | 1:9:A:ARG:HD2   | 1:9:A:ARG:H    | 9        | 0.13          |
| (1,146) | 1:9:A:ARG:HD3   | 1:9:A:ARG:H    | 9        | 0.13          |
| (1,57)  | 1:4:A:LEU:HA    | 1:7:A:PHE:HZ   | 1        | 0.13          |
| (1,57)  | 1:4:A:LEU:HA    | 1:7:A:PHE:HZ   | 4        | 0.13          |
| (1,57)  | 1:4:A:LEU:HA    | 1:7:A:PHE:HZ   | 16       | 0.13          |
| (1,250) | 1:17:A:LYS:HG2  | 1:17:A:LYS:H   | 17       | 0.12          |
| (1,250) | 1:17:A:LYS:HG3  | 1:17:A:LYS:H   | 17       | 0.12          |
| (1,250) | 1:17:A:LYS:HG2  | 1:17:A:LYS:H   | 19       | 0.12          |
| (1,250) | 1:17:A:LYS:HG3  | 1:17:A:LYS:H   | 19       | 0.12          |
| (1,242) | 1:16:A:LYS:HB2  | 1:17:A:LYS:H   | 2        | 0.12          |
| (1,242) | 1:16:A:LYS:HB3  | 1:17:A:LYS:H   | 2        | 0.12          |
| (1,241) | 1:16:A:LYS:HA   | 1:17:A:LYS:H   | 2        | 0.12          |
| (1,232) | 1:15:A:ARG:HA   | 1:17:A:LYS:H   | 6        | 0.12          |
| (1,232) | 1:15:A:ARG:HA   | 1:17:A:LYS:H   | 8        | 0.12          |
| (1,232) | 1:15:A:ARG:HA   | 1:17:A:LYS:H   | 9        | 0.12          |
| (1,201) | 1:13:A:LEU:H    | 1:14:A:GLN:H   | 2        | 0.12          |
| (1,201) | 1:13:A:LEU:H    | 1:14:A:GLN:H   | 6        | 0.12          |
| (1,196) | 1:13:A:LEU:HD11 | 1:13:A:LEU:H   | 7        | 0.12          |
| (1,196) | 1:13:A:LEU:HD12 | 1:13:A:LEU:H   | 7        | 0.12          |
| (1,196) | 1:13:A:LEU:HD13 | 1:13:A:LEU:H   | 7        | 0.12          |
| (1,196) | 1:13:A:LEU:HD21 | 1:13:A:LEU:H   | 7        | 0.12          |
| (1,196) | 1:13:A:LEU:HD22 | 1:13:A:LEU:H   | 7        | 0.12          |
| (1,196) | 1:13:A:LEU:HD23 | 1:13:A:LEU:H   | 7        | 0.12          |
| (1,196) | 1:13:A:LEU:HD11 | 1:13:A:LEU:H   | 9        | 0.12          |
| (1,196) | 1:13:A:LEU:HD12 | 1:13:A:LEU:H   | 9        | 0.12          |
| (1,196) | 1:13:A:LEU:HD13 | 1:13:A:LEU:H   | 9        | 0.12          |
| (1,196) | 1:13:A:LEU:HD21 | 1:13:A:LEU:H   | 9        | 0.12          |
| (1,196) | 1:13:A:LEU:HD22 | 1:13:A:LEU:H   | 9        | 0.12          |
| (1,196) | 1:13:A:LEU:HD23 | 1:13:A:LEU:H   | 9        | 0.12          |
| (1,187) | 1:12:A:ILE:HG12 | 1:13:A:LEU:H   | 11       | 0.12          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,187) | 1:12:A:ILE:HG13 | 1:13:A:LEU:H    | 11       | 0.12          |
| (1,187) | 1:12:A:ILE:HG12 | 1:13:A:LEU:H    | 15       | 0.12          |
| (1,187) | 1:12:A:ILE:HG13 | 1:13:A:LEU:H    | 15       | 0.12          |
| (1,185) | 1:12:A:ILE:HD11 | 1:13:A:LEU:H    | 15       | 0.12          |
| (1,185) | 1:12:A:ILE:HD12 | 1:13:A:LEU:H    | 15       | 0.12          |
| (1,185) | 1:12:A:ILE:HD13 | 1:13:A:LEU:H    | 15       | 0.12          |
| (1,157) | 1:11:A:PHE:HA   | 1:11:A:PHE:HE1  | 6        | 0.12          |
| (1,157) | 1:11:A:PHE:HA   | 1:11:A:PHE:HE2  | 6        | 0.12          |
| (1,157) | 1:11:A:PHE:HA   | 1:11:A:PHE:HE1  | 13       | 0.12          |
| (1,157) | 1:11:A:PHE:HA   | 1:11:A:PHE:HE2  | 13       | 0.12          |
| (1,154) | 1:9:A:ARG:HG2   | 1:13:A:LEU:H    | 6        | 0.12          |
| (1,154) | 1:9:A:ARG:HG3   | 1:13:A:LEU:H    | 6        | 0.12          |
| (1,153) | 1:9:A:ARG:HG2   | 1:13:A:LEU:HD11 | 20       | 0.12          |
| (1,153) | 1:9:A:ARG:HG2   | 1:13:A:LEU:HD12 | 20       | 0.12          |
| (1,153) | 1:9:A:ARG:HG2   | 1:13:A:LEU:HD13 | 20       | 0.12          |
| (1,153) | 1:9:A:ARG:HG2   | 1:13:A:LEU:HD21 | 20       | 0.12          |
| (1,153) | 1:9:A:ARG:HG2   | 1:13:A:LEU:HD22 | 20       | 0.12          |
| (1,153) | 1:9:A:ARG:HG2   | 1:13:A:LEU:HD23 | 20       | 0.12          |
| (1,153) | 1:9:A:ARG:HG3   | 1:13:A:LEU:HD11 | 20       | 0.12          |
| (1,153) | 1:9:A:ARG:HG3   | 1:13:A:LEU:HD12 | 20       | 0.12          |
| (1,153) | 1:9:A:ARG:HG3   | 1:13:A:LEU:HD13 | 20       | 0.12          |
| (1,153) | 1:9:A:ARG:HG3   | 1:13:A:LEU:HD21 | 20       | 0.12          |
| (1,153) | 1:9:A:ARG:HG3   | 1:13:A:LEU:HD22 | 20       | 0.12          |
| (1,153) | 1:9:A:ARG:HG3   | 1:13:A:LEU:HD23 | 20       | 0.12          |
| (1,146) | 1:9:A:ARG:HD2   | 1:9:A:ARG:H     | 4        | 0.12          |
| (1,146) | 1:9:A:ARG:HD3   | 1:9:A:ARG:H     | 4        | 0.12          |
| (1,139) | 1:9:A:ARG:HA    | 1:9:A:ARG:HD2   | 20       | 0.12          |
| (1,139) | 1:9:A:ARG:HA    | 1:9:A:ARG:HD3   | 20       | 0.12          |
| (1,102) | 1:6:A:LYS:H     | 1:7:A:PHE:H     | 7        | 0.12          |
| (1,250) | 1:17:A:LYS:HG2  | 1:17:A:LYS:H    | 10       | 0.11          |
| (1,250) | 1:17:A:LYS:HG3  | 1:17:A:LYS:H    | 10       | 0.11          |
| (1,232) | 1:15:A:ARG:HA   | 1:17:A:LYS:H    | 13       | 0.11          |
| (1,203) | 1:13:A:LEU:HD11 | 1:15:A:ARG:HA   | 17       | 0.11          |
| (1,203) | 1:13:A:LEU:HD12 | 1:15:A:ARG:HA   | 17       | 0.11          |
| (1,203) | 1:13:A:LEU:HD13 | 1:15:A:ARG:HA   | 17       | 0.11          |
| (1,203) | 1:13:A:LEU:HD21 | 1:15:A:ARG:HA   | 17       | 0.11          |
| (1,203) | 1:13:A:LEU:HD22 | 1:15:A:ARG:HA   | 17       | 0.11          |
| (1,203) | 1:13:A:LEU:HD23 | 1:15:A:ARG:HA   | 17       | 0.11          |
| (1,203) | 1:13:A:LEU:HD11 | 1:15:A:ARG:HA   | 19       | 0.11          |
| (1,203) | 1:13:A:LEU:HD12 | 1:15:A:ARG:HA   | 19       | 0.11          |
| (1,203) | 1:13:A:LEU:HD13 | 1:15:A:ARG:HA   | 19       | 0.11          |
| (1,203) | 1:13:A:LEU:HD21 | 1:15:A:ARG:HA   | 19       | 0.11          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,203) | 1:13:A:LEU:HD22 | 1:15:A:ARG:HA  | 19       | 0.11          |
| (1,203) | 1:13:A:LEU:HD23 | 1:15:A:ARG:HA  | 19       | 0.11          |
| (1,201) | 1:13:A:LEU:H    | 1:14:A:GLN:H   | 11       | 0.11          |
| (1,187) | 1:12:A:ILE:HG12 | 1:13:A:LEU:H   | 8        | 0.11          |
| (1,187) | 1:12:A:ILE:HG13 | 1:13:A:LEU:H   | 8        | 0.11          |
| (1,187) | 1:12:A:ILE:HG12 | 1:13:A:LEU:H   | 9        | 0.11          |
| (1,187) | 1:12:A:ILE:HG13 | 1:13:A:LEU:H   | 9        | 0.11          |
| (1,185) | 1:12:A:ILE:HD11 | 1:13:A:LEU:H   | 2        | 0.11          |
| (1,185) | 1:12:A:ILE:HD12 | 1:13:A:LEU:H   | 2        | 0.11          |
| (1,185) | 1:12:A:ILE:HD13 | 1:13:A:LEU:H   | 2        | 0.11          |
| (1,185) | 1:12:A:ILE:HD11 | 1:13:A:LEU:H   | 10       | 0.11          |
| (1,185) | 1:12:A:ILE:HD12 | 1:13:A:LEU:H   | 10       | 0.11          |
| (1,185) | 1:12:A:ILE:HD13 | 1:13:A:LEU:H   | 10       | 0.11          |
| (1,185) | 1:12:A:ILE:HD11 | 1:13:A:LEU:H   | 11       | 0.11          |
| (1,185) | 1:12:A:ILE:HD12 | 1:13:A:LEU:H   | 11       | 0.11          |
| (1,185) | 1:12:A:ILE:HD13 | 1:13:A:LEU:H   | 11       | 0.11          |
| (1,185) | 1:12:A:ILE:HD11 | 1:13:A:LEU:H   | 13       | 0.11          |
| (1,185) | 1:12:A:ILE:HD12 | 1:13:A:LEU:H   | 13       | 0.11          |
| (1,185) | 1:12:A:ILE:HD13 | 1:13:A:LEU:H   | 13       | 0.11          |
| (1,157) | 1:11:A:PHE:HA   | 1:11:A:PHE:HE1 | 2        | 0.11          |
| (1,157) | 1:11:A:PHE:HA   | 1:11:A:PHE:HE2 | 2        | 0.11          |
| (1,157) | 1:11:A:PHE:HA   | 1:11:A:PHE:HE1 | 7        | 0.11          |
| (1,157) | 1:11:A:PHE:HA   | 1:11:A:PHE:HE2 | 7        | 0.11          |
| (1,157) | 1:11:A:PHE:HA   | 1:11:A:PHE:HE1 | 8        | 0.11          |
| (1,157) | 1:11:A:PHE:HA   | 1:11:A:PHE:HE2 | 8        | 0.11          |
| (1,157) | 1:11:A:PHE:HA   | 1:11:A:PHE:HE1 | 19       | 0.11          |
| (1,157) | 1:11:A:PHE:HA   | 1:11:A:PHE:HE2 | 19       | 0.11          |
| (1,154) | 1:9:A:ARG:HG2   | 1:13:A:LEU:H   | 19       | 0.11          |
| (1,154) | 1:9:A:ARG:HG3   | 1:13:A:LEU:H   | 19       | 0.11          |
| (1,105) | 1:6:A:LYS:HA    | 1:9:A:ARG:HD2  | 18       | 0.11          |
| (1,105) | 1:6:A:LYS:HA    | 1:9:A:ARG:HD3  | 18       | 0.11          |
| (1,102) | 1:6:A:LYS:H     | 1:7:A:PHE:H    | 14       | 0.11          |
| (1,102) | 1:6:A:LYS:H     | 1:7:A:PHE:H    | 18       | 0.11          |
| (1,65)  | 1:4:A:LEU:HD11  | 1:8:A:PHE:HZ   | 11       | 0.11          |
| (1,65)  | 1:4:A:LEU:HD12  | 1:8:A:PHE:HZ   | 11       | 0.11          |
| (1,65)  | 1:4:A:LEU:HD13  | 1:8:A:PHE:HZ   | 11       | 0.11          |
| (1,65)  | 1:4:A:LEU:HD21  | 1:8:A:PHE:HZ   | 11       | 0.11          |
| (1,65)  | 1:4:A:LEU:HD22  | 1:8:A:PHE:HZ   | 11       | 0.11          |
| (1,65)  | 1:4:A:LEU:HD23  | 1:8:A:PHE:HZ   | 11       | 0.11          |
| (1,57)  | 1:4:A:LEU:HA    | 1:7:A:PHE:HZ   | 2        | 0.11          |
| (1,57)  | 1:4:A:LEU:HA    | 1:7:A:PHE:HZ   | 6        | 0.11          |
| (1,57)  | 1:4:A:LEU:HA    | 1:7:A:PHE:HZ   | 13       | 0.11          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,28)  | 1:3:A:ARG:H    | 1:4:A:LEU:H    | 14       | 0.11          |
| (1,19)  | 1:3:A:ARG:HD2  | 1:3:A:ARG:HE   | 4        | 0.11          |
| (1,19)  | 1:3:A:ARG:HD3  | 1:3:A:ARG:HE   | 4        | 0.11          |
| (1,19)  | 1:3:A:ARG:HD2  | 1:3:A:ARG:HE   | 11       | 0.11          |
| (1,19)  | 1:3:A:ARG:HD3  | 1:3:A:ARG:HE   | 11       | 0.11          |
| (1,19)  | 1:3:A:ARG:HD2  | 1:3:A:ARG:HE   | 12       | 0.11          |
| (1,19)  | 1:3:A:ARG:HD3  | 1:3:A:ARG:HE   | 12       | 0.11          |
| (1,19)  | 1:3:A:ARG:HD2  | 1:3:A:ARG:HE   | 13       | 0.11          |
| (1,19)  | 1:3:A:ARG:HD3  | 1:3:A:ARG:HE   | 13       | 0.11          |
| (1,19)  | 1:3:A:ARG:HD2  | 1:3:A:ARG:HE   | 14       | 0.11          |
| (1,19)  | 1:3:A:ARG:HD3  | 1:3:A:ARG:HE   | 14       | 0.11          |
| (1,19)  | 1:3:A:ARG:HD2  | 1:3:A:ARG:HE   | 19       | 0.11          |
| (1,19)  | 1:3:A:ARG:HD3  | 1:3:A:ARG:HE   | 19       | 0.11          |
| (1,6)   | 1:2:A:MET:HB2  | 1:4:A:LEU:HD11 | 9        | 0.11          |
| (1,6)   | 1:2:A:MET:HB2  | 1:4:A:LEU:HD12 | 9        | 0.11          |
| (1,6)   | 1:2:A:MET:HB2  | 1:4:A:LEU:HD13 | 9        | 0.11          |
| (1,6)   | 1:2:A:MET:HB2  | 1:4:A:LEU:HD21 | 9        | 0.11          |
| (1,6)   | 1:2:A:MET:HB2  | 1:4:A:LEU:HD22 | 9        | 0.11          |
| (1,6)   | 1:2:A:MET:HB2  | 1:4:A:LEU:HD23 | 9        | 0.11          |
| (1,6)   | 1:2:A:MET:HB3  | 1:4:A:LEU:HD11 | 9        | 0.11          |
| (1,6)   | 1:2:A:MET:HB3  | 1:4:A:LEU:HD12 | 9        | 0.11          |
| (1,6)   | 1:2:A:MET:HB3  | 1:4:A:LEU:HD13 | 9        | 0.11          |
| (1,6)   | 1:2:A:MET:HB3  | 1:4:A:LEU:HD21 | 9        | 0.11          |
| (1,6)   | 1:2:A:MET:HB3  | 1:4:A:LEU:HD22 | 9        | 0.11          |
| (1,6)   | 1:2:A:MET:HB3  | 1:4:A:LEU:HD23 | 9        | 0.11          |
| (1,250) | 1:17:A:LYS:HG2 | 1:17:A:LYS:H   | 6        | 0.1           |
| (1,250) | 1:17:A:LYS:HG3 | 1:17:A:LYS:H   | 6        | 0.1           |
| (1,250) | 1:17:A:LYS:HG2 | 1:17:A:LYS:H   | 20       | 0.1           |
| (1,250) | 1:17:A:LYS:HG3 | 1:17:A:LYS:H   | 20       | 0.1           |
| (1,241) | 1:16:A:LYS:HA  | 1:17:A:LYS:H   | 3        | 0.1           |
| (1,241) | 1:16:A:LYS:HA  | 1:17:A:LYS:H   | 4        | 0.1           |
| (1,241) | 1:16:A:LYS:HA  | 1:17:A:LYS:H   | 5        | 0.1           |
| (1,241) | 1:16:A:LYS:HA  | 1:17:A:LYS:H   | 10       | 0.1           |
| (1,241) | 1:16:A:LYS:HA  | 1:17:A:LYS:H   | 15       | 0.1           |
| (1,175) | 1:12:A:ILE:HB  | 1:12:A:ILE:H   | 4        | 0.1           |
| (1,157) | 1:11:A:PHE:HA  | 1:11:A:PHE:HE1 | 17       | 0.1           |
| (1,157) | 1:11:A:PHE:HA  | 1:11:A:PHE:HE2 | 17       | 0.1           |
| (1,154) | 1:9:A:ARG:HG2  | 1:13:A:LEU:H   | 2        | 0.1           |
| (1,154) | 1:9:A:ARG:HG3  | 1:13:A:LEU:H   | 2        | 0.1           |
| (1,154) | 1:9:A:ARG:HG2  | 1:13:A:LEU:H   | 13       | 0.1           |
| (1,154) | 1:9:A:ARG:HG3  | 1:13:A:LEU:H   | 13       | 0.1           |
| (1,139) | 1:9:A:ARG:HA   | 1:9:A:ARG:HD2  | 17       | 0.1           |

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| Key     | Atom-1       | Atom-2        | Model ID | Violation (Å) |
|---------|--------------|---------------|----------|---------------|
| (1,139) | 1:9:A:ARG:HA | 1:9:A:ARG:HD3 | 17       | 0.1           |
| (1,57)  | 1:4:A:LEU:HA | 1:7:A:PHE:HZ  | 20       | 0.1           |

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

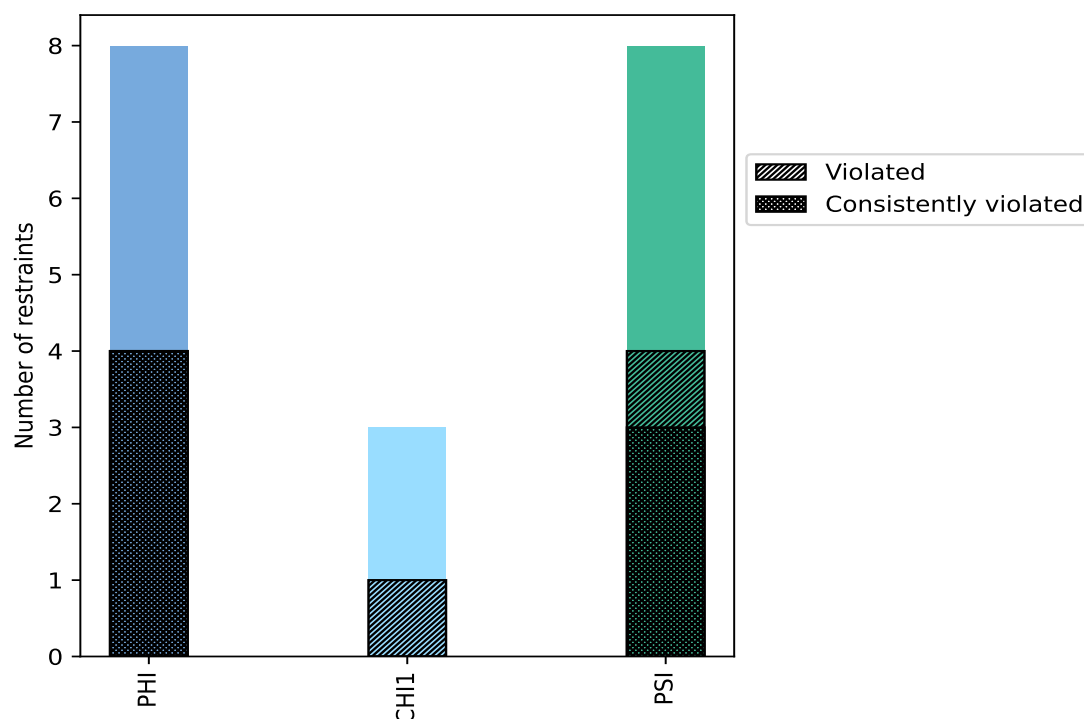
### 10.1 Summary of dihedral-angle violations [i](#)

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

| Angle type | Count | % <sup>1</sup> | Violated <sup>3</sup> |                |                | Consistently Violated <sup>4</sup> |                |                |
|------------|-------|----------------|-----------------------|----------------|----------------|------------------------------------|----------------|----------------|
|            |       |                | Count                 | % <sup>2</sup> | % <sup>1</sup> | Count                              | % <sup>2</sup> | % <sup>1</sup> |
| PHI        | 8     | 42.1           | 4                     | 50.0           | 21.1           | 4                                  | 50.0           | 21.1           |
| CHI1       | 3     | 15.8           | 1                     | 33.3           | 5.3            | 0                                  | 0.0            | 0.0            |
| PSI        | 8     | 42.1           | 4                     | 50.0           | 21.1           | 3                                  | 37.5           | 15.8           |
| Total      | 19    | 100.0          | 9                     | 47.4           | 47.4           | 7                                  | 36.8           | 36.8           |

<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 [i](#)



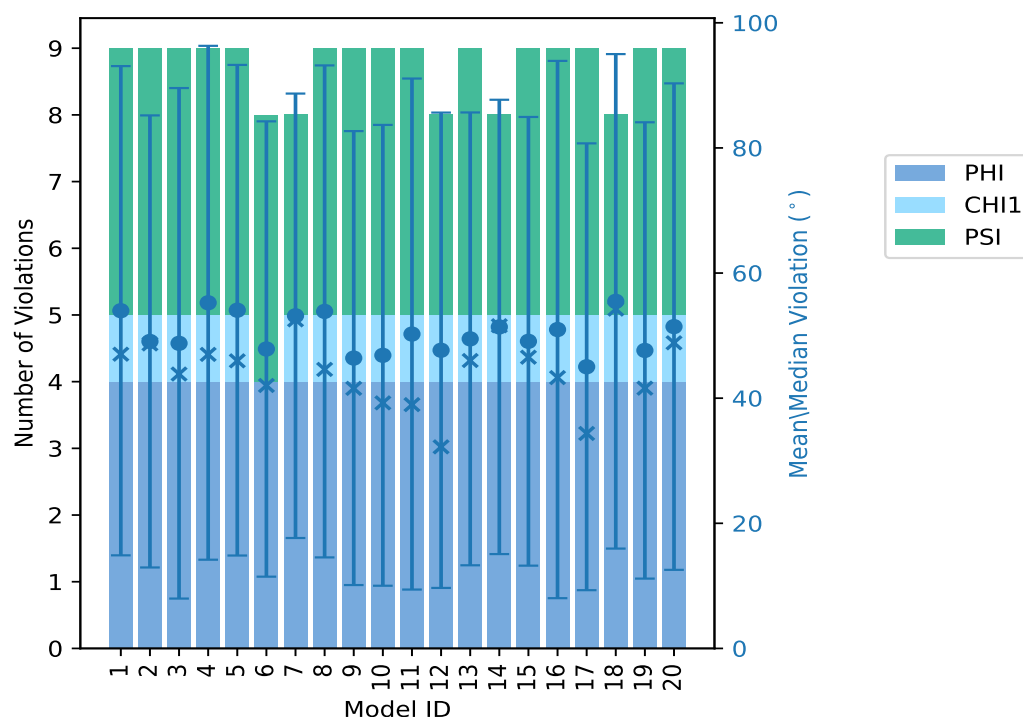
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

## 10.2 Dihedral-angle violation statistics for each model

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

| Model ID | Number of violations |      |     |       | Mean (°) | Max (°) | SD (°) | Median (°) |
|----------|----------------------|------|-----|-------|----------|---------|--------|------------|
|          | PHI                  | CHI1 | PSI | Total |          |         |        |            |
| 1        | 4                    | 1    | 4   | 9     | 53.98    | 118.85  | 39.1   | 47.03      |
| 2        | 4                    | 1    | 4   | 9     | 49.07    | 120.59  | 36.13  | 48.67      |
| 3        | 4                    | 1    | 4   | 9     | 48.77    | 142.57  | 40.8   | 43.86      |
| 4        | 4                    | 1    | 4   | 9     | 55.25    | 127.9   | 41.07  | 47.0       |
| 5        | 4                    | 1    | 4   | 9     | 54.06    | 118.49  | 39.21  | 45.97      |
| 6        | 4                    | 0    | 4   | 8     | 47.86    | 117.77  | 36.39  | 42.03      |
| 7        | 4                    | 1    | 3   | 8     | 53.17    | 116.71  | 35.52  | 52.52      |
| 8        | 4                    | 1    | 4   | 9     | 53.87    | 119.34  | 39.32  | 44.6       |
| 9        | 4                    | 1    | 4   | 9     | 46.41    | 120.51  | 36.28  | 41.57      |
| 10       | 4                    | 1    | 4   | 9     | 46.85    | 121.88  | 36.83  | 39.25      |
| 11       | 4                    | 1    | 4   | 9     | 50.25    | 120.76  | 40.84  | 38.97      |
| 12       | 4                    | 1    | 3   | 8     | 47.66    | 109.9   | 37.99  | 32.22      |
| 13       | 4                    | 1    | 4   | 9     | 49.48    | 120.58  | 36.19  | 46.02      |
| 14       | 4                    | 1    | 3   | 8     | 51.39    | 119.8   | 36.31  | 51.58      |
| 15       | 4                    | 1    | 4   | 9     | 49.09    | 120.27  | 35.86  | 46.55      |
| 16       | 4                    | 1    | 4   | 9     | 50.97    | 136.62  | 42.94  | 43.29      |
| 17       | 4                    | 1    | 4   | 9     | 45.02    | 113.81  | 35.71  | 34.36      |
| 18       | 4                    | 1    | 3   | 8     | 55.48    | 117.74  | 39.52  | 54.24      |
| 19       | 4                    | 1    | 4   | 9     | 47.63    | 118.58  | 36.47  | 41.6       |
| 20       | 4                    | 1    | 4   | 9     | 51.44    | 116.9   | 38.88  | 48.85      |

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



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

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

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

| Number of violated restraints |      |     |       | Fraction of the ensemble |      |
|-------------------------------|------|-----|-------|--------------------------|------|
| PHI                           | CHI1 | PSI | Total | Count <sup>1</sup>       | %    |
| 0                             | 0    | 0   | 0     | 1                        | 5.0  |
| 0                             | 0    | 0   | 0     | 2                        | 10.0 |
| 0                             | 0    | 0   | 0     | 3                        | 15.0 |
| 0                             | 0    | 0   | 0     | 4                        | 20.0 |
| 0                             | 0    | 0   | 0     | 5                        | 25.0 |
| 0                             | 0    | 0   | 0     | 6                        | 30.0 |
| 0                             | 0    | 0   | 0     | 7                        | 35.0 |
| 0                             | 0    | 0   | 0     | 8                        | 40.0 |
| 0                             | 0    | 0   | 0     | 9                        | 45.0 |
| 0                             | 0    | 0   | 0     | 10                       | 50.0 |
| 0                             | 0    | 0   | 0     | 11                       | 55.0 |

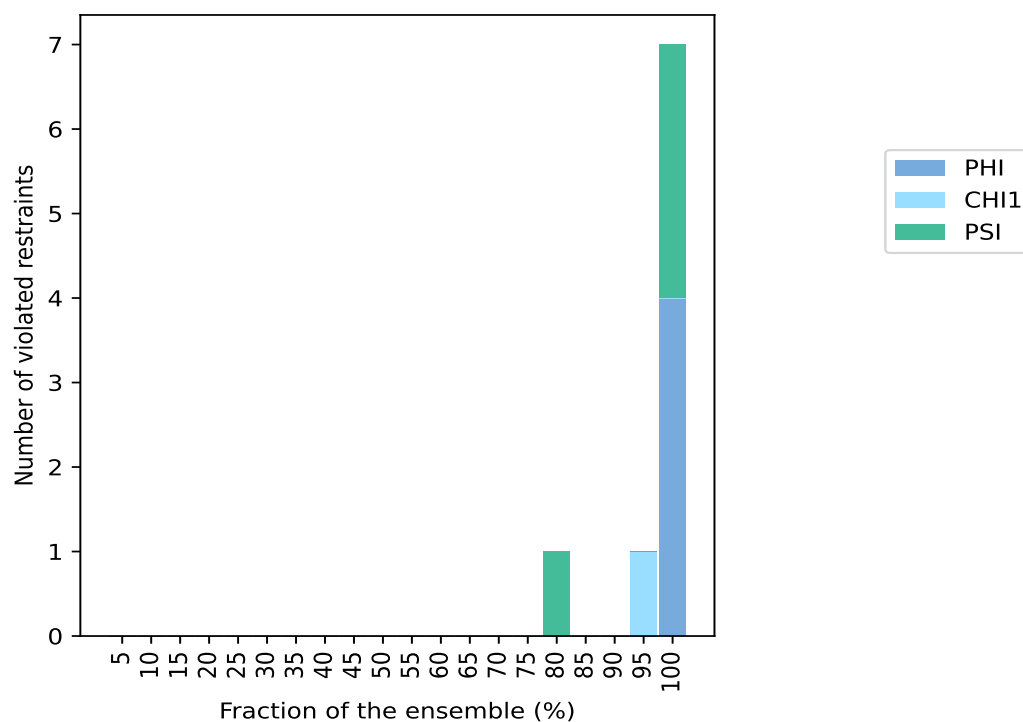
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| Number of violated restraints |      |     |       | Fraction of the ensemble |       |
|-------------------------------|------|-----|-------|--------------------------|-------|
| PHI                           | CHI1 | PSI | Total | Count <sup>1</sup>       | %     |
| 0                             | 0    | 0   | 0     | 12                       | 60.0  |
| 0                             | 0    | 0   | 0     | 13                       | 65.0  |
| 0                             | 0    | 0   | 0     | 14                       | 70.0  |
| 0                             | 0    | 0   | 0     | 15                       | 75.0  |
| 0                             | 0    | 1   | 1     | 16                       | 80.0  |
| 0                             | 0    | 0   | 0     | 17                       | 85.0  |
| 0                             | 0    | 0   | 0     | 18                       | 90.0  |
| 0                             | 1    | 0   | 1     | 19                       | 95.0  |
| 4                             | 0    | 3   | 7     | 20                       | 100.0 |

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

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

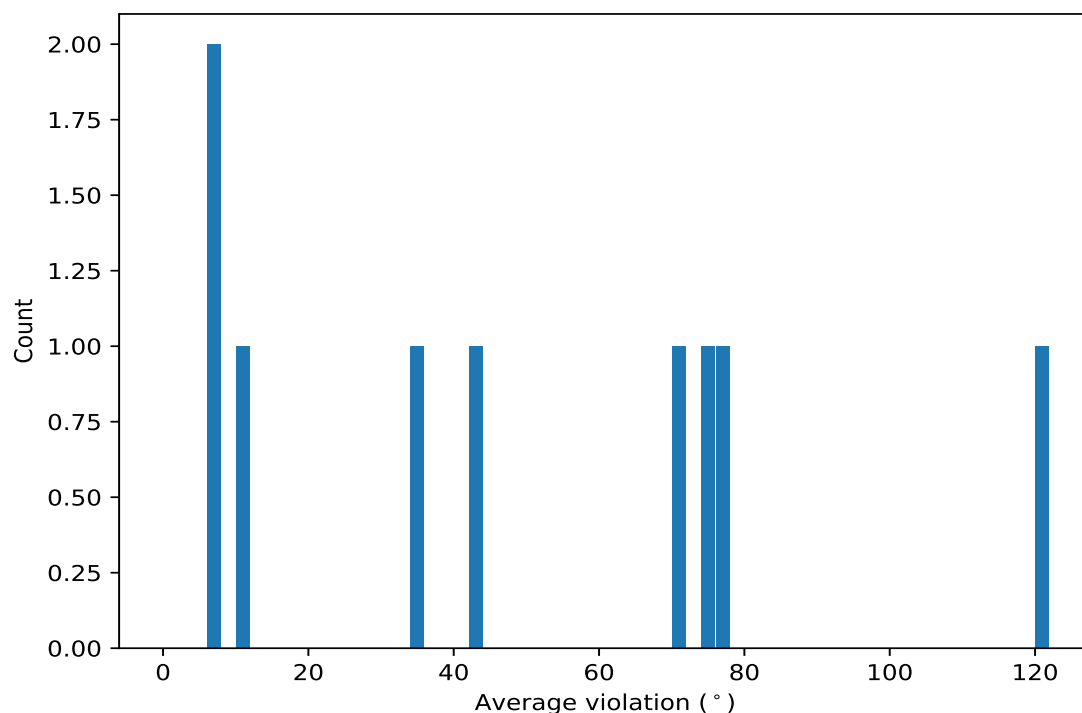


## 10.4 Most violated dihedral-angle restraints in the ensemble [i](#)

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

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

in the ensemble



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

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

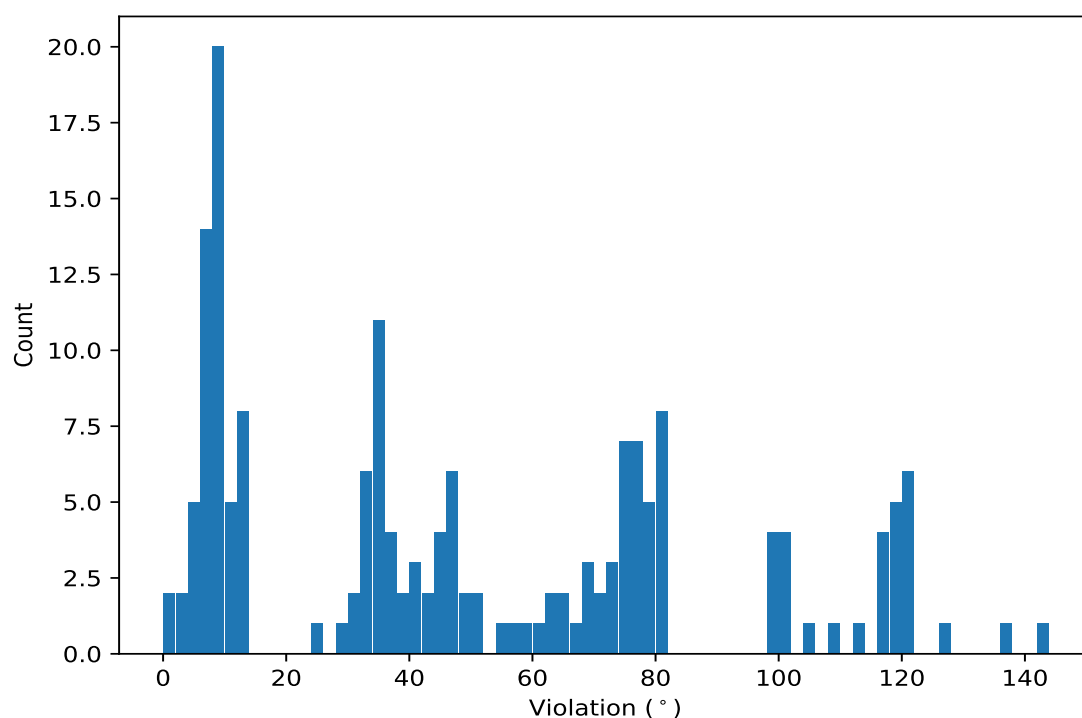
| Key    | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Models <sup>1</sup> | Mean   | SD <sup>2</sup> | Median |
|--------|--------------|---------------|---------------|--------------|---------------------|--------|-----------------|--------|
| (2,16) | 1:12:A:ILE:N | 1:12:A:ILE:CA | 1:12:A:ILE:C  | 1:13:A:LEU:N | 20                  | 120.35 | 7.94            | 119.57 |
| (2,4)  | 1:5:A:SER:N  | 1:5:A:SER:CA  | 1:5:A:SER:C   | 1:6:A:LYS:N  | 20                  | 77.1   | 3.56            | 77.69  |
| (2,15) | 1:11:A:PHE:C | 1:12:A:ILE:N  | 1:12:A:ILE:CA | 1:12:A:ILE:C | 20                  | 71.14  | 16.87           | 74.73  |
| (2,5)  | 1:5:A:SER:C  | 1:6:A:LYS:N   | 1:6:A:LYS:CA  | 1:6:A:LYS:C  | 20                  | 43.41  | 5.75            | 45.78  |
| (2,7)  | 1:6:A:LYS:C  | 1:7:A:PHE:N   | 1:7:A:PHE:CA  | 1:7:A:PHE:C  | 20                  | 34.65  | 1.27            | 34.76  |
| (2,9)  | 1:7:A:PHE:C  | 1:8:A:PHE:N   | 1:8:A:PHE:CA  | 1:8:A:PHE:C  | 20                  | 10.16  | 3.04            | 11.75  |
| (2,8)  | 1:7:A:PHE:N  | 1:7:A:PHE:CA  | 1:7:A:PHE:C   | 1:8:A:PHE:N  | 20                  | 7.92   | 0.99            | 8.26   |
| (1,1)  | 1:4:A:LEU:N  | 1:4:A:LEU:CA  | 1:4:A:LEU:CB  | 1:4:A:LEU:CG | 19                  | 74.63  | 23.76           | 66.37  |
| (2,6)  | 1:6:A:LYS:N  | 1:6:A:LYS:CA  | 1:6:A:LYS:C   | 1:7:A:PHE:N  | 16                  | 6.3    | 2.64            | 7.09   |

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

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

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

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



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

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

| Key    | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Model ID | Violation (°) |
|--------|--------------|---------------|---------------|--------------|----------|---------------|
| (2,16) | 1:12:A:ILE:N | 1:12:A:ILE:CA | 1:12:A:ILE:C  | 1:13:A:LEU:N | 3        | 142.57        |
| (2,16) | 1:12:A:ILE:N | 1:12:A:ILE:CA | 1:12:A:ILE:C  | 1:13:A:LEU:N | 16       | 136.62        |
| (2,16) | 1:12:A:ILE:N | 1:12:A:ILE:CA | 1:12:A:ILE:C  | 1:13:A:LEU:N | 4        | 127.9         |
| (2,16) | 1:12:A:ILE:N | 1:12:A:ILE:CA | 1:12:A:ILE:C  | 1:13:A:LEU:N | 10       | 121.88        |
| (2,16) | 1:12:A:ILE:N | 1:12:A:ILE:CA | 1:12:A:ILE:C  | 1:13:A:LEU:N | 11       | 120.76        |
| (2,16) | 1:12:A:ILE:N | 1:12:A:ILE:CA | 1:12:A:ILE:C  | 1:13:A:LEU:N | 2        | 120.59        |
| (2,16) | 1:12:A:ILE:N | 1:12:A:ILE:CA | 1:12:A:ILE:C  | 1:13:A:LEU:N | 13       | 120.58        |
| (2,16) | 1:12:A:ILE:N | 1:12:A:ILE:CA | 1:12:A:ILE:C  | 1:13:A:LEU:N | 9        | 120.51        |
| (2,16) | 1:12:A:ILE:N | 1:12:A:ILE:CA | 1:12:A:ILE:C  | 1:13:A:LEU:N | 15       | 120.27        |
| (2,16) | 1:12:A:ILE:N | 1:12:A:ILE:CA | 1:12:A:ILE:C  | 1:13:A:LEU:N | 14       | 119.8         |
| (2,16) | 1:12:A:ILE:N | 1:12:A:ILE:CA | 1:12:A:ILE:C  | 1:13:A:LEU:N | 8        | 119.34        |
| (2,16) | 1:12:A:ILE:N | 1:12:A:ILE:CA | 1:12:A:ILE:C  | 1:13:A:LEU:N | 1        | 118.85        |
| (2,16) | 1:12:A:ILE:N | 1:12:A:ILE:CA | 1:12:A:ILE:C  | 1:13:A:LEU:N | 19       | 118.58        |
| (2,16) | 1:12:A:ILE:N | 1:12:A:ILE:CA | 1:12:A:ILE:C  | 1:13:A:LEU:N | 5        | 118.49        |
| (2,16) | 1:12:A:ILE:N | 1:12:A:ILE:CA | 1:12:A:ILE:C  | 1:13:A:LEU:N | 6        | 117.77        |
| (2,16) | 1:12:A:ILE:N | 1:12:A:ILE:CA | 1:12:A:ILE:C  | 1:13:A:LEU:N | 18       | 117.74        |
| (2,15) | 1:11:A:PHE:C | 1:12:A:ILE:N  | 1:12:A:ILE:CA | 1:12:A:ILE:C | 20       | 116.9         |
| (2,16) | 1:12:A:ILE:N | 1:12:A:ILE:CA | 1:12:A:ILE:C  | 1:13:A:LEU:N | 7        | 116.71        |
| (2,16) | 1:12:A:ILE:N | 1:12:A:ILE:CA | 1:12:A:ILE:C  | 1:13:A:LEU:N | 17       | 113.81        |
| (2,16) | 1:12:A:ILE:N | 1:12:A:ILE:CA | 1:12:A:ILE:C  | 1:13:A:LEU:N | 12       | 109.9         |
| (2,16) | 1:12:A:ILE:N | 1:12:A:ILE:CA | 1:12:A:ILE:C  | 1:13:A:LEU:N | 20       | 104.39        |

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| Key    | Atom-1       | Atom-2       | Atom-3        | Atom-4       | Model ID | Violation (°) |
|--------|--------------|--------------|---------------|--------------|----------|---------------|
| (1,1)  | 1:4:A:LEU:N  | 1:4:A:LEU:CA | 1:4:A:LEU:CB  | 1:4:A:LEU:CG | 18       | 100.81        |
| (1,1)  | 1:4:A:LEU:N  | 1:4:A:LEU:CA | 1:4:A:LEU:CB  | 1:4:A:LEU:CG | 11       | 100.73        |
| (1,1)  | 1:4:A:LEU:N  | 1:4:A:LEU:CA | 1:4:A:LEU:CB  | 1:4:A:LEU:CG | 16       | 100.54        |
| (1,1)  | 1:4:A:LEU:N  | 1:4:A:LEU:CA | 1:4:A:LEU:CB  | 1:4:A:LEU:CG | 8        | 100.43        |
| (1,1)  | 1:4:A:LEU:N  | 1:4:A:LEU:CA | 1:4:A:LEU:CB  | 1:4:A:LEU:CG | 12       | 99.86         |
| (1,1)  | 1:4:A:LEU:N  | 1:4:A:LEU:CA | 1:4:A:LEU:CB  | 1:4:A:LEU:CG | 4        | 99.81         |
| (1,1)  | 1:4:A:LEU:N  | 1:4:A:LEU:CA | 1:4:A:LEU:CB  | 1:4:A:LEU:CG | 5        | 99.77         |
| (1,1)  | 1:4:A:LEU:N  | 1:4:A:LEU:CA | 1:4:A:LEU:CB  | 1:4:A:LEU:CG | 1        | 99.62         |
| (2,15) | 1:11:A:PHE:C | 1:12:A:ILE:N | 1:12:A:ILE:CA | 1:12:A:ILE:C | 19       | 81.57         |
| (2,4)  | 1:5:A:SER:N  | 1:5:A:SER:CA | 1:5:A:SER:C   | 1:6:A:LYS:N  | 5        | 80.83         |
| (2,4)  | 1:5:A:SER:N  | 1:5:A:SER:CA | 1:5:A:SER:C   | 1:6:A:LYS:N  | 8        | 80.77         |
| (2,4)  | 1:5:A:SER:N  | 1:5:A:SER:CA | 1:5:A:SER:C   | 1:6:A:LYS:N  | 1        | 80.69         |
| (2,15) | 1:11:A:PHE:C | 1:12:A:ILE:N | 1:12:A:ILE:CA | 1:12:A:ILE:C | 17       | 80.53         |
| (2,4)  | 1:5:A:SER:N  | 1:5:A:SER:CA | 1:5:A:SER:C   | 1:6:A:LYS:N  | 4        | 80.52         |
| (2,4)  | 1:5:A:SER:N  | 1:5:A:SER:CA | 1:5:A:SER:C   | 1:6:A:LYS:N  | 20       | 80.16         |
| (2,4)  | 1:5:A:SER:N  | 1:5:A:SER:CA | 1:5:A:SER:C   | 1:6:A:LYS:N  | 15       | 80.01         |
| (2,4)  | 1:5:A:SER:N  | 1:5:A:SER:CA | 1:5:A:SER:C   | 1:6:A:LYS:N  | 13       | 79.56         |
| (2,4)  | 1:5:A:SER:N  | 1:5:A:SER:CA | 1:5:A:SER:C   | 1:6:A:LYS:N  | 2        | 79.22         |
| (2,4)  | 1:5:A:SER:N  | 1:5:A:SER:CA | 1:5:A:SER:C   | 1:6:A:LYS:N  | 19       | 79.22         |
| (2,15) | 1:11:A:PHE:C | 1:12:A:ILE:N | 1:12:A:ILE:CA | 1:12:A:ILE:C | 4        | 78.37         |
| (2,4)  | 1:5:A:SER:N  | 1:5:A:SER:CA | 1:5:A:SER:C   | 1:6:A:LYS:N  | 17       | 78.07         |
| (2,15) | 1:11:A:PHE:C | 1:12:A:ILE:N | 1:12:A:ILE:CA | 1:12:A:ILE:C | 5        | 77.45         |
| (2,4)  | 1:5:A:SER:N  | 1:5:A:SER:CA | 1:5:A:SER:C   | 1:6:A:LYS:N  | 7        | 77.32         |
| (2,4)  | 1:5:A:SER:N  | 1:5:A:SER:CA | 1:5:A:SER:C   | 1:6:A:LYS:N  | 3        | 77.28         |
| (2,15) | 1:11:A:PHE:C | 1:12:A:ILE:N | 1:12:A:ILE:CA | 1:12:A:ILE:C | 7        | 77.26         |
| (2,4)  | 1:5:A:SER:N  | 1:5:A:SER:CA | 1:5:A:SER:C   | 1:6:A:LYS:N  | 16       | 76.7          |
| (2,4)  | 1:5:A:SER:N  | 1:5:A:SER:CA | 1:5:A:SER:C   | 1:6:A:LYS:N  | 9        | 76.42         |
| (2,4)  | 1:5:A:SER:N  | 1:5:A:SER:CA | 1:5:A:SER:C   | 1:6:A:LYS:N  | 10       | 76.21         |
| (2,15) | 1:11:A:PHE:C | 1:12:A:ILE:N | 1:12:A:ILE:CA | 1:12:A:ILE:C | 2        | 75.88         |
| (2,15) | 1:11:A:PHE:C | 1:12:A:ILE:N | 1:12:A:ILE:CA | 1:12:A:ILE:C | 8        | 75.55         |
| (2,15) | 1:11:A:PHE:C | 1:12:A:ILE:N | 1:12:A:ILE:CA | 1:12:A:ILE:C | 13       | 75.52         |
| (2,15) | 1:11:A:PHE:C | 1:12:A:ILE:N | 1:12:A:ILE:CA | 1:12:A:ILE:C | 1        | 75.43         |
| (2,4)  | 1:5:A:SER:N  | 1:5:A:SER:CA | 1:5:A:SER:C   | 1:6:A:LYS:N  | 6        | 74.35         |
| (2,4)  | 1:5:A:SER:N  | 1:5:A:SER:CA | 1:5:A:SER:C   | 1:6:A:LYS:N  | 11       | 74.26         |
| (2,15) | 1:11:A:PHE:C | 1:12:A:ILE:N | 1:12:A:ILE:CA | 1:12:A:ILE:C | 18       | 74.03         |
| (2,15) | 1:11:A:PHE:C | 1:12:A:ILE:N | 1:12:A:ILE:CA | 1:12:A:ILE:C | 15       | 73.97         |
| (2,15) | 1:11:A:PHE:C | 1:12:A:ILE:N | 1:12:A:ILE:CA | 1:12:A:ILE:C | 6        | 73.94         |
| (2,15) | 1:11:A:PHE:C | 1:12:A:ILE:N | 1:12:A:ILE:CA | 1:12:A:ILE:C | 14       | 73.15         |
| (2,4)  | 1:5:A:SER:N  | 1:5:A:SER:CA | 1:5:A:SER:C   | 1:6:A:LYS:N  | 18       | 71.75         |
| (2,4)  | 1:5:A:SER:N  | 1:5:A:SER:CA | 1:5:A:SER:C   | 1:6:A:LYS:N  | 14       | 70.55         |
| (1,1)  | 1:4:A:LEU:N  | 1:4:A:LEU:CA | 1:4:A:LEU:CB  | 1:4:A:LEU:CG | 14       | 69.39         |
| (2,15) | 1:11:A:PHE:C | 1:12:A:ILE:N | 1:12:A:ILE:CA | 1:12:A:ILE:C | 11       | 69.08         |
| (2,4)  | 1:5:A:SER:N  | 1:5:A:SER:CA | 1:5:A:SER:C   | 1:6:A:LYS:N  | 12       | 68.19         |
| (1,1)  | 1:4:A:LEU:N  | 1:4:A:LEU:CA | 1:4:A:LEU:CB  | 1:4:A:LEU:CG | 10       | 66.37         |
| (1,1)  | 1:4:A:LEU:N  | 1:4:A:LEU:CA | 1:4:A:LEU:CB  | 1:4:A:LEU:CG | 3        | 65.41         |
| (1,1)  | 1:4:A:LEU:N  | 1:4:A:LEU:CA | 1:4:A:LEU:CB  | 1:4:A:LEU:CG | 7        | 64.96         |
| (1,1)  | 1:4:A:LEU:N  | 1:4:A:LEU:CA | 1:4:A:LEU:CB  | 1:4:A:LEU:CG | 9        | 62.71         |
| (2,15) | 1:11:A:PHE:C | 1:12:A:ILE:N | 1:12:A:ILE:CA | 1:12:A:ILE:C | 10       | 62.13         |
| (2,15) | 1:11:A:PHE:C | 1:12:A:ILE:N | 1:12:A:ILE:CA | 1:12:A:ILE:C | 9        | 61.65         |
| (1,1)  | 1:4:A:LEU:N  | 1:4:A:LEU:CA | 1:4:A:LEU:CB  | 1:4:A:LEU:CG | 13       | 59.96         |
| (1,1)  | 1:4:A:LEU:N  | 1:4:A:LEU:CA | 1:4:A:LEU:CB  | 1:4:A:LEU:CG | 15       | 56.88         |

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| Key    | Atom-1       | Atom-2       | Atom-3        | Atom-4       | Model ID | Violation (°) |
|--------|--------------|--------------|---------------|--------------|----------|---------------|
| (1,1)  | 1:4:A:LEU:N  | 1:4:A:LEU:CA | 1:4:A:LEU:CB  | 1:4:A:LEU:CG | 2        | 54.66         |
| (2,5)  | 1:5:A:SER:C  | 1:6:A:LYS:N  | 1:6:A:LYS:CA  | 1:6:A:LYS:C  | 20       | 51.22         |
| (2,5)  | 1:5:A:SER:C  | 1:6:A:LYS:N  | 1:6:A:LYS:CA  | 1:6:A:LYS:C  | 6        | 50.71         |
| (1,1)  | 1:4:A:LEU:N  | 1:4:A:LEU:CA | 1:4:A:LEU:CB  | 1:4:A:LEU:CG | 20       | 48.85         |
| (2,5)  | 1:5:A:SER:C  | 1:6:A:LYS:N  | 1:6:A:LYS:CA  | 1:6:A:LYS:C  | 2        | 48.67         |
| (2,5)  | 1:5:A:SER:C  | 1:6:A:LYS:N  | 1:6:A:LYS:CA  | 1:6:A:LYS:C  | 19       | 47.17         |
| (2,5)  | 1:5:A:SER:C  | 1:6:A:LYS:N  | 1:6:A:LYS:CA  | 1:6:A:LYS:C  | 3        | 47.11         |
| (2,5)  | 1:5:A:SER:C  | 1:6:A:LYS:N  | 1:6:A:LYS:CA  | 1:6:A:LYS:C  | 1        | 47.03         |
| (2,5)  | 1:5:A:SER:C  | 1:6:A:LYS:N  | 1:6:A:LYS:CA  | 1:6:A:LYS:C  | 4        | 47.0          |
| (2,5)  | 1:5:A:SER:C  | 1:6:A:LYS:N  | 1:6:A:LYS:CA  | 1:6:A:LYS:C  | 15       | 46.55         |
| (2,5)  | 1:5:A:SER:C  | 1:6:A:LYS:N  | 1:6:A:LYS:CA  | 1:6:A:LYS:C  | 13       | 46.02         |
| (2,5)  | 1:5:A:SER:C  | 1:6:A:LYS:N  | 1:6:A:LYS:CA  | 1:6:A:LYS:C  | 5        | 45.97         |
| (2,5)  | 1:5:A:SER:C  | 1:6:A:LYS:N  | 1:6:A:LYS:CA  | 1:6:A:LYS:C  | 17       | 45.58         |
| (2,15) | 1:11:A:PHE:C | 1:12:A:ILE:N | 1:12:A:ILE:CA | 1:12:A:ILE:C | 16       | 44.67         |
| (2,5)  | 1:5:A:SER:C  | 1:6:A:LYS:N  | 1:6:A:LYS:CA  | 1:6:A:LYS:C  | 8        | 44.6          |
| (2,15) | 1:11:A:PHE:C | 1:12:A:ILE:N | 1:12:A:ILE:CA | 1:12:A:ILE:C | 3        | 43.86         |
| (2,5)  | 1:5:A:SER:C  | 1:6:A:LYS:N  | 1:6:A:LYS:CA  | 1:6:A:LYS:C  | 16       | 43.29         |
| (1,1)  | 1:4:A:LEU:N  | 1:4:A:LEU:CA | 1:4:A:LEU:CB  | 1:4:A:LEU:CG | 19       | 41.6          |
| (2,5)  | 1:5:A:SER:C  | 1:6:A:LYS:N  | 1:6:A:LYS:CA  | 1:6:A:LYS:C  | 9        | 41.57         |
| (2,5)  | 1:5:A:SER:C  | 1:6:A:LYS:N  | 1:6:A:LYS:CA  | 1:6:A:LYS:C  | 7        | 40.09         |
| (2,5)  | 1:5:A:SER:C  | 1:6:A:LYS:N  | 1:6:A:LYS:CA  | 1:6:A:LYS:C  | 10       | 39.25         |
| (2,5)  | 1:5:A:SER:C  | 1:6:A:LYS:N  | 1:6:A:LYS:CA  | 1:6:A:LYS:C  | 11       | 38.97         |
| (2,7)  | 1:6:A:LYS:C  | 1:7:A:PHE:N  | 1:7:A:PHE:CA  | 1:7:A:PHE:C  | 3        | 37.92         |
| (2,5)  | 1:5:A:SER:C  | 1:6:A:LYS:N  | 1:6:A:LYS:CA  | 1:6:A:LYS:C  | 18       | 36.72         |
| (2,7)  | 1:6:A:LYS:C  | 1:7:A:PHE:N  | 1:7:A:PHE:CA  | 1:7:A:PHE:C  | 10       | 36.55         |
| (2,7)  | 1:6:A:LYS:C  | 1:7:A:PHE:N  | 1:7:A:PHE:CA  | 1:7:A:PHE:C  | 16       | 36.02         |
| (2,7)  | 1:6:A:LYS:C  | 1:7:A:PHE:N  | 1:7:A:PHE:CA  | 1:7:A:PHE:C  | 13       | 35.46         |
| (2,7)  | 1:6:A:LYS:C  | 1:7:A:PHE:N  | 1:7:A:PHE:CA  | 1:7:A:PHE:C  | 9        | 35.45         |
| (2,7)  | 1:6:A:LYS:C  | 1:7:A:PHE:N  | 1:7:A:PHE:CA  | 1:7:A:PHE:C  | 1        | 35.02         |
| (2,7)  | 1:6:A:LYS:C  | 1:7:A:PHE:N  | 1:7:A:PHE:CA  | 1:7:A:PHE:C  | 15       | 35.01         |
| (2,7)  | 1:6:A:LYS:C  | 1:7:A:PHE:N  | 1:7:A:PHE:CA  | 1:7:A:PHE:C  | 2        | 34.83         |
| (2,7)  | 1:6:A:LYS:C  | 1:7:A:PHE:N  | 1:7:A:PHE:CA  | 1:7:A:PHE:C  | 7        | 34.79         |
| (2,7)  | 1:6:A:LYS:C  | 1:7:A:PHE:N  | 1:7:A:PHE:CA  | 1:7:A:PHE:C  | 4        | 34.78         |
| (2,7)  | 1:6:A:LYS:C  | 1:7:A:PHE:N  | 1:7:A:PHE:CA  | 1:7:A:PHE:C  | 19       | 34.75         |
| (2,7)  | 1:6:A:LYS:C  | 1:7:A:PHE:N  | 1:7:A:PHE:CA  | 1:7:A:PHE:C  | 5        | 34.65         |
| (2,7)  | 1:6:A:LYS:C  | 1:7:A:PHE:N  | 1:7:A:PHE:CA  | 1:7:A:PHE:C  | 17       | 34.36         |
| (2,7)  | 1:6:A:LYS:C  | 1:7:A:PHE:N  | 1:7:A:PHE:CA  | 1:7:A:PHE:C  | 8        | 34.18         |
| (2,7)  | 1:6:A:LYS:C  | 1:7:A:PHE:N  | 1:7:A:PHE:CA  | 1:7:A:PHE:C  | 20       | 33.93         |
| (2,7)  | 1:6:A:LYS:C  | 1:7:A:PHE:N  | 1:7:A:PHE:CA  | 1:7:A:PHE:C  | 14       | 33.76         |
| (2,7)  | 1:6:A:LYS:C  | 1:7:A:PHE:N  | 1:7:A:PHE:CA  | 1:7:A:PHE:C  | 6        | 33.35         |
| (2,7)  | 1:6:A:LYS:C  | 1:7:A:PHE:N  | 1:7:A:PHE:CA  | 1:7:A:PHE:C  | 11       | 33.15         |
| (2,7)  | 1:6:A:LYS:C  | 1:7:A:PHE:N  | 1:7:A:PHE:CA  | 1:7:A:PHE:C  | 12       | 32.57         |
| (2,7)  | 1:6:A:LYS:C  | 1:7:A:PHE:N  | 1:7:A:PHE:CA  | 1:7:A:PHE:C  | 18       | 32.52         |
| (2,15) | 1:11:A:PHE:C | 1:12:A:ILE:N | 1:12:A:ILE:CA | 1:12:A:ILE:C | 12       | 31.88         |
| (2,5)  | 1:5:A:SER:C  | 1:6:A:LYS:N  | 1:6:A:LYS:CA  | 1:6:A:LYS:C  | 14       | 30.81         |
| (2,5)  | 1:5:A:SER:C  | 1:6:A:LYS:N  | 1:6:A:LYS:CA  | 1:6:A:LYS:C  | 12       | 29.93         |
| (1,1)  | 1:4:A:LEU:N  | 1:4:A:LEU:CA | 1:4:A:LEU:CB  | 1:4:A:LEU:CG | 17       | 25.65         |
| (2,9)  | 1:7:A:PHE:C  | 1:8:A:PHE:N  | 1:8:A:PHE:CA  | 1:8:A:PHE:C  | 6        | 13.79         |
| (2,9)  | 1:7:A:PHE:C  | 1:8:A:PHE:N  | 1:8:A:PHE:CA  | 1:8:A:PHE:C  | 8        | 13.05         |
| (2,9)  | 1:7:A:PHE:C  | 1:8:A:PHE:N  | 1:8:A:PHE:CA  | 1:8:A:PHE:C  | 17       | 12.84         |
| (2,9)  | 1:7:A:PHE:C  | 1:8:A:PHE:N  | 1:8:A:PHE:CA  | 1:8:A:PHE:C  | 20       | 12.82         |

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| Key   | Atom-1      | Atom-2       | Atom-3       | Atom-4      | Model ID | Violation (°) |
|-------|-------------|--------------|--------------|-------------|----------|---------------|
| (2,9) | 1:7:A:PHE:C | 1:8:A:PHE:N  | 1:8:A:PHE:CA | 1:8:A:PHE:C | 15       | 12.63         |
| (2,9) | 1:7:A:PHE:C | 1:8:A:PHE:N  | 1:8:A:PHE:CA | 1:8:A:PHE:C | 1        | 12.45         |
| (2,9) | 1:7:A:PHE:C | 1:8:A:PHE:N  | 1:8:A:PHE:CA | 1:8:A:PHE:C | 5        | 12.41         |
| (2,9) | 1:7:A:PHE:C | 1:8:A:PHE:N  | 1:8:A:PHE:CA | 1:8:A:PHE:C | 13       | 12.16         |
| (2,9) | 1:7:A:PHE:C | 1:8:A:PHE:N  | 1:8:A:PHE:CA | 1:8:A:PHE:C | 4        | 11.97         |
| (2,9) | 1:7:A:PHE:C | 1:8:A:PHE:N  | 1:8:A:PHE:CA | 1:8:A:PHE:C | 2        | 11.79         |
| (2,9) | 1:7:A:PHE:C | 1:8:A:PHE:N  | 1:8:A:PHE:CA | 1:8:A:PHE:C | 19       | 11.71         |
| (2,9) | 1:7:A:PHE:C | 1:8:A:PHE:N  | 1:8:A:PHE:CA | 1:8:A:PHE:C | 3        | 10.9          |
| (2,6) | 1:6:A:LYS:N | 1:6:A:LYS:CA | 1:6:A:LYS:C  | 1:7:A:PHE:N | 6        | 10.35         |
| (2,9) | 1:7:A:PHE:C | 1:8:A:PHE:N  | 1:8:A:PHE:CA | 1:8:A:PHE:C | 16       | 9.48          |
| (2,8) | 1:7:A:PHE:N | 1:7:A:PHE:CA | 1:7:A:PHE:C  | 1:8:A:PHE:N | 3        | 9.37          |
| (2,8) | 1:7:A:PHE:N | 1:7:A:PHE:CA | 1:7:A:PHE:C  | 1:8:A:PHE:N | 10       | 8.93          |
| (2,8) | 1:7:A:PHE:N | 1:7:A:PHE:CA | 1:7:A:PHE:C  | 1:8:A:PHE:N | 13       | 8.8           |
| (2,9) | 1:7:A:PHE:C | 1:8:A:PHE:N  | 1:8:A:PHE:CA | 1:8:A:PHE:C | 10       | 8.7           |
| (2,9) | 1:7:A:PHE:C | 1:8:A:PHE:N  | 1:8:A:PHE:CA | 1:8:A:PHE:C | 9        | 8.66          |
| (2,8) | 1:7:A:PHE:N | 1:7:A:PHE:CA | 1:7:A:PHE:C  | 1:8:A:PHE:N | 6        | 8.61          |
| (2,8) | 1:7:A:PHE:N | 1:7:A:PHE:CA | 1:7:A:PHE:C  | 1:8:A:PHE:N | 2        | 8.58          |
| (2,6) | 1:6:A:LYS:N | 1:6:A:LYS:CA | 1:6:A:LYS:C  | 1:7:A:PHE:N | 8        | 8.56          |
| (2,6) | 1:6:A:LYS:N | 1:6:A:LYS:CA | 1:6:A:LYS:C  | 1:7:A:PHE:N | 4        | 8.53          |
| (2,6) | 1:6:A:LYS:N | 1:6:A:LYS:CA | 1:6:A:LYS:C  | 1:7:A:PHE:N | 5        | 8.52          |
| (2,8) | 1:7:A:PHE:N | 1:7:A:PHE:CA | 1:7:A:PHE:C  | 1:8:A:PHE:N | 1        | 8.51          |
| (2,8) | 1:7:A:PHE:N | 1:7:A:PHE:CA | 1:7:A:PHE:C  | 1:8:A:PHE:N | 5        | 8.46          |
| (2,8) | 1:7:A:PHE:N | 1:7:A:PHE:CA | 1:7:A:PHE:C  | 1:8:A:PHE:N | 15       | 8.41          |
| (2,8) | 1:7:A:PHE:N | 1:7:A:PHE:CA | 1:7:A:PHE:C  | 1:8:A:PHE:N | 4        | 8.34          |
| (2,8) | 1:7:A:PHE:N | 1:7:A:PHE:CA | 1:7:A:PHE:C  | 1:8:A:PHE:N | 8        | 8.34          |
| (2,8) | 1:7:A:PHE:N | 1:7:A:PHE:CA | 1:7:A:PHE:C  | 1:8:A:PHE:N | 9        | 8.18          |
| (2,6) | 1:6:A:LYS:N | 1:6:A:LYS:CA | 1:6:A:LYS:C  | 1:7:A:PHE:N | 1        | 8.18          |
| (2,6) | 1:6:A:LYS:N | 1:6:A:LYS:CA | 1:6:A:LYS:C  | 1:7:A:PHE:N | 15       | 8.06          |
| (2,8) | 1:7:A:PHE:N | 1:7:A:PHE:CA | 1:7:A:PHE:C  | 1:8:A:PHE:N | 20       | 8.04          |
| (2,8) | 1:7:A:PHE:N | 1:7:A:PHE:CA | 1:7:A:PHE:C  | 1:8:A:PHE:N | 14       | 7.73          |
| (2,8) | 1:7:A:PHE:N | 1:7:A:PHE:CA | 1:7:A:PHE:C  | 1:8:A:PHE:N | 19       | 7.67          |
| (2,8) | 1:7:A:PHE:N | 1:7:A:PHE:CA | 1:7:A:PHE:C  | 1:8:A:PHE:N | 7        | 7.63          |
| (2,8) | 1:7:A:PHE:N | 1:7:A:PHE:CA | 1:7:A:PHE:C  | 1:8:A:PHE:N | 17       | 7.45          |
| (2,9) | 1:7:A:PHE:C | 1:8:A:PHE:N  | 1:8:A:PHE:CA | 1:8:A:PHE:C | 11       | 7.4           |
| (2,6) | 1:6:A:LYS:N | 1:6:A:LYS:CA | 1:6:A:LYS:C  | 1:7:A:PHE:N | 2        | 7.37          |
| (2,6) | 1:6:A:LYS:N | 1:6:A:LYS:CA | 1:6:A:LYS:C  | 1:7:A:PHE:N | 13       | 7.27          |
| (2,8) | 1:7:A:PHE:N | 1:7:A:PHE:CA | 1:7:A:PHE:C  | 1:8:A:PHE:N | 16       | 7.22          |
| (2,6) | 1:6:A:LYS:N | 1:6:A:LYS:CA | 1:6:A:LYS:C  | 1:7:A:PHE:N | 17       | 6.91          |
| (2,8) | 1:7:A:PHE:N | 1:7:A:PHE:CA | 1:7:A:PHE:C  | 1:8:A:PHE:N | 11       | 6.83          |
| (2,6) | 1:6:A:LYS:N | 1:6:A:LYS:CA | 1:6:A:LYS:C  | 1:7:A:PHE:N | 20       | 6.65          |
| (2,9) | 1:7:A:PHE:C | 1:8:A:PHE:N  | 1:8:A:PHE:CA | 1:8:A:PHE:C | 7        | 6.61          |
| (2,6) | 1:6:A:LYS:N | 1:6:A:LYS:CA | 1:6:A:LYS:C  | 1:7:A:PHE:N | 19       | 6.41          |
| (2,8) | 1:7:A:PHE:N | 1:7:A:PHE:CA | 1:7:A:PHE:C  | 1:8:A:PHE:N | 18       | 6.37          |
| (2,9) | 1:7:A:PHE:C | 1:8:A:PHE:N  | 1:8:A:PHE:CA | 1:8:A:PHE:C | 14       | 5.95          |
| (2,8) | 1:7:A:PHE:N | 1:7:A:PHE:CA | 1:7:A:PHE:C  | 1:8:A:PHE:N | 12       | 4.9           |
| (2,6) | 1:6:A:LYS:N | 1:6:A:LYS:CA | 1:6:A:LYS:C  | 1:7:A:PHE:N | 3        | 4.47          |
| (2,6) | 1:6:A:LYS:N | 1:6:A:LYS:CA | 1:6:A:LYS:C  | 1:7:A:PHE:N | 16       | 4.23          |
| (2,9) | 1:7:A:PHE:C | 1:8:A:PHE:N  | 1:8:A:PHE:CA | 1:8:A:PHE:C | 12       | 4.01          |
| (2,9) | 1:7:A:PHE:C | 1:8:A:PHE:N  | 1:8:A:PHE:CA | 1:8:A:PHE:C | 18       | 3.89          |
| (2,6) | 1:6:A:LYS:N | 1:6:A:LYS:CA | 1:6:A:LYS:C  | 1:7:A:PHE:N | 9        | 2.54          |
| (2,6) | 1:6:A:LYS:N | 1:6:A:LYS:CA | 1:6:A:LYS:C  | 1:7:A:PHE:N | 10       | 1.64          |

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| Key   | Atom-1      | Atom-2       | Atom-3      | Atom-4      | Model ID | Violation (°) |
|-------|-------------|--------------|-------------|-------------|----------|---------------|
| (2,6) | 1:6:A:LYS:N | 1:6:A:LYS:CA | 1:6:A:LYS:C | 1:7:A:PHE:N | 11       | 1.08          |