



# Full wwPDB NMR Structure Validation Report ⓘ

Mar 8, 2026 – 09:56 AM UTC

PDB ID : 9YM4 / pdb\_00009ym4  
BMRB ID : 31275  
Title : Backbone Modification in the Villin Headpiece Miniprotein: HP35 with beta3Phe at Position 6  
Authors : Lin, Y.; David, R.M.; Amin, D.M.; Osborne, S.W.J.; Horne, W.S.  
Deposited on : 2025-10-09

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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  
Mogul : 2022.3.0, CSD as543be (2022)  
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

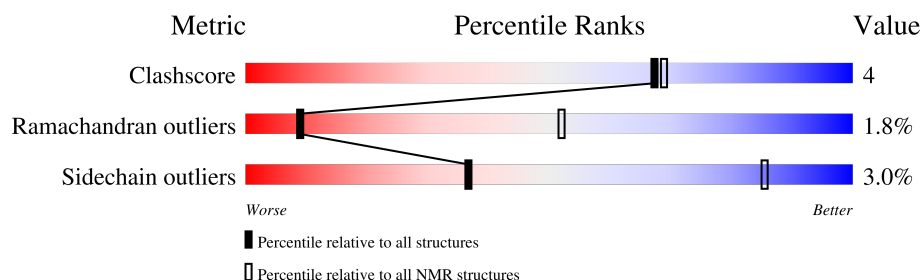
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 53%.

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     | 36     |                  |

## 2 Ensemble composition and analysis

This entry contains 10 models. Model 2 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:7-A:11, A:13-A:35 (28) | 0.86              | 2            |

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

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

The models can be grouped into 3 clusters and 2 single-model clusters were found.

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

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 586 atoms, of which 298 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Villin-1.

| Mol | Chain | Residues | Atoms |     |     |    |    | Trace |
|-----|-------|----------|-------|-----|-----|----|----|-------|
| 1   | A     | 36       | Total | C   | H   | N  | O  | 1     |
|     |       |          | 586   | 189 | 298 | 49 | 50 |       |

There are 3 discrepancies between the modelled and reference sequences:

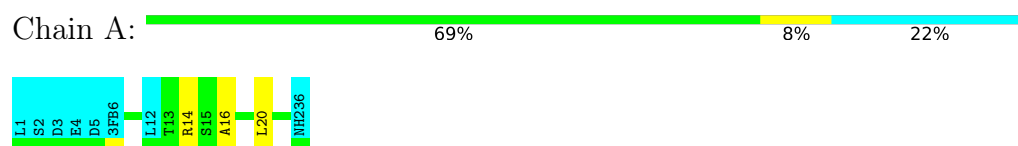
| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| A     | 6       | 3FB      | PHE    | engineered mutation | UNP P02640 |
| A     | 12      | NLE      | MET    | engineered mutation | UNP P02640 |
| A     | 36      | NH2      | -      | amidation           | UNP P02640 |

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

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

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

- Molecule 1: Villin-1

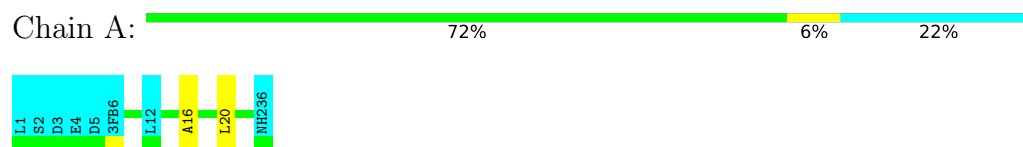


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section [4.1](#) above.

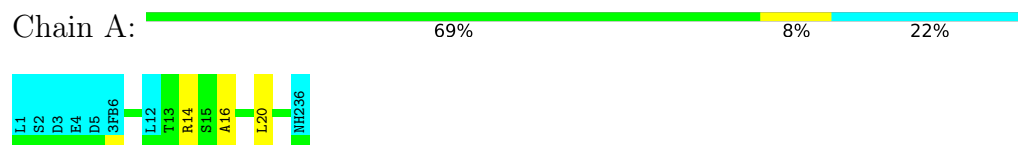
#### 4.2.1 Score per residue for model 1

- Molecule 1: Villin-1



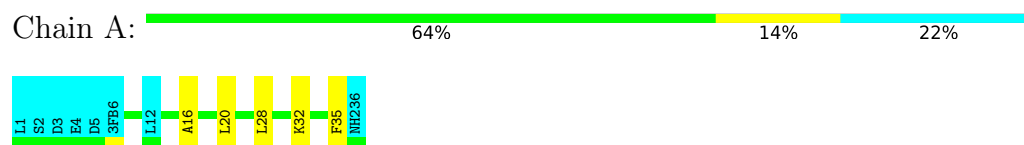
#### 4.2.2 Score per residue for model 2 (medoid)

- Molecule 1: Villin-1



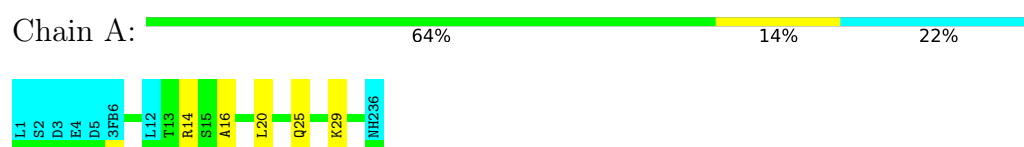
### 4.2.3 Score per residue for model 3

- Molecule 1: Villin-1



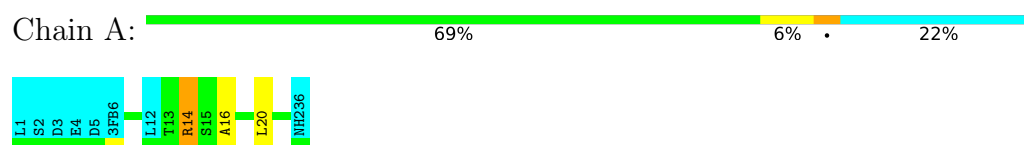
### 4.2.4 Score per residue for model 4

- Molecule 1: Villin-1



### 4.2.5 Score per residue for model 5

- Molecule 1: Villin-1



### 4.2.6 Score per residue for model 6

- Molecule 1: Villin-1



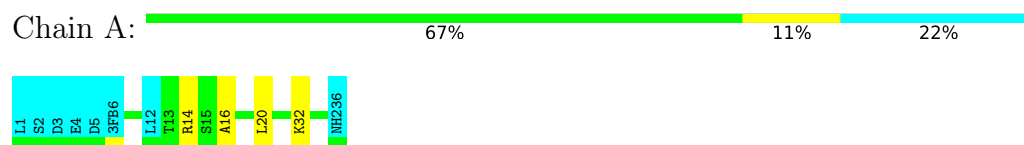
### 4.2.7 Score per residue for model 7

- Molecule 1: Villin-1



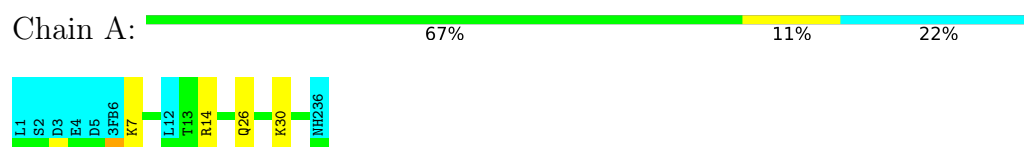
#### 4.2.8 Score per residue for model 8

- Molecule 1: Villin-1



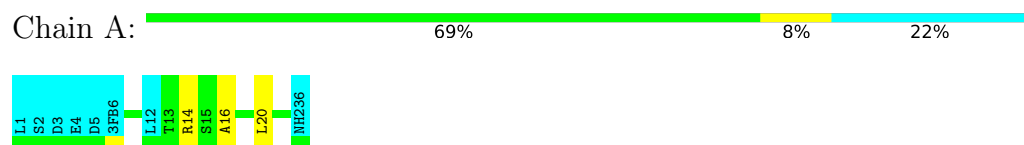
#### 4.2.9 Score per residue for model 9

- Molecule 1: Villin-1



#### 4.2.10 Score per residue for model 10

- Molecule 1: Villin-1



## 5 Refinement protocol and experimental data overview

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

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

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

| Software name | Classification        | Version |
|---------------|-----------------------|---------|
| ARIA          | structure calculation |         |

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

|                                              |                |
|----------------------------------------------|----------------|
| Chemical shift file(s)                       | working_cs.cif |
| Number of chemical shift lists               | 1              |
| Total number of shifts                       | 270            |
| Number of shifts mapped to atoms             | 270            |
| Number of unparsed shifts                    | 0              |
| Number of shifts with mapping errors         | 0              |
| Number of shifts with mapping warnings       | 0              |
| Assignment completeness (well-defined parts) | 53%            |



## 6 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: 3FB, NH2, NLE

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     | 228   | 242      | 242      | 2±1     |
| All | All   | 2280  | 2420     | 2420     | 18      |

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 4.

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

| Atom-1        | Atom-2         | Clash(Å) | Distance(Å) | Models |       |
|---------------|----------------|----------|-------------|--------|-------|
|               |                |          |             | Worst  | Total |
| 1:A:16:ALA:O  | 1:A:20:LEU:HG  | 0.56     | 1.99        | 7      | 9     |
| 1:A:28:LEU:O  | 1:A:32:LYS:HG2 | 0.52     | 2.05        | 7      | 1     |
| 1:A:14:ARG:NE | 1:A:14:ARG:HA  | 0.49     | 2.22        | 4      | 2     |
| 1:A:26:GLN:O  | 1:A:30:LYS:HG3 | 0.47     | 2.09        | 9      | 1     |
| 1:A:25:GLN:O  | 1:A:29:LYS:HG3 | 0.46     | 2.11        | 6      | 2     |
| 1:A:29:LYS:HA | 1:A:35:PHE:O   | 0.46     | 2.10        | 7      | 1     |
| 1:A:7:LYS:HD2 | 1:A:7:LYS:N    | 0.44     | 2.28        | 9      | 1     |
| 1:A:28:LEU:O  | 1:A:32:LYS:HG3 | 0.43     | 2.14        | 3      | 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     | 28/36 (78%)   | 24±1 (88±5%) | 3±1 (11±3%) | 0±1 (2±2%) | 9           | 52 |
| All | All   | 280/360 (78%) | 245 (88%)    | 30 (11%)    | 5 (2%)     | 9           | 52 |

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

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 35  | PHE  | 2              |
| 1   | A     | 14  | ARG  | 2              |
| 1   | A     | 32  | LYS  | 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     | 23/28 (82%)   | 22±1 (97±3%) | 1±1 (3±3%) | 37          | 85 |
| All | All   | 230/280 (82%) | 223 (97%)    | 7 (3%)     | 37          | 85 |

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     | 14  | ARG  | 4              |
| 1   | A     | 32  | LYS  | 2              |
| 1   | A     | 13  | THR  | 1              |

### 6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 6.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length is the number of standard deviations the observed value is removed from the expected value. A bond length with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

| Mol | Type | Chain | Res | Link | Bond lengths |           |            |
|-----|------|-------|-----|------|--------------|-----------|------------|
|     |      |       |     |      | Counts       | RMSZ      | #Z>2       |
| 1   | NLE  | A     | 12  | 1    | 6,7,8        | 0.46±0.02 | 0±0 (0±0%) |

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

| Mol | Type | Chain | Res | Link | Bond angles |           |            |
|-----|------|-------|-----|------|-------------|-----------|------------|
|     |      |       |     |      | Counts      | RMSZ      | #Z>2       |
| 1   | NLE  | A     | 12  | 1    | 2,7,9       | 0.47±0.02 | 0±0 (0±0%) |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res | Link | Chirals | Torsions  | Rings |
|-----|------|-------|-----|------|---------|-----------|-------|
| 1   | NLE  | A     | 12  | 1    | -       | 0±0,5,6,8 | -     |

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 6.7 Other polymers [i](#)

There are no such molecules in this entry.

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

There are no chain breaks in this entry.

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

The completeness of assignment taking into account all chemical shift lists is 53% for the well-defined parts and 52% for the entire structure.

### 7.1 Chemical shift list 1

File name: `working_cs.cif`

Chemical shift list name: *starch\_output*

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

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

|                                         |     |
|-----------------------------------------|-----|
| Total number of shifts                  | 270 |
| Number of shifts mapped to atoms        | 270 |
| 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 53%, i.e. 219 atoms were assigned a chemical shift out of a possible 410. 0 out of 5 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total         | <sup>1</sup> H | <sup>13</sup> C | <sup>15</sup> N |
|-----------|---------------|----------------|-----------------|-----------------|
| Backbone  | 55/140 (39%)  | 55/57 (96%)    | 0/56 (0%)       | 0/27 (0%)       |
| Sidechain | 146/228 (64%) | 146/147 (99%)  | 0/69 (0%)       | 0/12 (0%)       |
| Aromatic  | 18/42 (43%)   | 18/21 (86%)    | 0/20 (0%)       | 0/1 (0%)        |
| Overall   | 219/410 (53%) | 219/225 (97%)  | 0/145 (0%)      | 0/40 (0%)       |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 52%, i.e. 244 atoms were assigned a chemical shift out of a possible 466. 0 out of 6 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total         | <sup>1</sup> H | <sup>13</sup> C | <sup>15</sup> N |
|-----------|---------------|----------------|-----------------|-----------------|
| Backbone  | 64/165 (39%)  | 64/67 (96%)    | 0/66 (0%)       | 0/32 (0%)       |
| Sidechain | 162/259 (63%) | 162/166 (98%)  | 0/81 (0%)       | 0/12 (0%)       |
| Aromatic  | 18/42 (43%)   | 18/21 (86%)    | 0/20 (0%)       | 0/1 (0%)        |
| Overall   | 244/466 (52%) | 244/254 (96%)  | 0/167 (0%)      | 0/45 (0%)       |

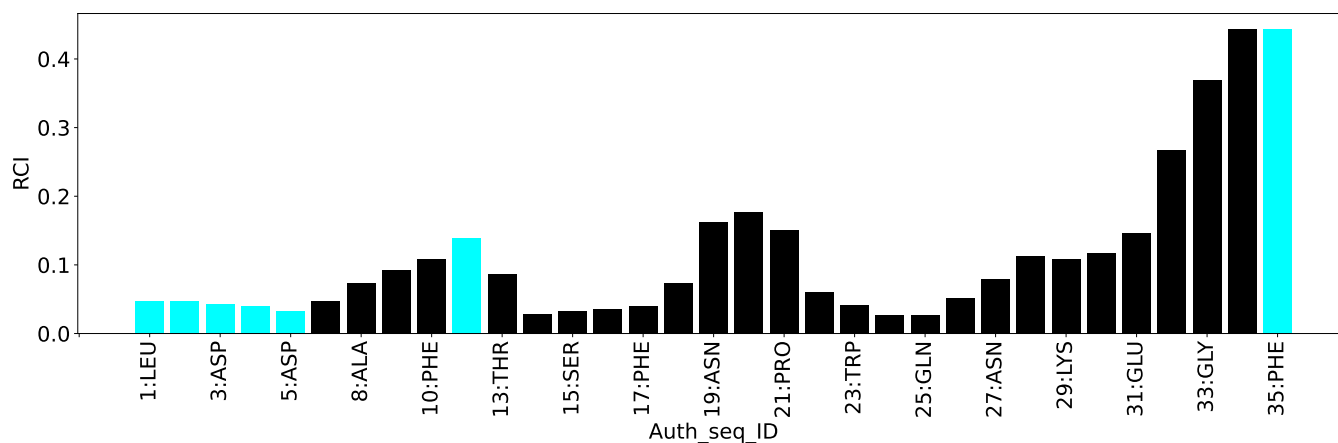
### 7.1.4 Statistically unusual chemical shifts [i](#)

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                                | 728   |
| Intra-residue ( $ i-j =0$ )                              | 353   |
| Sequential ( $ i-j =1$ )                                 | 153   |
| Medium range ( $ i-j >1$ and $ i-j <5$ )                 | 130   |
| Long range ( $ i-j \geq 5$ )                             | 62    |
| Inter-chain                                              | 0     |
| Hydrogen bond restraints                                 | 30    |
| Disulfide bond restraints                                | 0     |
| Total dihedral-angle restraints                          | 0     |
| Number of unmapped restraints                            | 0     |
| Number of restraints per residue                         | 20.2  |
| Number of long range restraints per residue <sup>1</sup> | 1.7   |

<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)  | 21.8                                   | 0.2     |
| 0.2-0.5 (Medium) | 41.3                                   | 0.5     |
| >0.5 (Large)     | 58.8                                   | 6.78    |

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

Dihedral-angle violations less than  $1^\circ$  are not included in the calculation. There are no dihedral-angle violations



## 9 Distance violation analysis ⓘ

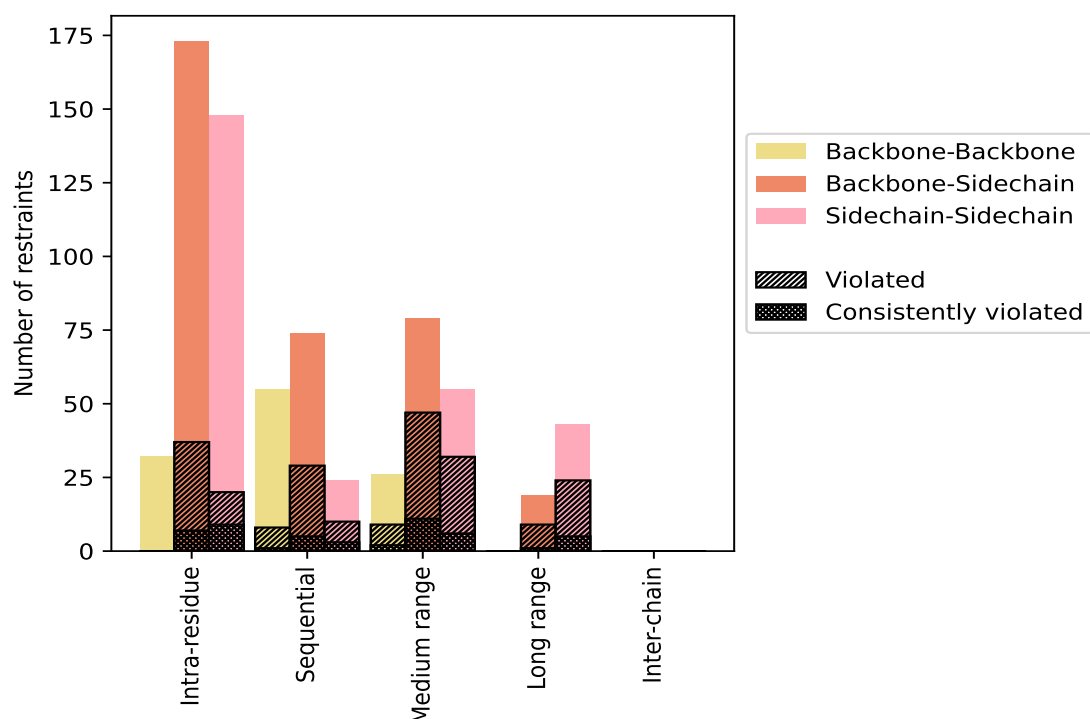
### 9.1 Summary of distance violations ⓘ

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>      |
| <a href="#">Intra-residue ( i-j =0)</a>                    | <a href="#">353</a> | <a href="#">48.5</a>  | <a href="#">57</a>    | <a href="#">16.1</a> | <a href="#">7.8</a>  | <a href="#">16</a>                 | <a href="#">4.5</a>  | <a href="#">2.2</a> |
| Backbone-Backbone                                          | 32                  | 4.4                   | 0                     | 0.0                  | 0.0                  | 0                                  | 0.0                  | 0.0                 |
| Backbone-Sidechain                                         | 173                 | 23.8                  | 37                    | 21.4                 | 5.1                  | 7                                  | 4.0                  | 1.0                 |
| Sidechain-Sidechain                                        | 148                 | 20.3                  | 20                    | 13.5                 | 2.7                  | 9                                  | 6.1                  | 1.2                 |
| <a href="#">Sequential ( i-j =1)</a>                       | <a href="#">153</a> | <a href="#">21.0</a>  | <a href="#">47</a>    | <a href="#">30.7</a> | <a href="#">6.5</a>  | <a href="#">9</a>                  | <a href="#">5.9</a>  | <a href="#">1.2</a> |
| Backbone-Backbone                                          | 55                  | 7.6                   | 8                     | 14.5                 | 1.1                  | 1                                  | 1.8                  | 0.1                 |
| Backbone-Sidechain                                         | 74                  | 10.2                  | 29                    | 39.2                 | 4.0                  | 5                                  | 6.8                  | 0.7                 |
| Sidechain-Sidechain                                        | 24                  | 3.3                   | 10                    | 41.7                 | 1.4                  | 3                                  | 12.5                 | 0.4                 |
| <a href="#">Medium range ( i-j &gt;1 &amp;  i-j &lt;5)</a> | <a href="#">130</a> | <a href="#">17.9</a>  | <a href="#">61</a>    | <a href="#">46.9</a> | <a href="#">8.4</a>  | <a href="#">14</a>                 | <a href="#">10.8</a> | <a href="#">1.9</a> |
| Backbone-Backbone                                          | 26                  | 3.6                   | 9                     | 34.6                 | 1.2                  | 2                                  | 7.7                  | 0.3                 |
| Backbone-Sidechain                                         | 49                  | 6.7                   | 20                    | 40.8                 | 2.7                  | 6                                  | 12.2                 | 0.8                 |
| Sidechain-Sidechain                                        | 55                  | 7.6                   | 32                    | 58.2                 | 4.4                  | 6                                  | 10.9                 | 0.8                 |
| <a href="#">Long range ( i-j ≥5)</a>                       | <a href="#">62</a>  | <a href="#">8.5</a>   | <a href="#">33</a>    | <a href="#">53.2</a> | <a href="#">4.5</a>  | <a href="#">6</a>                  | <a href="#">9.7</a>  | <a href="#">0.8</a> |
| Backbone-Backbone                                          | 0                   | 0.0                   | 0                     | 0.0                  | 0.0                  | 0                                  | 0.0                  | 0.0                 |
| Backbone-Sidechain                                         | 19                  | 2.6                   | 9                     | 47.4                 | 1.2                  | 1                                  | 5.3                  | 0.1                 |
| Sidechain-Sidechain                                        | 43                  | 5.9                   | 24                    | 55.8                 | 3.3                  | 5                                  | 11.6                 | 0.7                 |
| <a href="#">Inter-chain</a>                                | <a href="#">0</a>   | <a href="#">0.0</a>   | <a href="#">0</a>     | <a href="#">0.0</a>  | <a href="#">0.0</a>  | <a href="#">0</a>                  | <a href="#">0.0</a>  | <a href="#">0.0</a> |
| Backbone-Backbone                                          | 0                   | 0.0                   | 0                     | 0.0                  | 0.0                  | 0                                  | 0.0                  | 0.0                 |
| Backbone-Sidechain                                         | 0                   | 0.0                   | 0                     | 0.0                  | 0.0                  | 0                                  | 0.0                  | 0.0                 |
| Sidechain-Sidechain                                        | 0                   | 0.0                   | 0                     | 0.0                  | 0.0                  | 0                                  | 0.0                  | 0.0                 |
| <a href="#">Hydrogen bond</a>                              | <a href="#">30</a>  | <a href="#">4.1</a>   | <a href="#">27</a>    | <a href="#">90.0</a> | <a href="#">3.7</a>  | <a href="#">5</a>                  | <a href="#">16.7</a> | <a href="#">0.7</a> |
| <a href="#">Disulfide bond</a>                             | <a href="#">0</a>   | <a href="#">0.0</a>   | <a href="#">0</a>     | <a href="#">0.0</a>  | <a href="#">0.0</a>  | <a href="#">0</a>                  | <a href="#">0.0</a>  | <a href="#">0.0</a> |
| <a href="#">Total</a>                                      | <a href="#">728</a> | <a href="#">100.0</a> | <a href="#">225</a>   | <a href="#">30.9</a> | <a href="#">30.9</a> | <a href="#">50</a>                 | <a href="#">6.9</a>  | <a href="#">6.9</a> |
| Backbone-Backbone                                          | 113                 | 15.5                  | 17                    | 15.0                 | 2.3                  | 3                                  | 2.7                  | 0.4                 |
| Backbone-Sidechain                                         | 345                 | 47.4                  | 122                   | 35.4                 | 16.8                 | 24                                 | 7.0                  | 3.3                 |
| Sidechain-Sidechain                                        | 270                 | 37.1                  | 86                    | 31.9                 | 11.8                 | 23                                 | 8.5                  | 3.2                 |

<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

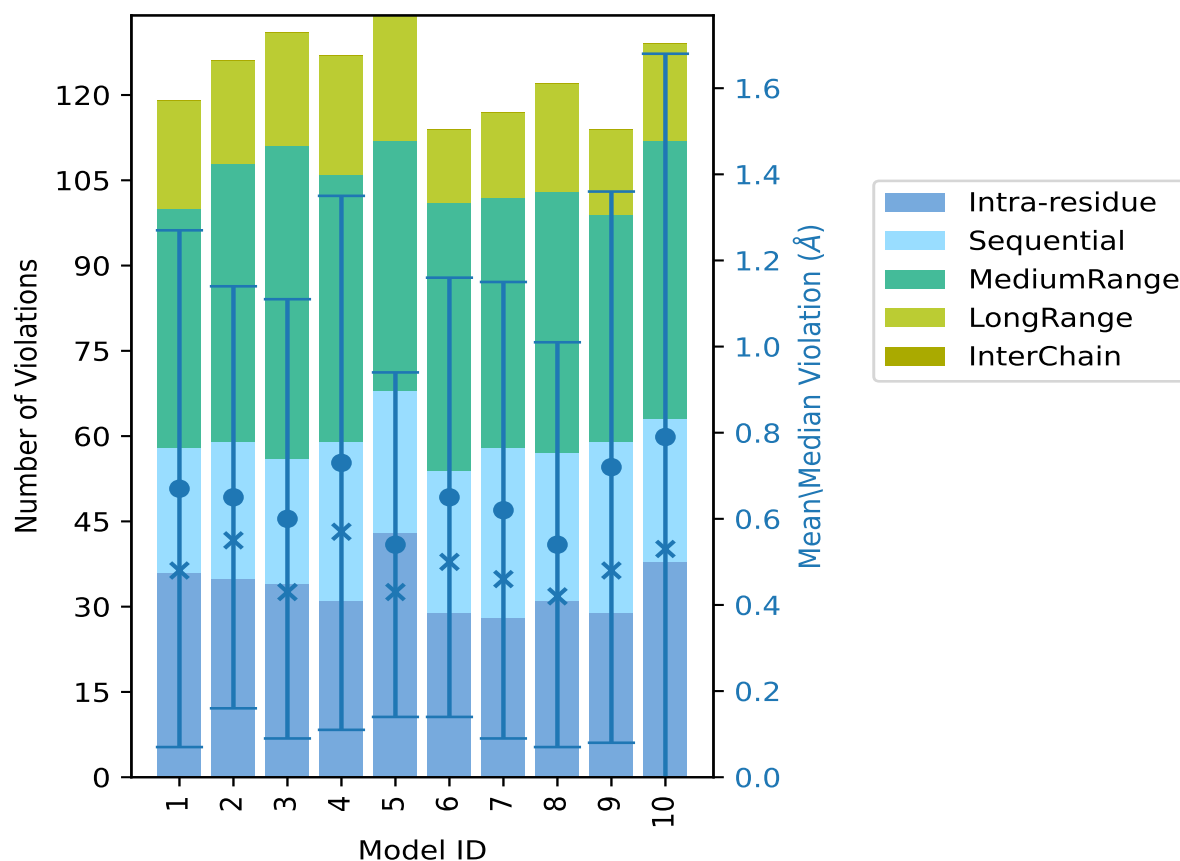
## 9.2 Distance violation statistics for each model [i](#)

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        | 36                   | 22              | 42              | 19              | 0               | 119   | 0.67     | 3.78    | 0.6                 | 0.48       |
| 2        | 35                   | 24              | 49              | 18              | 0               | 126   | 0.65     | 2.47    | 0.49                | 0.55       |
| 3        | 34                   | 22              | 55              | 20              | 0               | 131   | 0.6      | 3.34    | 0.51                | 0.43       |
| 4        | 31                   | 28              | 47              | 21              | 0               | 127   | 0.73     | 3.16    | 0.62                | 0.57       |
| 5        | 43                   | 25              | 44              | 22              | 0               | 134   | 0.54     | 2.31    | 0.4                 | 0.43       |
| 6        | 29                   | 25              | 47              | 13              | 0               | 114   | 0.65     | 2.87    | 0.51                | 0.5        |
| 7        | 28                   | 30              | 44              | 15              | 0               | 117   | 0.62     | 2.77    | 0.53                | 0.46       |
| 8        | 31                   | 26              | 46              | 19              | 0               | 122   | 0.54     | 3.24    | 0.47                | 0.42       |
| 9        | 29                   | 30              | 40              | 15              | 0               | 114   | 0.72     | 3.86    | 0.64                | 0.48       |
| 10       | 38                   | 25              | 49              | 17              | 0               | 129   | 0.79     | 6.78    | 0.89                | 0.53       |

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

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



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

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

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 500(IR:296, SQ:106, MR:69, LR:29, 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>       | %    |
| 9                             | 12              | 9               | 2               | 0               | 32    | 1                        | 10.0 |
| 3                             | 4               | 7               | 1               | 0               | 15    | 2                        | 20.0 |
| 7                             | 8               | 5               | 6               | 0               | 26    | 3                        | 30.0 |

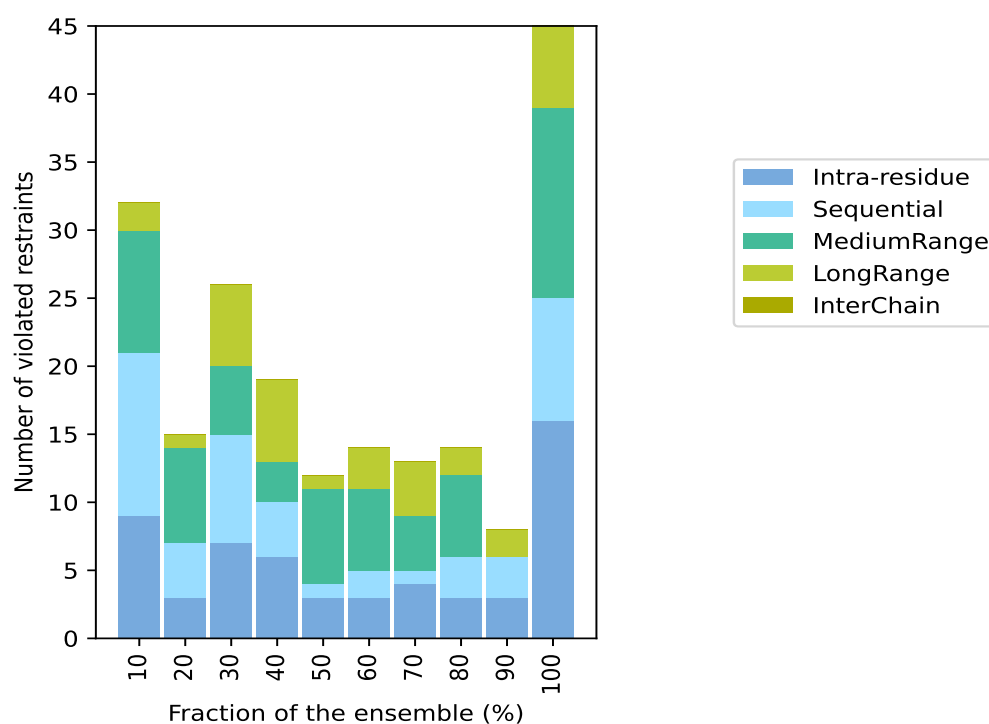
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| Number of violated restraints |                 |                 |                 |                 |       | Fraction of the ensemble |       |
|-------------------------------|-----------------|-----------------|-----------------|-----------------|-------|--------------------------|-------|
| IR <sup>1</sup>               | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total | Count <sup>6</sup>       | %     |
| 6                             | 4               | 3               | 6               | 0               | 19    | 4                        | 40.0  |
| 3                             | 1               | 7               | 1               | 0               | 12    | 5                        | 50.0  |
| 3                             | 2               | 6               | 3               | 0               | 14    | 6                        | 60.0  |
| 4                             | 1               | 4               | 4               | 0               | 13    | 7                        | 70.0  |
| 3                             | 3               | 6               | 2               | 0               | 14    | 8                        | 80.0  |
| 3                             | 3               | 0               | 2               | 0               | 8     | 9                        | 90.0  |
| 16                            | 9               | 14              | 6               | 0               | 45    | 10                       | 100.0 |

<sup>1</sup>Intra-residue restraints, <sup>2</sup>Sequential restraints, <sup>3</sup>Medium range restraints, <sup>4</sup>Long range restraints, <sup>5</sup>Inter-chain restraints, <sup>6</sup> Number of models with violations

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

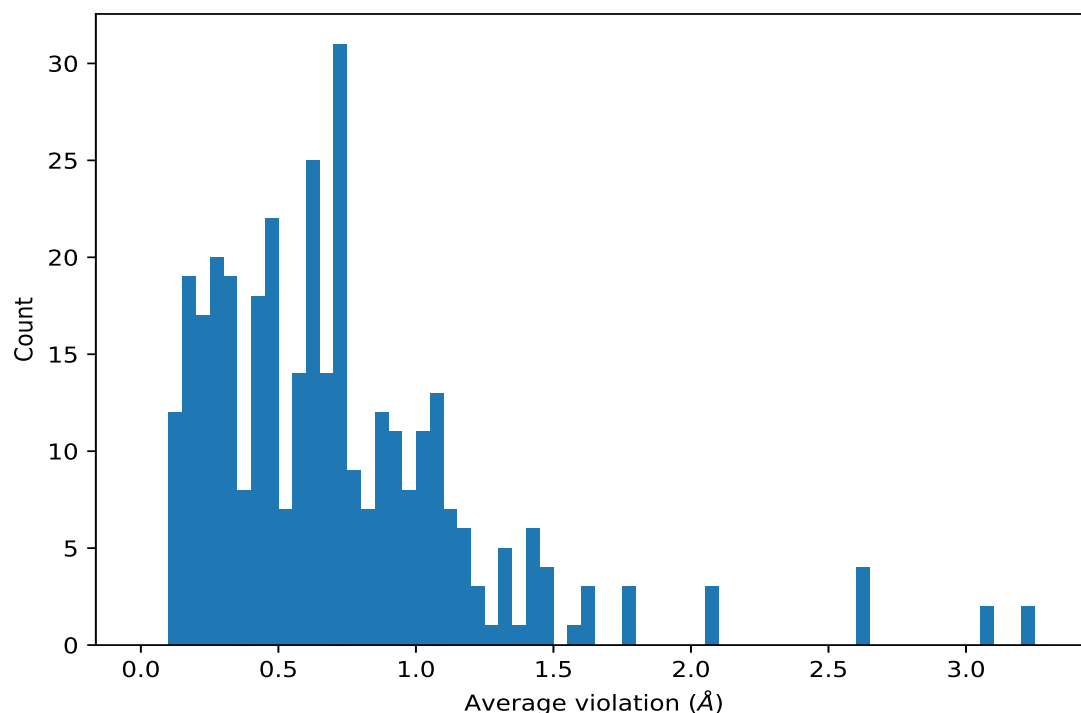


## 9.4 Most violated distance restraints in the ensemble ⓘ

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

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

in the ensemble



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

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

| Key     | Atom-1          | Atom-2         | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|-----------------|----------------|---------------------|----------|---------------------|------------|
| (1,528) | 1:18:A:ALA:HB1  | 1:17:A:PHE:HB2 | 10                  | 1.77     | 0.05                | 1.77       |
| (1,528) | 1:18:A:ALA:HB2  | 1:17:A:PHE:HB2 | 10                  | 1.77     | 0.05                | 1.77       |
| (1,528) | 1:18:A:ALA:HB3  | 1:17:A:PHE:HB2 | 10                  | 1.77     | 0.05                | 1.77       |
| (3,11)  | 1:17:A:PHE:H    | 1:13:A:THR:O   | 10                  | 1.56     | 0.97                | 0.94       |
| (2,6)   | 1:13:A:THR:HG21 | 1:17:A:PHE:H   | 10                  | 1.46     | 0.36                | 1.41       |
| (2,6)   | 1:13:A:THR:HG23 | 1:17:A:PHE:H   | 10                  | 1.46     | 0.36                | 1.41       |
| (2,6)   | 1:13:A:THR:HG22 | 1:17:A:PHE:H   | 10                  | 1.46     | 0.36                | 1.41       |
| (3,12)  | 1:17:A:PHE:N    | 1:13:A:THR:O   | 10                  | 1.28     | 0.87                | 0.74       |
| (2,1)   | 1:28:A:LEU:HD13 | 1:17:A:PHE:H   | 10                  | 1.17     | 0.37                | 1.06       |
| (2,1)   | 1:28:A:LEU:HD12 | 1:17:A:PHE:H   | 10                  | 1.17     | 0.37                | 1.06       |
| (2,1)   | 1:28:A:LEU:HD11 | 1:17:A:PHE:H   | 10                  | 1.17     | 0.37                | 1.06       |
| (3,15)  | 1:19:A:ASN:H    | 1:15:A:SER:O   | 10                  | 1.09     | 0.48                | 0.94       |
| (2,65)  | 1:12:A:NLE:HE1  | 1:23:A:TRP:HZ2 | 10                  | 1.07     | 0.5                 | 0.87       |
| (2,65)  | 1:22:A:LEU:HD11 | 1:23:A:TRP:HD1 | 10                  | 1.07     | 0.5                 | 0.87       |
| (2,65)  | 1:22:A:LEU:HD12 | 1:23:A:TRP:HD1 | 10                  | 1.07     | 0.5                 | 0.87       |

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| Key     | Atom-1          | Atom-2         | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|-----------------|----------------|---------------------|----------|---------------------|------------|
| (2,65)  | 1:28:A:LEU:HD12 | 1:19:A:ASN:H   | 10                  | 1.07     | 0.5                 | 0.87       |
| (2,65)  | 1:22:A:LEU:HD13 | 1:23:A:TRP:HD1 | 10                  | 1.07     | 0.5                 | 0.87       |
| (2,7)   | 1:8:A:ALA:HB3   | 1:10:A:PHE:H   | 10                  | 1.07     | 0.13                | 1.1        |
| (2,7)   | 1:8:A:ALA:HB1   | 1:10:A:PHE:H   | 10                  | 1.07     | 0.13                | 1.1        |
| (2,7)   | 1:8:A:ALA:HB2   | 1:10:A:PHE:H   | 10                  | 1.07     | 0.13                | 1.1        |
| (1,533) | 1:22:A:LEU:HD22 | 1:26:A:GLN:HG2 | 10                  | 1.04     | 0.33                | 1.21       |
| (1,533) | 1:22:A:LEU:HD21 | 1:26:A:GLN:HG2 | 10                  | 1.04     | 0.33                | 1.21       |
| (1,533) | 1:22:A:LEU:HD23 | 1:26:A:GLN:HG2 | 10                  | 1.04     | 0.33                | 1.21       |
| (2,23)  | 1:27:A:ASN:HB2  | 1:23:A:TRP:HZ3 | 10                  | 0.99     | 0.23                | 0.94       |
| (2,23)  | 1:27:A:ASN:HB3  | 1:23:A:TRP:HZ3 | 10                  | 0.99     | 0.23                | 0.94       |
| (2,23)  | 1:17:A:PHE:HB3  | 1:17:A:PHE:HE2 | 10                  | 0.99     | 0.23                | 0.94       |
| (3,13)  | 1:18:A:ALA:H    | 1:14:A:ARG:O   | 10                  | 0.98     | 0.63                | 0.84       |
| (1,71)  | 1:4:A:GLU:HG3   | 1:4:A:GLU:H    | 10                  | 0.93     | 0.04                | 0.94       |
| (1,71)  | 1:4:A:GLU:HG2   | 1:4:A:GLU:H    | 10                  | 0.93     | 0.04                | 0.94       |
| (2,84)  | 1:20:A:LEU:HD11 | 1:24:A:LYS:HB2 | 10                  | 0.9      | 0.24                | 0.98       |
| (2,84)  | 1:20:A:LEU:HD13 | 1:16:A:ALA:HB3 | 10                  | 0.9      | 0.24                | 0.98       |
| (2,84)  | 1:20:A:LEU:HD12 | 1:16:A:ALA:HB2 | 10                  | 0.9      | 0.24                | 0.98       |
| (2,84)  | 1:20:A:LEU:HD12 | 1:16:A:ALA:HB3 | 10                  | 0.9      | 0.24                | 0.98       |
| (2,84)  | 1:20:A:LEU:HD12 | 1:24:A:LYS:HB2 | 10                  | 0.9      | 0.24                | 0.98       |
| (2,84)  | 1:20:A:LEU:HD13 | 1:16:A:ALA:HB1 | 10                  | 0.9      | 0.24                | 0.98       |
| (2,25)  | 1:21:A:PRO:HD3  | 1:23:A:TRP:HH2 | 10                  | 0.88     | 0.35                | 0.96       |
| (2,25)  | 1:23:A:TRP:HB3  | 1:23:A:TRP:HH2 | 10                  | 0.88     | 0.35                | 0.96       |
| (1,108) | 1:24:A:LYS:HE3  | 1:23:A:TRP:HH2 | 10                  | 0.85     | 0.25                | 0.92       |
| (1,262) | 1:25:A:GLN:HG2  | 1:17:A:PHE:HE1 | 10                  | 0.82     | 0.23                | 0.84       |
| (1,262) | 1:25:A:GLN:HG2  | 1:17:A:PHE:HE2 | 10                  | 0.82     | 0.23                | 0.84       |
| (2,12)  | 1:28:A:LEU:HG   | 1:29:A:LYS:H   | 10                  | 0.82     | 0.21                | 0.82       |
| (2,12)  | 1:29:A:LYS:HD2  | 1:29:A:LYS:H   | 10                  | 0.82     | 0.21                | 0.82       |
| (2,12)  | 1:29:A:LYS:HD3  | 1:29:A:LYS:H   | 10                  | 0.82     | 0.21                | 0.82       |
| (2,13)  | 1:25:A:GLN:HG3  | 1:26:A:GLN:H   | 10                  | 0.82     | 0.04                | 0.83       |
| (1,467) | 1:22:A:LEU:HB2  | 1:21:A:PRO:HA  | 10                  | 0.77     | 0.14                | 0.85       |
| (2,8)   | 1:16:A:ALA:HB1  | 1:13:A:THR:H   | 10                  | 0.77     | 0.43                | 0.45       |
| (2,8)   | 1:29:A:LYS:HG3  | 1:30:A:LYS:H   | 10                  | 0.77     | 0.43                | 0.45       |
| (2,8)   | 1:16:A:ALA:HB3  | 1:13:A:THR:H   | 10                  | 0.77     | 0.43                | 0.45       |
| (2,8)   | 1:29:A:LYS:HG2  | 1:30:A:LYS:H   | 10                  | 0.77     | 0.43                | 0.45       |
| (2,8)   | 1:16:A:ALA:HB2  | 1:13:A:THR:H   | 10                  | 0.77     | 0.43                | 0.45       |
| (1,323) | 1:28:A:LEU:HD13 | 1:28:A:LEU:HA  | 10                  | 0.74     | 0.04                | 0.74       |
| (1,323) | 1:28:A:LEU:HD11 | 1:28:A:LEU:HA  | 10                  | 0.74     | 0.04                | 0.74       |
| (1,323) | 1:28:A:LEU:HD12 | 1:28:A:LEU:HA  | 10                  | 0.74     | 0.04                | 0.74       |
| (2,100) | 1:8:A:ALA:HB3   | 1:9:A:VAL:HA   | 10                  | 0.74     | 0.06                | 0.74       |
| (2,100) | 1:8:A:ALA:HB1   | 1:9:A:VAL:HA   | 10                  | 0.74     | 0.06                | 0.74       |
| (2,100) | 1:8:A:ALA:HB2   | 1:9:A:VAL:HA   | 10                  | 0.74     | 0.06                | 0.74       |
| (1,294) | 1:28:A:LEU:HD21 | 1:17:A:PHE:HD1 | 10                  | 0.71     | 0.29                | 0.69       |

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| Key     | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,294) | 1:28:A:LEU:HD22 | 1:17:A:PHE:HD1  | 10                  | 0.71     | 0.29                | 0.69       |
| (1,294) | 1:28:A:LEU:HD23 | 1:17:A:PHE:HD1  | 10                  | 0.71     | 0.29                | 0.69       |
| (1,360) | 1:28:A:LEU:HD22 | 1:20:A:LEU:HD11 | 10                  | 0.7      | 0.23                | 0.64       |
| (1,360) | 1:28:A:LEU:HD23 | 1:20:A:LEU:HD11 | 10                  | 0.7      | 0.23                | 0.64       |
| (1,360) | 1:28:A:LEU:HD21 | 1:20:A:LEU:HD13 | 10                  | 0.7      | 0.23                | 0.64       |
| (1,360) | 1:28:A:LEU:HD21 | 1:20:A:LEU:HD11 | 10                  | 0.7      | 0.23                | 0.64       |
| (1,360) | 1:28:A:LEU:HD22 | 1:20:A:LEU:HD13 | 10                  | 0.7      | 0.23                | 0.64       |
| (1,360) | 1:28:A:LEU:HD22 | 1:20:A:LEU:HD12 | 10                  | 0.7      | 0.23                | 0.64       |
| (1,360) | 1:28:A:LEU:HD23 | 1:20:A:LEU:HD12 | 10                  | 0.7      | 0.23                | 0.64       |
| (3,16)  | 1:19:A:ASN:N    | 1:15:A:SER:O    | 10                  | 0.67     | 0.46                | 0.51       |
| (1,530) | 1:24:A:LYS:HB2  | 1:21:A:PRO:HD3  | 10                  | 0.66     | 0.18                | 0.6        |
| (1,130) | 1:17:A:PHE:HB2  | 1:17:A:PHE:HE1  | 10                  | 0.63     | 0.02                | 0.64       |
| (2,33)  | 1:9:A:VAL:H     | 1:7:A:LYS:HA    | 10                  | 0.62     | 0.2                 | 0.66       |
| (2,60)  | 1:18:A:ALA:HB3  | 1:20:A:LEU:H    | 10                  | 0.6      | 0.11                | 0.62       |
| (2,60)  | 1:18:A:ALA:HB1  | 1:20:A:LEU:H    | 10                  | 0.6      | 0.11                | 0.62       |
| (2,60)  | 1:16:A:ALA:HB1  | 1:20:A:LEU:H    | 10                  | 0.6      | 0.11                | 0.62       |
| (2,60)  | 1:16:A:ALA:HB2  | 1:20:A:LEU:H    | 10                  | 0.6      | 0.11                | 0.62       |
| (2,60)  | 1:18:A:ALA:HB2  | 1:20:A:LEU:H    | 10                  | 0.6      | 0.11                | 0.62       |
| (1,257) | 1:21:A:PRO:HG3  | 1:23:A:TRP:HZ2  | 10                  | 0.59     | 0.32                | 0.6        |
| (1,426) | 1:22:A:LEU:HG   | 1:22:A:LEU:HB3  | 10                  | 0.59     | 0.02                | 0.58       |
| (1,426) | 1:22:A:LEU:HG   | 1:22:A:LEU:HB2  | 10                  | 0.59     | 0.02                | 0.58       |
| (1,332) | 1:20:A:LEU:HD11 | 1:21:A:PRO:HD3  | 10                  | 0.56     | 0.1                 | 0.52       |
| (1,332) | 1:20:A:LEU:HD13 | 1:21:A:PRO:HD3  | 10                  | 0.56     | 0.1                 | 0.52       |
| (1,332) | 1:20:A:LEU:HD12 | 1:21:A:PRO:HD3  | 10                  | 0.56     | 0.1                 | 0.52       |
| (1,327) | 1:20:A:LEU:HD11 | 1:24:A:LYS:HA   | 10                  | 0.47     | 0.19                | 0.44       |
| (1,327) | 1:20:A:LEU:HD13 | 1:24:A:LYS:HA   | 10                  | 0.47     | 0.19                | 0.44       |
| (1,327) | 1:20:A:LEU:HD12 | 1:24:A:LYS:HA   | 10                  | 0.47     | 0.19                | 0.44       |
| (1,89)  | 1:10:A:PHE:HB3  | 1:10:A:PHE:H    | 10                  | 0.47     | 0.03                | 0.47       |
| (1,165) | 1:13:A:THR:H    | 1:11:A:GLY:HA3  | 10                  | 0.42     | 0.1                 | 0.44       |
| (2,16)  | 1:20:A:LEU:HB2  | 1:18:A:ALA:H    | 10                  | 0.41     | 0.06                | 0.4        |
| (1,254) | 1:20:A:LEU:HB2  | 1:25:A:GLN:HE22 | 10                  | 0.4      | 0.14                | 0.44       |
| (1,82)  | 1:6:A:3FB:HB1   | 1:7:A:LYS:H     | 10                  | 0.4      | 0.05                | 0.4        |
| (1,552) | 1:35:A:PHE:HD1  | 1:35:A:PHE:HE1  | 10                  | 0.39     | 0.0                 | 0.39       |
| (1,552) | 1:35:A:PHE:HD2  | 1:35:A:PHE:HE2  | 10                  | 0.39     | 0.0                 | 0.39       |
| (1,92)  | 1:17:A:PHE:HB2  | 1:18:A:ALA:H    | 10                  | 0.36     | 0.04                | 0.36       |
| (1,550) | 1:23:A:TRP:HZ3  | 1:23:A:TRP:HZ2  | 10                  | 0.34     | 0.0                 | 0.34       |
| (1,377) | 1:12:A:NLE:HD2  | 1:12:A:NLE:HG3  | 10                  | 0.3      | 0.03                | 0.28       |
| (1,377) | 1:12:A:NLE:HD2  | 1:12:A:NLE:HG2  | 10                  | 0.3      | 0.03                | 0.28       |
| (1,541) | 1:17:A:PHE:HD2  | 1:17:A:PHE:HE2  | 10                  | 0.25     | 0.0                 | 0.25       |
| (1,541) | 1:17:A:PHE:HD1  | 1:17:A:PHE:HE1  | 10                  | 0.25     | 0.0                 | 0.25       |
| (1,569) | 1:17:A:PHE:HD2  | 1:17:A:PHE:H    | 10                  | 0.22     | 0.02                | 0.23       |
| (1,569) | 1:17:A:PHE:HD1  | 1:17:A:PHE:H    | 10                  | 0.22     | 0.02                | 0.23       |

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| Key     | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,38)  | 1:28:A:LEU:HB3  | 1:28:A:LEU:H    | 10                  | 0.22     | 0.01                | 0.22       |
| (1,170) | 1:9:A:VAL:HA    | 1:10:A:PHE:H    | 10                  | 0.2      | 0.01                | 0.2        |
| (1,457) | 1:21:A:PRO:HG2  | 1:21:A:PRO:HA   | 10                  | 0.19     | 0.02                | 0.2        |
| (1,125) | 1:14:A:ARG:HD3  | 1:14:A:ARG:HH22 | 10                  | 0.13     | 0.01                | 0.13       |
| (1,125) | 1:14:A:ARG:HD2  | 1:14:A:ARG:HH22 | 10                  | 0.13     | 0.01                | 0.13       |
| (1,252) | 1:25:A:GLN:HG2  | 1:25:A:GLN:HE22 | 10                  | 0.12     | 0.0                 | 0.12       |
| (1,252) | 1:25:A:GLN:HG3  | 1:25:A:GLN:HE22 | 10                  | 0.12     | 0.0                 | 0.12       |
| (1,542) | 1:23:A:TRP:HZ3  | 1:23:A:TRP:HH2  | 10                  | 0.12     | 0.0                 | 0.12       |
| (1,151) | 1:29:A:LYS:HA   | 1:14:A:ARG:HH21 | 9                   | 3.23     | 1.49                | 3.24       |
| (1,151) | 1:29:A:LYS:HA   | 1:14:A:ARG:HH22 | 9                   | 3.23     | 1.49                | 3.24       |
| (3,9)   | 1:16:A:ALA:H    | 1:12:A:NLE:O    | 9                   | 2.06     | 0.5                 | 2.31       |
| (3,10)  | 1:16:A:ALA:N    | 1:12:A:NLE:O    | 9                   | 1.13     | 0.4                 | 1.34       |
| (1,290) | 1:9:A:VAL:HG21  | 1:10:A:PHE:HD2  | 9                   | 0.67     | 0.32                | 0.63       |
| (1,290) | 1:9:A:VAL:HG23  | 1:10:A:PHE:HD2  | 9                   | 0.67     | 0.32                | 0.63       |
| (1,290) | 1:9:A:VAL:HG22  | 1:10:A:PHE:HD2  | 9                   | 0.67     | 0.32                | 0.63       |
| (1,109) | 1:19:A:ASN:HB3  | 1:19:A:ASN:HD22 | 9                   | 0.52     | 0.01                | 0.52       |
| (1,265) | 1:28:A:LEU:HG   | 1:17:A:PHE:HD1  | 9                   | 0.49     | 0.21                | 0.48       |
| (3,25)  | 1:30:A:LYS:H    | 1:26:A:GLN:O    | 9                   | 0.43     | 0.23                | 0.28       |
| (1,75)  | 1:6:A:3FB:HC1   | 1:7:A:LYS:H     | 9                   | 0.32     | 0.05                | 0.33       |
| (1,101) | 1:6:A:3FB:HB1   | 1:6:A:3FB:H     | 9                   | 0.17     | 0.04                | 0.16       |
| (1,171) | 1:29:A:LYS:HA   | 1:30:A:LYS:H    | 9                   | 0.16     | 0.03                | 0.18       |
| (1,2)   | 1:9:A:VAL:HG13  | 1:9:A:VAL:H     | 9                   | 0.14     | 0.02                | 0.15       |
| (1,2)   | 1:9:A:VAL:HG12  | 1:9:A:VAL:H     | 9                   | 0.14     | 0.02                | 0.15       |
| (1,2)   | 1:9:A:VAL:HG11  | 1:9:A:VAL:H     | 9                   | 0.14     | 0.02                | 0.15       |
| (2,75)  | 1:28:A:LEU:HD21 | 1:6:A:3FB:HE1   | 8                   | 1.31     | 0.62                | 1.31       |
| (2,75)  | 1:28:A:LEU:HD22 | 1:6:A:3FB:HE2   | 8                   | 1.31     | 0.62                | 1.31       |
| (2,75)  | 1:28:A:LEU:HD23 | 1:14:A:ARG:HH21 | 8                   | 1.31     | 0.62                | 1.31       |
| (2,75)  | 1:28:A:LEU:HD21 | 1:6:A:3FB:HE2   | 8                   | 1.31     | 0.62                | 1.31       |
| (2,75)  | 1:28:A:LEU:HD22 | 1:6:A:3FB:HE1   | 8                   | 1.31     | 0.62                | 1.31       |
| (2,85)  | 1:24:A:LYS:HG2  | 1:12:A:NLE:HD2  | 8                   | 0.94     | 0.34                | 1.05       |
| (2,85)  | 1:24:A:LYS:HG3  | 1:13:A:THR:HG22 | 8                   | 0.94     | 0.34                | 1.05       |
| (3,14)  | 1:18:A:ALA:N    | 1:14:A:ARG:O    | 8                   | 0.93     | 0.54                | 1.03       |
| (1,329) | 1:12:A:NLE:HE1  | 1:10:A:PHE:HB2  | 8                   | 0.62     | 0.2                 | 0.58       |
| (1,329) | 1:12:A:NLE:HE2  | 1:10:A:PHE:HB2  | 8                   | 0.62     | 0.2                 | 0.58       |
| (1,329) | 1:12:A:NLE:HE3  | 1:10:A:PHE:HB2  | 8                   | 0.62     | 0.2                 | 0.58       |
| (1,264) | 1:20:A:LEU:HG   | 1:17:A:PHE:HD1  | 8                   | 0.6      | 0.17                | 0.56       |
| (3,7)   | 1:10:A:PHE:H    | 1:6:A:3FB:O     | 8                   | 0.57     | 0.41                | 0.46       |
| (2,78)  | 1:9:A:VAL:HG23  | 1:8:A:ALA:HA    | 8                   | 0.48     | 0.08                | 0.48       |
| (2,78)  | 1:9:A:VAL:HG21  | 1:8:A:ALA:HA    | 8                   | 0.48     | 0.08                | 0.48       |
| (2,78)  | 1:9:A:VAL:HG22  | 1:8:A:ALA:HA    | 8                   | 0.48     | 0.08                | 0.48       |
| (2,78)  | 1:34:A:LEU:HD11 | 1:1:A:LEU:HA    | 8                   | 0.48     | 0.08                | 0.48       |
| (1,17)  | 1:14:A:ARG:HB3  | 1:14:A:ARG:H    | 8                   | 0.47     | 0.16                | 0.56       |

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| Key     | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,286) | 1:20:A:LEU:HD12 | 1:17:A:PHE:HE1  | 8                   | 0.46     | 0.22                | 0.39       |
| (1,286) | 1:20:A:LEU:HD11 | 1:17:A:PHE:HE1  | 8                   | 0.46     | 0.22                | 0.39       |
| (1,107) | 1:24:A:LYS:HE2  | 1:23:A:TRP:HH2  | 8                   | 0.43     | 0.1                 | 0.41       |
| (1,535) | 1:22:A:LEU:HD22 | 1:26:A:GLN:HG3  | 8                   | 0.41     | 0.2                 | 0.36       |
| (1,535) | 1:22:A:LEU:HD21 | 1:26:A:GLN:HG3  | 8                   | 0.41     | 0.2                 | 0.36       |
| (1,535) | 1:22:A:LEU:HD23 | 1:26:A:GLN:HG3  | 8                   | 0.41     | 0.2                 | 0.36       |
| (1,376) | 1:12:A:NLE:HD2  | 1:12:A:NLE:HB3  | 8                   | 0.38     | 0.05                | 0.36       |
| (1,415) | 1:19:A:ASN:HB3  | 1:16:A:ALA:HA   | 8                   | 0.31     | 0.12                | 0.3        |
| (2,46)  | 1:21:A:PRO:HA   | 1:23:A:TRP:HD1  | 8                   | 0.25     | 0.06                | 0.25       |
| (1,238) | 1:23:A:TRP:HA   | 1:23:A:TRP:HE3  | 8                   | 0.14     | 0.03                | 0.13       |
| (1,154) | 1:8:A:ALA:HA    | 1:9:A:VAL:H     | 8                   | 0.11     | 0.01                | 0.11       |
| (1,373) | 1:1:A:LEU:HG    | 1:5:A:ASP:HB3   | 7                   | 1.35     | 0.6                 | 1.32       |
| (2,17)  | 1:7:A:LYS:HE2   | 1:14:A:ARG:H    | 7                   | 1.23     | 1.09                | 0.93       |
| (2,17)  | 1:7:A:LYS:HE3   | 1:14:A:ARG:H    | 7                   | 1.23     | 1.09                | 0.93       |
| (1,554) | 1:23:A:TRP:HE3  | 1:27:A:ASN:HD22 | 7                   | 1.17     | 0.47                | 1.31       |
| (2,55)  | 1:32:A:LYS:HD3  | 1:10:A:PHE:HD2  | 7                   | 1.12     | 0.78                | 1.03       |
| (2,55)  | 1:32:A:LYS:HD3  | 1:14:A:ARG:HH21 | 7                   | 1.12     | 0.78                | 1.03       |
| (2,55)  | 1:32:A:LYS:HD2  | 1:10:A:PHE:HD2  | 7                   | 1.12     | 0.78                | 1.03       |
| (2,63)  | 1:13:A:THR:HG22 | 1:10:A:PHE:HE2  | 7                   | 1.04     | 0.46                | 0.86       |
| (2,63)  | 1:13:A:THR:HG21 | 1:10:A:PHE:HE2  | 7                   | 1.04     | 0.46                | 0.86       |
| (2,63)  | 1:13:A:THR:HG22 | 1:6:A:3FB:HD1   | 7                   | 1.04     | 0.46                | 0.86       |
| (2,63)  | 1:13:A:THR:HG23 | 1:6:A:3FB:HD2   | 7                   | 1.04     | 0.46                | 0.86       |
| (2,63)  | 1:13:A:THR:HG21 | 1:6:A:3FB:HD2   | 7                   | 1.04     | 0.46                | 0.86       |
| (2,63)  | 1:13:A:THR:HG21 | 1:6:A:3FB:HD1   | 7                   | 1.04     | 0.46                | 0.86       |
| (1,319) | 1:22:A:LEU:HD13 | 1:22:A:LEU:HA   | 7                   | 0.75     | 0.03                | 0.76       |
| (1,319) | 1:22:A:LEU:HD11 | 1:22:A:LEU:HA   | 7                   | 0.75     | 0.03                | 0.76       |
| (1,319) | 1:22:A:LEU:HD12 | 1:22:A:LEU:HA   | 7                   | 0.75     | 0.03                | 0.76       |
| (2,10)  | 1:32:A:LYS:HD2  | 1:33:A:GLY:H    | 7                   | 0.72     | 0.22                | 0.61       |
| (2,10)  | 1:32:A:LYS:HD3  | 1:33:A:GLY:H    | 7                   | 0.72     | 0.22                | 0.61       |
| (2,10)  | 1:28:A:LEU:HB3  | 1:30:A:LYS:H    | 7                   | 0.72     | 0.22                | 0.61       |
| (3,1)   | 1:7:A:LYS:H     | 1:3:A:ASP:O     | 7                   | 0.67     | 0.47                | 0.48       |
| (1,9)   | 1:34:A:LEU:HD12 | 1:34:A:LEU:H    | 7                   | 0.47     | 0.3                 | 0.29       |
| (1,9)   | 1:34:A:LEU:HD11 | 1:34:A:LEU:H    | 7                   | 0.47     | 0.3                 | 0.29       |
| (1,9)   | 1:34:A:LEU:HD13 | 1:34:A:LEU:H    | 7                   | 0.47     | 0.3                 | 0.29       |
| (1,493) | 1:7:A:LYS:HD3   | 1:7:A:LYS:HA    | 7                   | 0.43     | 0.13                | 0.39       |
| (1,493) | 1:7:A:LYS:HD2   | 1:7:A:LYS:HA    | 7                   | 0.43     | 0.13                | 0.39       |
| (1,156) | 1:24:A:LYS:HA   | 1:27:A:ASN:HD22 | 7                   | 0.35     | 0.18                | 0.28       |
| (1,351) | 1:20:A:LEU:HD13 | 1:12:A:NLE:HD2  | 7                   | 0.31     | 0.15                | 0.39       |
| (1,351) | 1:20:A:LEU:HD12 | 1:12:A:NLE:HD2  | 7                   | 0.31     | 0.15                | 0.39       |
| (1,351) | 1:20:A:LEU:HD11 | 1:12:A:NLE:HD2  | 7                   | 0.31     | 0.15                | 0.39       |
| (1,61)  | 1:31:A:GLU:HB2  | 1:30:A:LYS:H    | 7                   | 0.29     | 0.09                | 0.29       |
| (1,349) | 1:34:A:LEU:HD11 | 1:34:A:LEU:HB3  | 7                   | 0.16     | 0.05                | 0.14       |

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| Key     | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,349) | 1:34:A:LEU:HD13 | 1:34:A:LEU:HB2  | 7                   | 0.16     | 0.05                | 0.14       |
| (1,349) | 1:34:A:LEU:HD12 | 1:34:A:LEU:HB2  | 7                   | 0.16     | 0.05                | 0.14       |
| (1,349) | 1:34:A:LEU:HD12 | 1:34:A:LEU:HB3  | 7                   | 0.16     | 0.05                | 0.14       |
| (1,134) | 1:17:A:PHE:HB2  | 1:14:A:ARG:HH22 | 6                   | 1.45     | 1.22                | 1.14       |
| (1,475) | 1:30:A:LYS:HA   | 1:30:A:LYS:HD2  | 6                   | 1.16     | 0.07                | 1.15       |
| (1,475) | 1:30:A:LYS:HA   | 1:30:A:LYS:HD3  | 6                   | 1.16     | 0.07                | 1.15       |
| (1,427) | 1:1:A:LEU:HG    | 1:5:A:ASP:HB2   | 6                   | 1.1      | 0.42                | 0.94       |
| (1,54)  | 1:30:A:LYS:HB3  | 1:30:A:LYS:H    | 6                   | 1.01     | 0.01                | 1.02       |
| (1,574) | 1:23:A:TRP:HZ3  | 1:27:A:ASN:HD22 | 6                   | 0.96     | 0.45                | 1.12       |
| (2,86)  | 1:1:A:LEU:HD21  | 1:34:A:LEU:HB2  | 6                   | 0.73     | 0.65                | 0.61       |
| (2,86)  | 1:1:A:LEU:HD22  | 1:34:A:LEU:HB2  | 6                   | 0.73     | 0.65                | 0.61       |
| (2,86)  | 1:1:A:LEU:HD23  | 1:34:A:LEU:HB2  | 6                   | 0.73     | 0.65                | 0.61       |
| (2,86)  | 1:1:A:LEU:HD22  | 1:34:A:LEU:HB3  | 6                   | 0.73     | 0.65                | 0.61       |
| (1,352) | 1:20:A:LEU:HD13 | 1:13:A:THR:HG21 | 6                   | 0.68     | 0.36                | 0.6        |
| (1,352) | 1:20:A:LEU:HD12 | 1:13:A:THR:HG23 | 6                   | 0.68     | 0.36                | 0.6        |
| (1,352) | 1:20:A:LEU:HD12 | 1:13:A:THR:HG21 | 6                   | 0.68     | 0.36                | 0.6        |
| (1,352) | 1:20:A:LEU:HD13 | 1:13:A:THR:HG23 | 6                   | 0.68     | 0.36                | 0.6        |
| (1,352) | 1:20:A:LEU:HD11 | 1:13:A:THR:HG23 | 6                   | 0.68     | 0.36                | 0.6        |
| (2,105) | 1:23:A:TRP:HH2  | 1:23:A:TRP:HE3  | 6                   | 0.44     | 0.01                | 0.45       |
| (2,105) | 1:27:A:ASN:HD21 | 1:23:A:TRP:HE3  | 6                   | 0.44     | 0.01                | 0.45       |
| (1,529) | 1:12:A:NLE:HG3  | 1:10:A:PHE:HB2  | 6                   | 0.33     | 0.18                | 0.29       |
| (1,25)  | 1:14:A:ARG:HG2  | 1:15:A:SER:H    | 6                   | 0.32     | 0.2                 | 0.22       |
| (1,452) | 1:26:A:GLN:HG2  | 1:23:A:TRP:HA   | 6                   | 0.31     | 0.1                 | 0.3        |
| (1,298) | 1:18:A:ALA:HB3  | 1:25:A:GLN:HE21 | 6                   | 0.29     | 0.07                | 0.3        |
| (1,298) | 1:18:A:ALA:HB2  | 1:25:A:GLN:HE21 | 6                   | 0.29     | 0.07                | 0.3        |
| (1,278) | 1:24:A:LYS:HB3  | 1:23:A:TRP:HZ2  | 6                   | 0.19     | 0.05                | 0.18       |
| (3,19)  | 1:27:A:ASN:H    | 1:23:A:TRP:O    | 6                   | 0.15     | 0.06                | 0.12       |
| (2,37)  | 1:31:A:GLU:HA   | 1:32:A:LYS:H    | 6                   | 0.15     | 0.03                | 0.16       |
| (2,87)  | 1:1:A:LEU:HD22  | 1:34:A:LEU:HD13 | 5                   | 1.44     | 0.64                | 1.68       |
| (2,87)  | 1:12:A:NLE:HE2  | 1:20:A:LEU:HD23 | 5                   | 1.44     | 0.64                | 1.68       |
| (2,87)  | 1:12:A:NLE:HE3  | 1:20:A:LEU:HD23 | 5                   | 1.44     | 0.64                | 1.68       |
| (2,87)  | 1:12:A:NLE:HE2  | 1:20:A:LEU:HD22 | 5                   | 1.44     | 0.64                | 1.68       |
| (1,29)  | 1:29:A:LYS:HG2  | 1:29:A:LYS:H    | 5                   | 0.87     | 0.02                | 0.86       |
| (1,29)  | 1:29:A:LYS:HG3  | 1:29:A:LYS:H    | 5                   | 0.87     | 0.02                | 0.86       |
| (1,582) | 1:24:A:LYS:HZ3  | 1:27:A:ASN:HD22 | 5                   | 0.71     | 0.69                | 0.25       |
| (1,582) | 1:24:A:LYS:HZ1  | 1:27:A:ASN:HD22 | 5                   | 0.71     | 0.69                | 0.25       |
| (1,582) | 1:24:A:LYS:HZ2  | 1:27:A:ASN:HD22 | 5                   | 0.71     | 0.69                | 0.25       |
| (2,24)  | 1:6:A:3FB:HB2   | 1:10:A:PHE:HD2  | 5                   | 0.68     | 0.18                | 0.64       |
| (2,24)  | 1:35:A:PHE:HB3  | 1:14:A:ARG:HH21 | 5                   | 0.68     | 0.18                | 0.64       |
| (3,2)   | 1:7:A:LYS:N     | 1:3:A:ASP:O     | 5                   | 0.55     | 0.39                | 0.43       |
| (2,94)  | 1:35:A:PHE:HB3  | 1:32:A:LYS:HA   | 5                   | 0.55     | 0.16                | 0.53       |
| (2,94)  | 1:6:A:3FB:HB2   | 1:32:A:LYS:HA   | 5                   | 0.55     | 0.16                | 0.53       |

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| Key     | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (2,20)  | 1:10:A:PHE:HB3  | 1:13:A:THR:H    | 5                   | 0.4      | 0.18                | 0.36       |
| (1,581) | 1:34:A:LEU:H    | 1:35:A:PHE:H    | 5                   | 0.38     | 0.16                | 0.36       |
| (2,88)  | 1:28:A:LEU:HD11 | 1:25:A:GLN:HG2  | 5                   | 0.31     | 0.11                | 0.35       |
| (2,88)  | 1:28:A:LEU:HD13 | 1:25:A:GLN:HG2  | 5                   | 0.31     | 0.11                | 0.35       |
| (2,88)  | 1:12:A:NLE:HE3  | 1:12:A:NLE:HB3  | 5                   | 0.31     | 0.11                | 0.35       |
| (2,88)  | 1:12:A:NLE:HE2  | 1:12:A:NLE:HB3  | 5                   | 0.31     | 0.11                | 0.35       |
| (1,194) | 1:28:A:LEU:HA   | 1:30:A:LYS:H    | 5                   | 0.23     | 0.08                | 0.18       |
| (1,558) | 1:23:A:TRP:HE3  | 1:27:A:ASN:H    | 5                   | 0.21     | 0.09                | 0.17       |
| (1,518) | 1:14:A:ARG:HB3  | 1:14:A:ARG:HD3  | 5                   | 0.19     | 0.06                | 0.17       |
| (1,518) | 1:14:A:ARG:HB3  | 1:14:A:ARG:HD2  | 5                   | 0.19     | 0.06                | 0.17       |
| (1,235) | 1:23:A:TRP:HA   | 1:23:A:TRP:HD1  | 5                   | 0.12     | 0.01                | 0.12       |
| (1,365) | 1:1:A:LEU:HD13  | 1:34:A:LEU:HD11 | 4                   | 2.62     | 0.39                | 2.63       |
| (1,365) | 1:1:A:LEU:HD23  | 1:34:A:LEU:HD13 | 4                   | 2.62     | 0.39                | 2.63       |
| (1,365) | 1:1:A:LEU:HD11  | 1:34:A:LEU:HD13 | 4                   | 2.62     | 0.39                | 2.63       |
| (1,365) | 1:1:A:LEU:HD22  | 1:34:A:LEU:HD11 | 4                   | 2.62     | 0.39                | 2.63       |
| (1,312) | 1:34:A:LEU:HD11 | 1:34:A:LEU:HA   | 4                   | 1.2      | 0.04                | 1.2        |
| (3,29)  | 1:32:A:LYS:H    | 1:28:A:LEU:O    | 4                   | 1.04     | 1.08                | 0.58       |
| (1,266) | 1:1:A:LEU:HG    | 1:6:A:3FB:HE2   | 4                   | 0.85     | 0.56                | 0.66       |
| (1,266) | 1:1:A:LEU:HG    | 1:6:A:3FB:HE1   | 4                   | 0.85     | 0.56                | 0.66       |
| (1,403) | 1:5:A:ASP:HB2   | 1:6:A:3FB:HB2   | 4                   | 0.83     | 0.73                | 0.74       |
| (2,102) | 1:30:A:LYS:HB3  | 1:30:A:LYS:HE3  | 4                   | 0.7      | 0.02                | 0.7        |
| (2,102) | 1:29:A:LYS:HB2  | 1:29:A:LYS:HE3  | 4                   | 0.7      | 0.02                | 0.7        |
| (2,4)   | 1:28:A:LEU:HD12 | 1:13:A:THR:H    | 4                   | 0.62     | 0.3                 | 0.5        |
| (2,4)   | 1:12:A:NLE:HE2  | 1:13:A:THR:H    | 4                   | 0.62     | 0.3                 | 0.5        |
| (2,4)   | 1:28:A:LEU:HD11 | 1:13:A:THR:H    | 4                   | 0.62     | 0.3                 | 0.5        |
| (2,4)   | 1:1:A:LEU:HD23  | 1:33:A:GLY:H    | 4                   | 0.62     | 0.3                 | 0.5        |
| (1,513) | 1:32:A:LYS:HB2  | 1:35:A:PHE:HB3  | 4                   | 0.62     | 0.5                 | 0.44       |
| (2,52)  | 1:1:A:LEU:HG    | 1:6:A:3FB:HD2   | 4                   | 0.62     | 0.21                | 0.64       |
| (2,52)  | 1:1:A:LEU:HG    | 1:6:A:3FB:HD1   | 4                   | 0.62     | 0.21                | 0.64       |
| (2,52)  | 1:28:A:LEU:HG   | 1:17:A:PHE:HE1  | 4                   | 0.62     | 0.21                | 0.64       |
| (3,3)   | 1:8:A:ALA:H     | 1:4:A:GLU:O     | 4                   | 0.62     | 0.59                | 0.32       |
| (3,8)   | 1:10:A:PHE:N    | 1:6:A:3FB:O     | 4                   | 0.6      | 0.27                | 0.5        |
| (1,42)  | 1:32:A:LYS:HB3  | 1:33:A:GLY:H    | 4                   | 0.52     | 0.15                | 0.52       |
| (2,9)   | 1:30:A:LYS:HG2  | 1:30:A:LYS:H    | 4                   | 0.52     | 0.12                | 0.5        |
| (2,9)   | 1:32:A:LYS:HG3  | 1:33:A:GLY:H    | 4                   | 0.52     | 0.12                | 0.5        |
| (2,9)   | 1:32:A:LYS:HG2  | 1:33:A:GLY:H    | 4                   | 0.52     | 0.12                | 0.5        |
| (1,35)  | 1:32:A:LYS:HG3  | 1:32:A:LYS:H    | 4                   | 0.52     | 0.08                | 0.49       |
| (1,35)  | 1:32:A:LYS:HG2  | 1:32:A:LYS:H    | 4                   | 0.52     | 0.08                | 0.49       |
| (1,217) | 1:2:A:SER:HB2   | 1:3:A:ASP:H     | 4                   | 0.47     | 0.06                | 0.45       |
| (2,41)  | 1:12:A:NLE:HA   | 1:13:A:THR:H    | 4                   | 0.45     | 0.06                | 0.48       |
| (1,331) | 1:24:A:LYS:HG2  | 1:21:A:PRO:HD3  | 4                   | 0.37     | 0.17                | 0.34       |
| (3,27)  | 1:31:A:GLU:H    | 1:27:A:ASN:O    | 4                   | 0.3      | 0.16                | 0.26       |

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| Key     | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,288) | 1:9:A:VAL:HG21  | 1:6:A:3FB:HD2   | 4                   | 0.28     | 0.08                | 0.26       |
| (1,288) | 1:9:A:VAL:HG22  | 1:6:A:3FB:HD2   | 4                   | 0.28     | 0.08                | 0.26       |
| (1,288) | 1:9:A:VAL:HG23  | 1:6:A:3FB:HD1   | 4                   | 0.28     | 0.08                | 0.26       |
| (2,99)  | 1:6:A:3FB:HA    | 1:13:A:THR:HG22 | 4                   | 0.27     | 0.11                | 0.3        |
| (2,99)  | 1:6:A:3FB:HA    | 1:13:A:THR:HG21 | 4                   | 0.27     | 0.11                | 0.3        |
| (2,99)  | 1:10:A:PHE:HA   | 1:13:A:THR:HG22 | 4                   | 0.27     | 0.11                | 0.3        |
| (1,183) | 1:15:A:SER:HB3  | 1:15:A:SER:H    | 4                   | 0.2      | 0.01                | 0.2        |
| (2,27)  | 1:25:A:GLN:HA   | 1:25:A:GLN:HE22 | 4                   | 0.2      | 0.01                | 0.2        |
| (1,430) | 1:15:A:SER:HB2  | 1:15:A:SER:HA   | 4                   | 0.11     | 0.0                 | 0.11       |
| (1,336) | 1:22:A:LEU:HD21 | 1:25:A:GLN:HG3  | 3                   | 3.05     | 0.03                | 3.04       |
| (1,336) | 1:22:A:LEU:HD22 | 1:25:A:GLN:HG3  | 3                   | 3.05     | 0.03                | 3.04       |
| (1,334) | 1:22:A:LEU:HD22 | 1:25:A:GLN:HB2  | 3                   | 2.05     | 0.1                 | 1.99       |
| (1,334) | 1:22:A:LEU:HD23 | 1:25:A:GLN:HB2  | 3                   | 2.05     | 0.1                 | 1.99       |
| (1,268) | 1:32:A:LYS:HD3  | 1:6:A:3FB:HE2   | 3                   | 1.6      | 0.1                 | 1.54       |
| (1,268) | 1:32:A:LYS:HD3  | 1:6:A:3FB:HE1   | 3                   | 1.6      | 0.1                 | 1.54       |
| (1,268) | 1:32:A:LYS:HD2  | 1:6:A:3FB:HE2   | 3                   | 1.6      | 0.1                 | 1.54       |
| (1,318) | 1:22:A:LEU:HD21 | 1:22:A:LEU:HA   | 3                   | 1.09     | 0.04                | 1.11       |
| (1,318) | 1:22:A:LEU:HD22 | 1:22:A:LEU:HA   | 3                   | 1.09     | 0.04                | 1.11       |
| (2,95)  | 1:6:A:3FB:HB1   | 1:13:A:THR:HA   | 3                   | 0.99     | 0.38                | 1.04       |
| (2,95)  | 1:6:A:3FB:HB1   | 1:32:A:LYS:HA   | 3                   | 0.99     | 0.38                | 1.04       |
| (1,223) | 1:13:A:THR:HB   | 1:14:A:ARG:H    | 3                   | 0.96     | 0.08                | 1.0        |
| (1,19)  | 1:13:A:THR:HG21 | 1:14:A:ARG:H    | 3                   | 0.88     | 0.02                | 0.87       |
| (1,19)  | 1:13:A:THR:HG22 | 1:14:A:ARG:H    | 3                   | 0.88     | 0.02                | 0.87       |
| (2,72)  | 1:1:A:LEU:HD11  | 1:6:A:3FB:H     | 3                   | 0.88     | 0.36                | 1.12       |
| (2,72)  | 1:1:A:LEU:HD23  | 1:6:A:3FB:H     | 3                   | 0.88     | 0.36                | 1.12       |
| (2,72)  | 1:28:A:LEU:HD13 | 1:35:A:PHE:HE1  | 3                   | 0.88     | 0.36                | 1.12       |
| (1,469) | 1:32:A:LYS:HD3  | 1:32:A:LYS:HA   | 3                   | 0.73     | 0.42                | 1.02       |
| (1,469) | 1:32:A:LYS:HD2  | 1:32:A:LYS:HA   | 3                   | 0.73     | 0.42                | 1.02       |
| (1,16)  | 1:22:A:LEU:HG   | 1:22:A:LEU:H    | 3                   | 0.68     | 0.03                | 0.69       |
| (3,5)   | 1:9:A:VAL:H     | 1:5:A:ASP:O     | 3                   | 0.63     | 0.4                 | 0.39       |
| (1,356) | 1:28:A:LEU:HD21 | 1:13:A:THR:HG23 | 3                   | 0.61     | 0.26                | 0.6        |
| (1,356) | 1:28:A:LEU:HD22 | 1:13:A:THR:HG23 | 3                   | 0.61     | 0.26                | 0.6        |
| (1,356) | 1:28:A:LEU:HD21 | 1:13:A:THR:HG21 | 3                   | 0.61     | 0.26                | 0.6        |
| (2,45)  | 1:5:A:ASP:HA    | 1:9:A:VAL:H     | 3                   | 0.57     | 0.46                | 0.29       |
| (3,30)  | 1:32:A:LYS:N    | 1:28:A:LEU:O    | 3                   | 0.56     | 0.45                | 0.4        |
| (1,18)  | 1:14:A:ARG:HG3  | 1:14:A:ARG:H    | 3                   | 0.48     | 0.16                | 0.4        |
| (1,534) | 1:1:A:LEU:HD23  | 1:5:A:ASP:HB3   | 3                   | 0.47     | 0.33                | 0.23       |
| (1,534) | 1:1:A:LEU:HD12  | 1:5:A:ASP:HB3   | 3                   | 0.47     | 0.33                | 0.23       |
| (2,58)  | 1:29:A:LYS:HG3  | 1:35:A:PHE:HE1  | 3                   | 0.47     | 0.03                | 0.46       |
| (2,58)  | 1:18:A:ALA:HB2  | 1:25:A:GLN:HE22 | 3                   | 0.47     | 0.03                | 0.46       |
| (1,8)   | 1:28:A:LEU:HD11 | 1:29:A:LYS:H    | 3                   | 0.44     | 0.12                | 0.45       |
| (1,8)   | 1:28:A:LEU:HD12 | 1:29:A:LYS:H    | 3                   | 0.44     | 0.12                | 0.45       |

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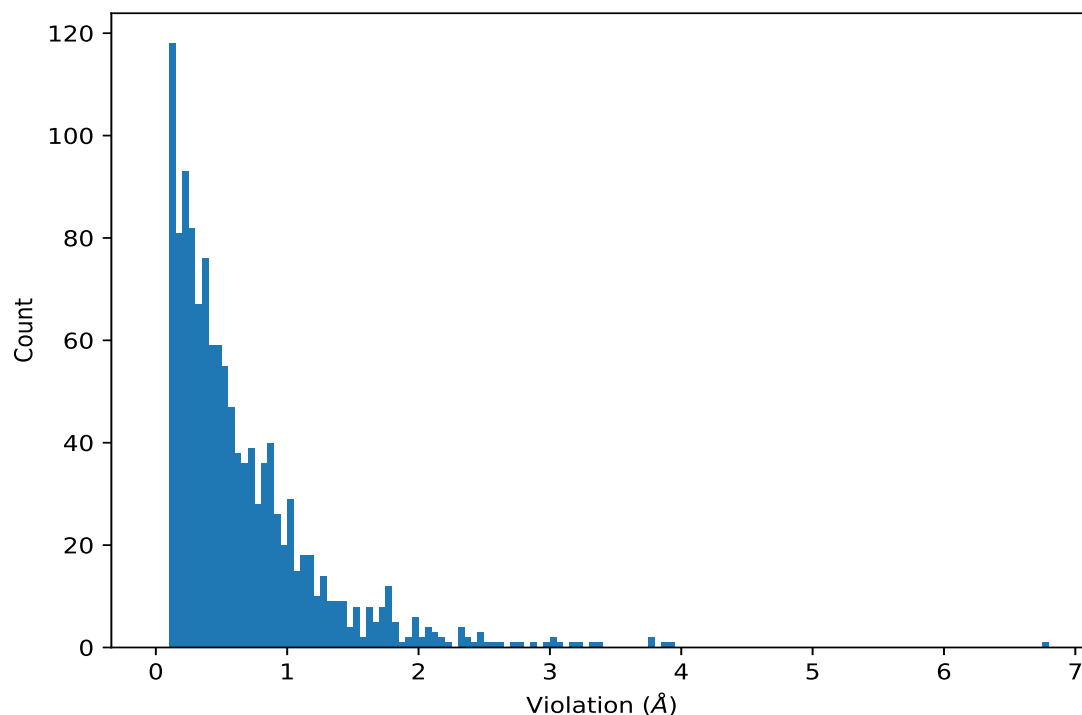
| Key     | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,27)  | 1:7:A:LYS:HG3   | 1:8:A:ALA:H     | 3                   | 0.4      | 0.14                | 0.32       |
| (3,26)  | 1:30:A:LYS:N    | 1:26:A:GLN:O    | 3                   | 0.33     | 0.1                 | 0.29       |
| (1,23)  | 1:16:A:ALA:HB1  | 1:17:A:PHE:H    | 3                   | 0.29     | 0.1                 | 0.23       |
| (1,23)  | 1:16:A:ALA:HB2  | 1:17:A:PHE:H    | 3                   | 0.29     | 0.1                 | 0.23       |
| (1,23)  | 1:16:A:ALA:HB3  | 1:17:A:PHE:H    | 3                   | 0.29     | 0.1                 | 0.23       |
| (3,23)  | 1:29:A:LYS:H    | 1:25:A:GLN:O    | 3                   | 0.29     | 0.03                | 0.31       |
| (2,97)  | 1:26:A:GLN:HA   | 1:29:A:LYS:HD2  | 3                   | 0.27     | 0.11                | 0.26       |
| (2,97)  | 1:26:A:GLN:HA   | 1:29:A:LYS:HD3  | 3                   | 0.27     | 0.11                | 0.26       |
| (1,122) | 1:6:A:3FB:HC1   | 1:6:A:3FB:HD1   | 3                   | 0.22     | 0.02                | 0.22       |
| (1,122) | 1:6:A:3FB:HC1   | 1:6:A:3FB:HD2   | 3                   | 0.22     | 0.02                | 0.22       |
| (2,80)  | 1:20:A:LEU:HD12 | 1:28:A:LEU:HG   | 3                   | 0.21     | 0.08                | 0.2        |
| (2,80)  | 1:20:A:LEU:HD11 | 1:28:A:LEU:HG   | 3                   | 0.21     | 0.08                | 0.2        |
| (2,80)  | 1:20:A:LEU:HD12 | 1:12:A:NLE:HB2  | 3                   | 0.21     | 0.08                | 0.2        |
| (1,401) | 1:6:A:3FB:HC2   | 1:6:A:3FB:HB1   | 3                   | 0.2      | 0.04                | 0.18       |
| (2,71)  | 1:24:A:LYS:HG2  | 1:23:A:TRP:HZ2  | 3                   | 0.2      | 0.1                 | 0.16       |
| (1,26)  | 1:12:A:NLE:HG3  | 1:11:A:GLY:H    | 3                   | 0.19     | 0.06                | 0.2        |
| (1,50)  | 1:30:A:LYS:HB3  | 1:31:A:GLU:H    | 3                   | 0.18     | 0.07                | 0.14       |
| (1,76)  | 1:26:A:GLN:HG2  | 1:26:A:GLN:H    | 3                   | 0.17     | 0.04                | 0.16       |
| (1,545) | 1:14:A:ARG:HH21 | 1:35:A:PHE:HD2  | 2                   | 1.44     | 1.04                | 1.44       |
| (1,545) | 1:14:A:ARG:HH21 | 1:35:A:PHE:HD1  | 2                   | 1.44     | 1.04                | 1.44       |
| (1,153) | 1:16:A:ALA:HA   | 1:19:A:ASN:HD22 | 2                   | 1.12     | 0.38                | 1.12       |
| (2,76)  | 1:12:A:NLE:HE1  | 1:10:A:PHE:HD1  | 2                   | 1.12     | 0.16                | 1.12       |
| (2,59)  | 1:16:A:ALA:HB3  | 1:19:A:ASN:HD22 | 2                   | 1.09     | 0.75                | 1.09       |
| (2,59)  | 1:16:A:ALA:HB1  | 1:19:A:ASN:HD22 | 2                   | 1.09     | 0.75                | 1.09       |
| (3,4)   | 1:8:A:ALA:N     | 1:4:A:GLU:O     | 2                   | 0.7      | 0.56                | 0.7        |
| (1,374) | 1:8:A:ALA:HB2   | 1:5:A:ASP:HB3   | 2                   | 0.59     | 0.36                | 0.59       |
| (1,175) | 1:15:A:SER:HA   | 1:18:A:ALA:H    | 2                   | 0.55     | 0.38                | 0.55       |
| (3,6)   | 1:9:A:VAL:N     | 1:5:A:ASP:O     | 2                   | 0.41     | 0.31                | 0.41       |
| (1,559) | 1:36:A:NH2:HN2  | 1:35:A:PHE:H    | 2                   | 0.36     | 0.04                | 0.36       |
| (1,191) | 1:34:A:LEU:HA   | 1:35:A:PHE:H    | 2                   | 0.34     | 0.14                | 0.34       |
| (2,90)  | 1:12:A:NLE:HD3  | 1:12:A:NLE:HB2  | 2                   | 0.32     | 0.02                | 0.32       |
| (3,28)  | 1:31:A:GLU:N    | 1:27:A:ASN:O    | 2                   | 0.28     | 0.12                | 0.28       |
| (2,18)  | 1:6:A:3FB:HB2   | 1:7:A:LYS:H     | 2                   | 0.26     | 0.08                | 0.26       |
| (1,503) | 1:7:A:LYS:HG3   | 1:7:A:LYS:HA    | 2                   | 0.24     | 0.01                | 0.24       |
| (1,41)  | 1:28:A:LEU:HG   | 1:27:A:ASN:H    | 2                   | 0.23     | 0.07                | 0.23       |
| (1,117) | 1:6:A:3FB:HC1   | 1:6:A:3FB:H     | 2                   | 0.17     | 0.05                | 0.17       |
| (2,70)  | 1:20:A:LEU:HD12 | 1:25:A:GLN:H    | 2                   | 0.16     | 0.03                | 0.16       |
| (2,70)  | 1:20:A:LEU:HD11 | 1:25:A:GLN:H    | 2                   | 0.16     | 0.03                | 0.16       |
| (1,208) | 1:27:A:ASN:HA   | 1:29:A:LYS:H    | 2                   | 0.15     | 0.01                | 0.15       |

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

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

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

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



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

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

| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,151) | 1:29:A:LYS:HA   | 1:14:A:ARG:HH21 | 10       | 6.78          |
| (1,134) | 1:17:A:PHE:HB2  | 1:14:A:ARG:HH22 | 10       | 3.94          |
| (1,151) | 1:29:A:LYS:HA   | 1:14:A:ARG:HH21 | 9        | 3.86          |
| (1,151) | 1:29:A:LYS:HA   | 1:14:A:ARG:HH21 | 1        | 3.78          |
| (2,17)  | 1:7:A:LYS:HE2   | 1:14:A:ARG:H    | 10       | 3.77          |
| (3,11)  | 1:17:A:PHE:H    | 1:13:A:THR:O    | 9        | 3.38          |
| (1,151) | 1:29:A:LYS:HA   | 1:14:A:ARG:HH21 | 3        | 3.34          |
| (1,151) | 1:29:A:LYS:HA   | 1:14:A:ARG:HH21 | 8        | 3.24          |
| (1,365) | 1:1:A:LEU:HD22  | 1:34:A:LEU:HD11 | 4        | 3.16          |
| (1,336) | 1:22:A:LEU:HD21 | 1:25:A:GLN:HG3  | 1        | 3.09          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,336) | 1:22:A:LEU:HD21 | 1:25:A:GLN:HG3  | 10       | 3.04          |
| (1,336) | 1:22:A:LEU:HD22 | 1:25:A:GLN:HG3  | 4        | 3.03          |
| (3,12)  | 1:17:A:PHE:N    | 1:13:A:THR:O    | 9        | 2.95          |
| (3,29)  | 1:32:A:LYS:H    | 1:28:A:LEU:O    | 6        | 2.87          |
| (3,11)  | 1:17:A:PHE:H    | 1:13:A:THR:O    | 7        | 2.77          |
| (1,365) | 1:1:A:LEU:HD13  | 1:34:A:LEU:HD11 | 10       | 2.72          |
| (1,151) | 1:29:A:LYS:HA   | 1:14:A:ARG:HH22 | 7        | 2.63          |
| (3,9)   | 1:16:A:ALA:H    | 1:12:A:NLE:O    | 10       | 2.58          |
| (1,365) | 1:1:A:LEU:HD11  | 1:34:A:LEU:HD13 | 3        | 2.54          |
| (2,55)  | 1:32:A:LYS:HD3  | 1:10:A:PHE:HD2  | 9        | 2.49          |
| (1,545) | 1:14:A:ARG:HH21 | 1:35:A:PHE:HD2  | 10       | 2.49          |
| (3,9)   | 1:16:A:ALA:H    | 1:12:A:NLE:O    | 2        | 2.47          |
| (3,9)   | 1:16:A:ALA:H    | 1:12:A:NLE:O    | 3        | 2.43          |
| (3,12)  | 1:17:A:PHE:N    | 1:13:A:THR:O    | 7        | 2.36          |
| (3,9)   | 1:16:A:ALA:H    | 1:12:A:NLE:O    | 8        | 2.35          |
| (1,373) | 1:1:A:LEU:HG    | 1:5:A:ASP:HB3   | 7        | 2.34          |
| (3,11)  | 1:17:A:PHE:H    | 1:13:A:THR:O    | 4        | 2.33          |
| (3,9)   | 1:16:A:ALA:H    | 1:12:A:NLE:O    | 5        | 2.31          |
| (3,11)  | 1:17:A:PHE:H    | 1:13:A:THR:O    | 6        | 2.3           |
| (3,9)   | 1:16:A:ALA:H    | 1:12:A:NLE:O    | 1        | 2.24          |
| (1,334) | 1:22:A:LEU:HD22 | 1:25:A:GLN:HB2  | 10       | 2.19          |
| (3,15)  | 1:19:A:ASN:H    | 1:15:A:SER:O    | 6        | 2.17          |
| (2,75)  | 1:28:A:LEU:HD21 | 1:6:A:3FB:HE1   | 1        | 2.11          |
| (2,75)  | 1:28:A:LEU:HD22 | 1:6:A:3FB:HE1   | 10       | 2.11          |
| (2,86)  | 1:1:A:LEU:HD21  | 1:34:A:LEU:HB2  | 1        | 2.1           |
| (2,6)   | 1:13:A:THR:HG22 | 1:17:A:PHE:H    | 4        | 2.09          |
| (1,365) | 1:1:A:LEU:HD23  | 1:34:A:LEU:HD13 | 2        | 2.07          |
| (1,151) | 1:29:A:LYS:HA   | 1:14:A:ARG:HH21 | 4        | 2.07          |
| (3,12)  | 1:17:A:PHE:N    | 1:13:A:THR:O    | 6        | 2.05          |
| (2,65)  | 1:22:A:LEU:HD11 | 1:23:A:TRP:HD1  | 10       | 2.04          |
| (2,64)  | 1:18:A:ALA:HB1  | 1:19:A:ASN:HD21 | 4        | 2.01          |
| (1,334) | 1:22:A:LEU:HD22 | 1:25:A:GLN:HB2  | 1        | 1.99          |
| (1,334) | 1:22:A:LEU:HD23 | 1:25:A:GLN:HB2  | 4        | 1.98          |
| (1,427) | 1:1:A:LEU:HG    | 1:5:A:ASP:HB2   | 2        | 1.97          |
| (1,151) | 1:29:A:LYS:HA   | 1:14:A:ARG:HH22 | 2        | 1.97          |
| (2,87)  | 1:12:A:NLE:HE2  | 1:20:A:LEU:HD22 | 10       | 1.96          |
| (3,13)  | 1:18:A:ALA:H    | 1:14:A:ARG:O    | 9        | 1.95          |
| (3,13)  | 1:18:A:ALA:H    | 1:14:A:ARG:O    | 4        | 1.91          |
| (2,65)  | 1:28:A:LEU:HD12 | 1:19:A:ASN:H    | 4        | 1.9           |
| (1,528) | 1:18:A:ALA:HB1  | 1:17:A:PHE:HB2  | 1        | 1.85          |
| (2,59)  | 1:16:A:ALA:HB1  | 1:19:A:ASN:HD22 | 4        | 1.84          |
| (2,6)   | 1:13:A:THR:HG21 | 1:17:A:PHE:H    | 9        | 1.84          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,528) | 1:18:A:ALA:HB1  | 1:17:A:PHE:HB2  | 9        | 1.84          |
| (2,6)   | 1:13:A:THR:HG23 | 1:17:A:PHE:H    | 7        | 1.81          |
| (1,528) | 1:18:A:ALA:HB2  | 1:17:A:PHE:HB2  | 8        | 1.8           |
| (2,1)   | 1:28:A:LEU:HD12 | 1:17:A:PHE:H    | 9        | 1.79          |
| (1,528) | 1:18:A:ALA:HB2  | 1:17:A:PHE:HB2  | 5        | 1.79          |
| (2,55)  | 1:32:A:LYS:HD2  | 1:10:A:PHE:HD2  | 8        | 1.78          |
| (1,373) | 1:1:A:LEU:HG    | 1:5:A:ASP:HB3   | 10       | 1.78          |
| (1,554) | 1:23:A:TRP:HE3  | 1:27:A:ASN:HD22 | 4        | 1.77          |
| (1,528) | 1:18:A:ALA:HB2  | 1:17:A:PHE:HB2  | 2        | 1.77          |
| (1,528) | 1:18:A:ALA:HB1  | 1:17:A:PHE:HB2  | 3        | 1.77          |
| (1,266) | 1:1:A:LEU:HG    | 1:6:A:3FB:HE2   | 7        | 1.77          |
| (3,12)  | 1:17:A:PHE:N    | 1:13:A:THR:O    | 4        | 1.76          |
| (2,87)  | 1:12:A:NLE:HE2  | 1:20:A:LEU:HD23 | 3        | 1.75          |
| (1,528) | 1:18:A:ALA:HB1  | 1:17:A:PHE:HB2  | 7        | 1.75          |
| (1,134) | 1:17:A:PHE:HB2  | 1:14:A:ARG:HH22 | 1        | 1.75          |
| (1,582) | 1:24:A:LYS:HZ3  | 1:27:A:ASN:HD22 | 10       | 1.74          |
| (1,528) | 1:18:A:ALA:HB2  | 1:17:A:PHE:HB2  | 4        | 1.74          |
| (1,268) | 1:32:A:LYS:HD3  | 1:6:A:3FB:HE1   | 10       | 1.74          |
| (1,373) | 1:1:A:LEU:HG    | 1:5:A:ASP:HB3   | 5        | 1.73          |
| (2,63)  | 1:13:A:THR:HG21 | 1:6:A:3FB:HD2   | 5        | 1.72          |
| (1,528) | 1:18:A:ALA:HB3  | 1:17:A:PHE:HB2  | 6        | 1.72          |
| (1,403) | 1:5:A:ASP:HB2   | 1:6:A:3FB:HB2   | 2        | 1.72          |
| (3,16)  | 1:19:A:ASN:N    | 1:15:A:SER:O    | 6        | 1.7           |
| (2,75)  | 1:28:A:LEU:HD22 | 1:6:A:3FB:HE2   | 2        | 1.69          |
| (1,528) | 1:18:A:ALA:HB3  | 1:17:A:PHE:HB2  | 10       | 1.69          |
| (2,87)  | 1:12:A:NLE:HE3  | 1:20:A:LEU:HD23 | 4        | 1.68          |
| (2,87)  | 1:12:A:NLE:HE2  | 1:20:A:LEU:HD23 | 2        | 1.65          |
| (2,75)  | 1:28:A:LEU:HD21 | 1:6:A:3FB:HE1   | 7        | 1.65          |
| (3,14)  | 1:18:A:ALA:N    | 1:14:A:ARG:O    | 4        | 1.64          |
| (3,14)  | 1:18:A:ALA:N    | 1:14:A:ARG:O    | 9        | 1.64          |
| (3,9)   | 1:16:A:ALA:H    | 1:12:A:NLE:O    | 4        | 1.64          |
| (2,1)   | 1:28:A:LEU:HD13 | 1:17:A:PHE:H    | 10       | 1.64          |
| (1,554) | 1:23:A:TRP:HE3  | 1:27:A:ASN:HD22 | 7        | 1.64          |
| (3,3)   | 1:8:A:ALA:H     | 1:4:A:GLU:O     | 3        | 1.63          |
| (2,1)   | 1:28:A:LEU:HD11 | 1:17:A:PHE:H    | 8        | 1.63          |
| (2,6)   | 1:13:A:THR:HG21 | 1:17:A:PHE:H    | 6        | 1.6           |
| (2,63)  | 1:13:A:THR:HG21 | 1:10:A:PHE:HE2  | 2        | 1.58          |
| (3,15)  | 1:19:A:ASN:H    | 1:15:A:SER:O    | 9        | 1.56          |
| (2,85)  | 1:24:A:LYS:HG2  | 1:12:A:NLE:HD2  | 6        | 1.54          |
| (1,268) | 1:32:A:LYS:HD3  | 1:6:A:3FB:HE2   | 1        | 1.54          |
| (3,1)   | 1:7:A:LYS:H     | 1:3:A:ASP:O     | 5        | 1.53          |
| (1,268) | 1:32:A:LYS:HD2  | 1:6:A:3FB:HE2   | 4        | 1.52          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,172) | 1:29:A:LYS:HA   | 1:32:A:LYS:H    | 6        | 1.52          |
| (3,15)  | 1:19:A:ASN:H    | 1:15:A:SER:O    | 4        | 1.5           |
| (3,10)  | 1:16:A:ALA:N    | 1:12:A:NLE:O    | 10       | 1.5           |
| (1,153) | 1:16:A:ALA:HA   | 1:19:A:ASN:HD22 | 4        | 1.5           |
| (2,55)  | 1:32:A:LYS:HD3  | 1:14:A:ARG:HH21 | 4        | 1.47          |
| (3,10)  | 1:16:A:ALA:N    | 1:12:A:NLE:O    | 2        | 1.46          |
| (3,13)  | 1:18:A:ALA:H    | 1:14:A:ARG:O    | 6        | 1.45          |
| (2,6)   | 1:13:A:THR:HG21 | 1:17:A:PHE:H    | 1        | 1.45          |
| (3,10)  | 1:16:A:ALA:N    | 1:12:A:NLE:O    | 3        | 1.44          |
| (1,533) | 1:22:A:LEU:HD22 | 1:26:A:GLN:HG2  | 10       | 1.44          |
| (1,513) | 1:32:A:LYS:HB2  | 1:35:A:PHE:HB3  | 2        | 1.44          |
| (2,95)  | 1:6:A:3FB:HB1   | 1:13:A:THR:HA   | 3        | 1.43          |
| (2,65)  | 1:12:A:NLE:HE1  | 1:23:A:TRP:HZ2  | 1        | 1.43          |
| (3,7)   | 1:10:A:PHE:H    | 1:6:A:3FB:O     | 9        | 1.42          |
| (1,554) | 1:23:A:TRP:HE3  | 1:27:A:ASN:HD22 | 2        | 1.42          |
| (3,13)  | 1:18:A:ALA:H    | 1:14:A:ARG:O    | 7        | 1.41          |
| (2,8)   | 1:29:A:LYS:HG3  | 1:30:A:LYS:H    | 6        | 1.41          |
| (1,574) | 1:23:A:TRP:HZ3  | 1:27:A:ASN:HD22 | 7        | 1.38          |
| (1,403) | 1:5:A:ASP:HB2   | 1:6:A:3FB:HB2   | 4        | 1.38          |
| (3,10)  | 1:16:A:ALA:N    | 1:12:A:NLE:O    | 5        | 1.37          |
| (2,6)   | 1:13:A:THR:HG23 | 1:17:A:PHE:H    | 2        | 1.37          |
| (1,151) | 1:29:A:LYS:HA   | 1:14:A:ARG:HH21 | 5        | 1.36          |
| (2,25)  | 1:23:A:TRP:HB3  | 1:23:A:TRP:HH2  | 6        | 1.35          |
| (2,25)  | 1:23:A:TRP:HB3  | 1:23:A:TRP:HH2  | 10       | 1.35          |
| (1,582) | 1:24:A:LYS:HZ3  | 1:27:A:ASN:HD22 | 1        | 1.35          |
| (1,574) | 1:23:A:TRP:HZ3  | 1:27:A:ASN:HD22 | 4        | 1.35          |
| (3,10)  | 1:16:A:ALA:N    | 1:12:A:NLE:O    | 8        | 1.34          |
| (2,23)  | 1:17:A:PHE:HB3  | 1:17:A:PHE:HE2  | 5        | 1.34          |
| (2,8)   | 1:29:A:LYS:HG3  | 1:30:A:LYS:H    | 4        | 1.34          |
| (2,23)  | 1:17:A:PHE:HB3  | 1:17:A:PHE:HE2  | 7        | 1.33          |
| (1,373) | 1:1:A:LEU:HG    | 1:5:A:ASP:HB3   | 9        | 1.32          |
| (1,574) | 1:23:A:TRP:HZ3  | 1:27:A:ASN:HD22 | 2        | 1.31          |
| (1,554) | 1:23:A:TRP:HE3  | 1:27:A:ASN:HD22 | 9        | 1.31          |
| (3,10)  | 1:16:A:ALA:N    | 1:12:A:NLE:O    | 1        | 1.3           |
| (3,9)   | 1:16:A:ALA:H    | 1:12:A:NLE:O    | 7        | 1.3           |
| (2,8)   | 1:29:A:LYS:HG3  | 1:30:A:LYS:H    | 7        | 1.28          |
| (2,6)   | 1:13:A:THR:HG21 | 1:17:A:PHE:H    | 8        | 1.28          |
| (1,533) | 1:22:A:LEU:HD21 | 1:26:A:GLN:HG2  | 6        | 1.28          |
| (1,533) | 1:22:A:LEU:HD21 | 1:26:A:GLN:HG2  | 8        | 1.28          |
| (2,76)  | 1:12:A:NLE:HE1  | 1:10:A:PHE:HD1  | 2        | 1.27          |
| (2,12)  | 1:28:A:LEU:HG   | 1:29:A:LYS:H    | 1        | 1.27          |
| (2,7)   | 1:8:A:ALA:HB2   | 1:10:A:PHE:H    | 9        | 1.27          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,475) | 1:30:A:LYS:HA   | 1:30:A:LYS:HD2  | 1        | 1.27          |
| (2,63)  | 1:13:A:THR:HG22 | 1:10:A:PHE:HE2  | 10       | 1.26          |
| (1,533) | 1:22:A:LEU:HD22 | 1:26:A:GLN:HG2  | 2        | 1.26          |
| (1,312) | 1:34:A:LEU:HD11 | 1:34:A:LEU:HA   | 9        | 1.26          |
| (3,4)   | 1:8:A:ALA:N     | 1:4:A:GLU:O     | 3        | 1.25          |
| (2,6)   | 1:13:A:THR:HG21 | 1:17:A:PHE:H    | 3        | 1.25          |
| (1,352) | 1:20:A:LEU:HD12 | 1:13:A:THR:HG23 | 2        | 1.25          |
| (2,23)  | 1:27:A:ASN:HB3  | 1:23:A:TRP:HZ3  | 4        | 1.24          |
| (1,427) | 1:1:A:LEU:HG    | 1:5:A:ASP:HB2   | 9        | 1.24          |
| (1,533) | 1:22:A:LEU:HD23 | 1:26:A:GLN:HG2  | 9        | 1.23          |
| (1,312) | 1:34:A:LEU:HD11 | 1:34:A:LEU:HA   | 1        | 1.22          |
| (3,9)   | 1:16:A:ALA:H    | 1:12:A:NLE:O    | 9        | 1.21          |
| (2,45)  | 1:5:A:ASP:HA    | 1:9:A:VAL:H     | 3        | 1.21          |
| (3,5)   | 1:9:A:VAL:H     | 1:5:A:ASP:O     | 3        | 1.2           |
| (2,17)  | 1:7:A:LYS:HE2   | 1:14:A:ARG:H    | 2        | 1.2           |
| (2,17)  | 1:7:A:LYS:HE3   | 1:14:A:ARG:H    | 5        | 1.2           |
| (1,533) | 1:22:A:LEU:HD21 | 1:26:A:GLN:HG2  | 3        | 1.2           |
| (3,14)  | 1:18:A:ALA:N    | 1:14:A:ARG:O    | 6        | 1.19          |
| (3,14)  | 1:18:A:ALA:N    | 1:14:A:ARG:O    | 7        | 1.19          |
| (2,25)  | 1:21:A:PRO:HD3  | 1:23:A:TRP:HH2  | 1        | 1.19          |
| (1,312) | 1:34:A:LEU:HD11 | 1:34:A:LEU:HA   | 5        | 1.19          |
| (1,290) | 1:9:A:VAL:HG23  | 1:10:A:PHE:HD2  | 2        | 1.19          |
| (3,2)   | 1:7:A:LYS:N     | 1:3:A:ASP:O     | 5        | 1.18          |
| (2,7)   | 1:8:A:ALA:HB1   | 1:10:A:PHE:H    | 6        | 1.18          |
| (1,475) | 1:30:A:LYS:HA   | 1:30:A:LYS:HD3  | 2        | 1.18          |
| (1,134) | 1:17:A:PHE:HB2  | 1:14:A:ARG:HH22 | 2        | 1.18          |
| (3,30)  | 1:32:A:LYS:N    | 1:28:A:LEU:O    | 6        | 1.17          |
| (2,1)   | 1:28:A:LEU:HD13 | 1:17:A:PHE:H    | 5        | 1.17          |
| (2,7)   | 1:8:A:ALA:HB2   | 1:10:A:PHE:H    | 4        | 1.16          |
| (1,475) | 1:30:A:LYS:HA   | 1:30:A:LYS:HD3  | 9        | 1.16          |
| (2,72)  | 1:1:A:LEU:HD23  | 1:6:A:3FB:H     | 3        | 1.15          |
| (1,475) | 1:30:A:LYS:HA   | 1:30:A:LYS:HD3  | 3        | 1.15          |
| (1,475) | 1:30:A:LYS:HA   | 1:30:A:LYS:HD2  | 10       | 1.15          |
| (1,312) | 1:34:A:LEU:HD11 | 1:34:A:LEU:HA   | 8        | 1.15          |
| (1,257) | 1:21:A:PRO:HG3  | 1:23:A:TRP:HZ2  | 6        | 1.15          |
| (2,85)  | 1:24:A:LYS:HG2  | 1:12:A:NLE:HD2  | 10       | 1.14          |
| (2,8)   | 1:29:A:LYS:HG2  | 1:30:A:LYS:H    | 9        | 1.14          |
| (1,262) | 1:25:A:GLN:HG2  | 1:17:A:PHE:HE2  | 10       | 1.14          |
| (3,16)  | 1:19:A:ASN:N    | 1:15:A:SER:O    | 9        | 1.13          |
| (2,84)  | 1:20:A:LEU:HD12 | 1:24:A:LYS:HB2  | 9        | 1.13          |
| (2,4)   | 1:28:A:LEU:HD12 | 1:13:A:THR:H    | 8        | 1.13          |
| (1,318) | 1:22:A:LEU:HD21 | 1:22:A:LEU:HA   | 10       | 1.13          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,262) | 1:25:A:GLN:HG2  | 1:17:A:PHE:HE2  | 6        | 1.13          |
| (3,1)   | 1:7:A:LYS:H     | 1:3:A:ASP:O     | 2        | 1.12          |
| (2,72)  | 1:1:A:LEU:HD11  | 1:6:A:3FB:H     | 2        | 1.12          |
| (1,294) | 1:28:A:LEU:HD23 | 1:17:A:PHE:HD1  | 6        | 1.12          |
| (1,294) | 1:28:A:LEU:HD22 | 1:17:A:PHE:HD1  | 10       | 1.12          |
| (2,84)  | 1:20:A:LEU:HD12 | 1:24:A:LYS:HB2  | 8        | 1.11          |
| (2,7)   | 1:8:A:ALA:HB3   | 1:10:A:PHE:H    | 1        | 1.11          |
| (2,7)   | 1:8:A:ALA:HB2   | 1:10:A:PHE:H    | 3        | 1.11          |
| (1,318) | 1:22:A:LEU:HD21 | 1:22:A:LEU:HA   | 1        | 1.11          |
| (1,134) | 1:17:A:PHE:HB2  | 1:14:A:ARG:HH22 | 3        | 1.11          |
| (1,108) | 1:24:A:LYS:HE3  | 1:23:A:TRP:HH2  | 1        | 1.11          |
| (3,13)  | 1:18:A:ALA:H    | 1:14:A:ARG:O    | 10       | 1.09          |
| (3,16)  | 1:19:A:ASN:N    | 1:15:A:SER:O    | 4        | 1.08          |
| (2,85)  | 1:24:A:LYS:HG3  | 1:13:A:THR:HG22 | 4        | 1.08          |
| (2,23)  | 1:27:A:ASN:HB2  | 1:23:A:TRP:HZ3  | 8        | 1.08          |
| (2,7)   | 1:8:A:ALA:HB2   | 1:10:A:PHE:H    | 7        | 1.08          |
| (1,108) | 1:24:A:LYS:HE3  | 1:23:A:TRP:HH2  | 2        | 1.08          |
| (2,85)  | 1:24:A:LYS:HG2  | 1:12:A:NLE:HD2  | 5        | 1.07          |
| (2,84)  | 1:20:A:LEU:HD13 | 1:16:A:ALA:HB1  | 10       | 1.07          |
| (2,7)   | 1:8:A:ALA:HB1   | 1:10:A:PHE:H    | 2        | 1.07          |
| (2,1)   | 1:28:A:LEU:HD11 | 1:17:A:PHE:H    | 3        | 1.07          |
| (3,8)   | 1:10:A:PHE:N    | 1:6:A:3FB:O     | 9        | 1.06          |
| (2,10)  | 1:28:A:LEU:HB3  | 1:30:A:LYS:H    | 10       | 1.06          |
| (2,1)   | 1:28:A:LEU:HD13 | 1:17:A:PHE:H    | 1        | 1.06          |
| (2,25)  | 1:21:A:PRO:HD3  | 1:23:A:TRP:HH2  | 3        | 1.05          |
| (1,257) | 1:21:A:PRO:HG3  | 1:23:A:TRP:HZ2  | 1        | 1.05          |
| (2,95)  | 1:6:A:3FB:HB1   | 1:13:A:THR:HA   | 8        | 1.04          |
| (1,469) | 1:32:A:LYS:HD3  | 1:32:A:LYS:HA   | 3        | 1.04          |
| (1,290) | 1:9:A:VAL:HG22  | 1:10:A:PHE:HD2  | 10       | 1.04          |
| (2,85)  | 1:24:A:LYS:HG2  | 1:12:A:NLE:HD2  | 9        | 1.03          |
| (2,84)  | 1:20:A:LEU:HD13 | 1:16:A:ALA:HB3  | 3        | 1.03          |
| (2,55)  | 1:32:A:LYS:HD3  | 1:10:A:PHE:HD2  | 3        | 1.03          |
| (1,427) | 1:1:A:LEU:HG    | 1:5:A:ASP:HB2   | 10       | 1.03          |
| (1,360) | 1:28:A:LEU:HD21 | 1:20:A:LEU:HD11 | 6        | 1.03          |
| (1,318) | 1:22:A:LEU:HD22 | 1:22:A:LEU:HA   | 4        | 1.03          |
| (1,54)  | 1:30:A:LYS:HB3  | 1:30:A:LYS:H    | 6        | 1.03          |
| (1,475) | 1:30:A:LYS:HA   | 1:30:A:LYS:HD3  | 8        | 1.02          |
| (1,469) | 1:32:A:LYS:HD2  | 1:32:A:LYS:HA   | 5        | 1.02          |
| (1,223) | 1:13:A:THR:HB   | 1:14:A:ARG:H    | 7        | 1.02          |
| (1,108) | 1:24:A:LYS:HE3  | 1:23:A:TRP:HH2  | 6        | 1.02          |
| (1,54)  | 1:30:A:LYS:HB3  | 1:30:A:LYS:H    | 8        | 1.02          |
| (1,54)  | 1:30:A:LYS:HB3  | 1:30:A:LYS:H    | 9        | 1.02          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (2,24)  | 1:6:A:3FB:HB2   | 1:10:A:PHE:HD2  | 9        | 1.01          |
| (2,23)  | 1:27:A:ASN:HB2  | 1:23:A:TRP:HZ3  | 3        | 1.01          |
| (1,530) | 1:24:A:LYS:HB2  | 1:21:A:PRO:HD3  | 1        | 1.01          |
| (1,108) | 1:24:A:LYS:HE3  | 1:23:A:TRP:HH2  | 5        | 1.01          |
| (1,71)  | 1:4:A:GLU:HG3   | 1:4:A:GLU:H     | 8        | 1.01          |
| (1,54)  | 1:30:A:LYS:HB3  | 1:30:A:LYS:H    | 4        | 1.01          |
| (2,1)   | 1:28:A:LEU:HD11 | 1:17:A:PHE:H    | 4        | 1.0           |
| (1,373) | 1:1:A:LEU:HG    | 1:5:A:ASP:HB3   | 2        | 1.0           |
| (1,360) | 1:28:A:LEU:HD23 | 1:20:A:LEU:HD11 | 10       | 1.0           |
| (1,294) | 1:28:A:LEU:HD21 | 1:17:A:PHE:HD1  | 8        | 1.0           |
| (1,223) | 1:13:A:THR:HB   | 1:14:A:ARG:H    | 9        | 1.0           |
| (1,54)  | 1:30:A:LYS:HB3  | 1:30:A:LYS:H    | 2        | 1.0           |
| (1,54)  | 1:30:A:LYS:HB3  | 1:30:A:LYS:H    | 5        | 1.0           |
| (3,11)  | 1:17:A:PHE:H    | 1:13:A:THR:O    | 5        | 0.99          |
| (2,25)  | 1:21:A:PRO:HD3  | 1:23:A:TRP:HH2  | 4        | 0.99          |
| (1,533) | 1:22:A:LEU:HD22 | 1:26:A:GLN:HG2  | 5        | 0.99          |
| (2,84)  | 1:20:A:LEU:HD11 | 1:24:A:LYS:HB2  | 1        | 0.98          |
| (2,6)   | 1:13:A:THR:HG23 | 1:17:A:PHE:H    | 5        | 0.98          |
| (1,108) | 1:24:A:LYS:HE3  | 1:23:A:TRP:HH2  | 8        | 0.98          |
| (3,15)  | 1:19:A:ASN:H    | 1:15:A:SER:O    | 1        | 0.97          |
| (2,84)  | 1:20:A:LEU:HD13 | 1:16:A:ALA:HB3  | 2        | 0.97          |
| (2,75)  | 1:28:A:LEU:HD21 | 1:6:A:3FB:HE1   | 3        | 0.97          |
| (2,12)  | 1:28:A:LEU:HG   | 1:29:A:LYS:H    | 10       | 0.97          |
| (1,360) | 1:28:A:LEU:HD23 | 1:20:A:LEU:HD12 | 9        | 0.97          |
| (2,84)  | 1:20:A:LEU:HD12 | 1:16:A:ALA:HB3  | 5        | 0.96          |
| (2,76)  | 1:12:A:NLE:HE1  | 1:10:A:PHE:HD1  | 6        | 0.96          |
| (2,12)  | 1:28:A:LEU:HG   | 1:29:A:LYS:H    | 9        | 0.96          |
| (1,352) | 1:20:A:LEU:HD12 | 1:13:A:THR:HG21 | 3        | 0.96          |
| (1,71)  | 1:4:A:GLU:HG2   | 1:4:A:GLU:H     | 10       | 0.96          |
| (2,65)  | 1:22:A:LEU:HD12 | 1:23:A:TRP:HD1  | 7        | 0.95          |
| (2,7)   | 1:8:A:ALA:HB3   | 1:10:A:PHE:H    | 10       | 0.95          |
| (1,374) | 1:8:A:ALA:HB2   | 1:5:A:ASP:HB3   | 3        | 0.95          |
| (1,290) | 1:9:A:VAL:HG21  | 1:10:A:PHE:HD2  | 1        | 0.95          |
| (3,15)  | 1:19:A:ASN:H    | 1:15:A:SER:O    | 3        | 0.94          |
| (2,25)  | 1:21:A:PRO:HD3  | 1:23:A:TRP:HH2  | 2        | 0.94          |
| (1,534) | 1:1:A:LEU:HD23  | 1:5:A:ASP:HB3   | 10       | 0.94          |
| (1,262) | 1:25:A:GLN:HG2  | 1:17:A:PHE:HE1  | 7        | 0.94          |
| (1,71)  | 1:4:A:GLU:HG3   | 1:4:A:GLU:H     | 1        | 0.94          |
| (1,71)  | 1:4:A:GLU:HG2   | 1:4:A:GLU:H     | 2        | 0.94          |
| (1,71)  | 1:4:A:GLU:HG3   | 1:4:A:GLU:H     | 3        | 0.94          |
| (1,71)  | 1:4:A:GLU:HG3   | 1:4:A:GLU:H     | 4        | 0.94          |
| (3,15)  | 1:19:A:ASN:H    | 1:15:A:SER:O    | 7        | 0.93          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (2,17)  | 1:7:A:LYS:HE3   | 1:14:A:ARG:H    | 6        | 0.93          |
| (2,12)  | 1:28:A:LEU:HG   | 1:29:A:LYS:H    | 8        | 0.93          |
| (1,574) | 1:23:A:TRP:HZ3  | 1:27:A:ASN:HD22 | 9        | 0.93          |
| (1,356) | 1:28:A:LEU:HD21 | 1:13:A:THR:HG23 | 8        | 0.93          |
| (1,175) | 1:15:A:SER:HA   | 1:18:A:ALA:H    | 6        | 0.93          |
| (2,10)  | 1:32:A:LYS:HD3  | 1:33:A:GLY:H    | 7        | 0.92          |
| (2,6)   | 1:13:A:THR:HG21 | 1:17:A:PHE:H    | 10       | 0.92          |
| (1,71)  | 1:4:A:GLU:HG3   | 1:4:A:GLU:H     | 6        | 0.92          |
| (1,19)  | 1:13:A:THR:HG22 | 1:14:A:ARG:H    | 7        | 0.91          |
| (3,25)  | 1:30:A:LYS:H    | 1:26:A:GLN:O    | 1        | 0.9           |
| (2,52)  | 1:1:A:LEU:HG    | 1:6:A:3FB:HD2   | 1        | 0.9           |
| (2,33)  | 1:9:A:VAL:H     | 1:7:A:LYS:HA    | 8        | 0.9           |
| (2,10)  | 1:32:A:LYS:HD3  | 1:33:A:GLY:H    | 5        | 0.9           |
| (2,7)   | 1:8:A:ALA:HB1   | 1:10:A:PHE:H    | 8        | 0.9           |
| (1,535) | 1:22:A:LEU:HD22 | 1:26:A:GLN:HG3  | 10       | 0.9           |
| (1,329) | 1:12:A:NLE:HE1  | 1:10:A:PHE:HB2  | 6        | 0.9           |
| (1,71)  | 1:4:A:GLU:HG3   | 1:4:A:GLU:H     | 5        | 0.9           |
| (3,11)  | 1:17:A:PHE:H    | 1:13:A:THR:O    | 1        | 0.89          |
| (2,1)   | 1:28:A:LEU:HD12 | 1:17:A:PHE:H    | 6        | 0.89          |
| (1,554) | 1:23:A:TRP:HE3  | 1:27:A:ASN:HD22 | 5        | 0.89          |
| (1,467) | 1:22:A:LEU:HB2  | 1:21:A:PRO:HA   | 8        | 0.89          |
| (1,29)  | 1:29:A:LYS:HG2  | 1:29:A:LYS:H    | 1        | 0.89          |
| (1,29)  | 1:29:A:LYS:HG2  | 1:29:A:LYS:H    | 8        | 0.89          |
| (2,75)  | 1:28:A:LEU:HD22 | 1:6:A:3FB:HE2   | 4        | 0.88          |
| (2,65)  | 1:22:A:LEU:HD13 | 1:23:A:TRP:HD1  | 6        | 0.88          |
| (1,530) | 1:24:A:LYS:HB2  | 1:21:A:PRO:HD3  | 6        | 0.88          |
| (1,71)  | 1:4:A:GLU:HG2   | 1:4:A:GLU:H     | 7        | 0.88          |
| (3,15)  | 1:19:A:ASN:H    | 1:15:A:SER:O    | 5        | 0.87          |
| (3,15)  | 1:19:A:ASN:H    | 1:15:A:SER:O    | 10       | 0.87          |
| (3,14)  | 1:18:A:ALA:N    | 1:14:A:ARG:O    | 10       | 0.87          |
| (2,13)  | 1:25:A:GLN:HG3  | 1:26:A:GLN:H    | 2        | 0.87          |
| (1,467) | 1:22:A:LEU:HB2  | 1:21:A:PRO:HA   | 9        | 0.87          |
| (1,262) | 1:25:A:GLN:HG2  | 1:17:A:PHE:HE2  | 3        | 0.87          |
| (1,71)  | 1:4:A:GLU:HG2   | 1:4:A:GLU:H     | 9        | 0.87          |
| (1,19)  | 1:13:A:THR:HG21 | 1:14:A:ARG:H    | 4        | 0.87          |
| (1,19)  | 1:13:A:THR:HG21 | 1:14:A:ARG:H    | 9        | 0.87          |
| (2,65)  | 1:22:A:LEU:HD12 | 1:23:A:TRP:HD1  | 3        | 0.86          |
| (2,63)  | 1:13:A:THR:HG22 | 1:10:A:PHE:HE2  | 1        | 0.86          |
| (2,23)  | 1:27:A:ASN:HB2  | 1:23:A:TRP:HZ3  | 1        | 0.86          |
| (1,467) | 1:22:A:LEU:HB2  | 1:21:A:PRO:HA   | 3        | 0.86          |
| (1,467) | 1:22:A:LEU:HB2  | 1:21:A:PRO:HA   | 6        | 0.86          |
| (1,467) | 1:22:A:LEU:HB2  | 1:21:A:PRO:HA   | 7        | 0.86          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,360) | 1:28:A:LEU:HD22 | 1:20:A:LEU:HD11 | 1        | 0.86          |
| (1,294) | 1:28:A:LEU:HD22 | 1:17:A:PHE:HD1  | 2        | 0.86          |
| (1,108) | 1:24:A:LYS:HE3  | 1:23:A:TRP:HH2  | 7        | 0.86          |
| (1,29)  | 1:29:A:LYS:HG3  | 1:29:A:LYS:H    | 2        | 0.86          |
| (1,29)  | 1:29:A:LYS:HG3  | 1:29:A:LYS:H    | 10       | 0.86          |
| (3,11)  | 1:17:A:PHE:H    | 1:13:A:THR:O    | 8        | 0.85          |
| (3,7)   | 1:10:A:PHE:H    | 1:6:A:3FB:O     | 5        | 0.85          |
| (2,33)  | 1:9:A:VAL:H     | 1:7:A:LYS:HA    | 4        | 0.85          |
| (2,23)  | 1:27:A:ASN:HB2  | 1:23:A:TRP:HZ3  | 9        | 0.85          |
| (2,12)  | 1:28:A:LEU:HG   | 1:29:A:LYS:H    | 2        | 0.85          |
| (1,427) | 1:1:A:LEU:HG    | 1:5:A:ASP:HB2   | 7        | 0.85          |
| (1,329) | 1:12:A:NLE:HE3  | 1:10:A:PHE:HB2  | 10       | 0.85          |
| (1,264) | 1:20:A:LEU:HG   | 1:17:A:PHE:HD1  | 6        | 0.85          |
| (1,262) | 1:25:A:GLN:HG2  | 1:17:A:PHE:HE1  | 4        | 0.85          |
| (1,223) | 1:13:A:THR:HB   | 1:14:A:ARG:H    | 4        | 0.85          |
| (2,13)  | 1:25:A:GLN:HG3  | 1:26:A:GLN:H    | 3        | 0.84          |
| (2,13)  | 1:25:A:GLN:HG3  | 1:26:A:GLN:H    | 4        | 0.84          |
| (1,467) | 1:22:A:LEU:HB2  | 1:21:A:PRO:HA   | 2        | 0.84          |
| (1,467) | 1:22:A:LEU:HB2  | 1:21:A:PRO:HA   | 5        | 0.84          |
| (1,352) | 1:20:A:LEU:HD13 | 1:13:A:THR:HG21 | 8        | 0.84          |
| (1,108) | 1:24:A:LYS:HE3  | 1:23:A:TRP:HH2  | 9        | 0.84          |
| (1,29)  | 1:29:A:LYS:HG3  | 1:29:A:LYS:H    | 9        | 0.84          |
| (1,13)  | 1:2:A:SER:H     | 1:1:A:LEU:HG    | 9        | 0.84          |
| (3,1)   | 1:7:A:LYS:H     | 1:3:A:ASP:O     | 9        | 0.83          |
| (2,100) | 1:8:A:ALA:HB2   | 1:9:A:VAL:HA    | 3        | 0.83          |
| (2,63)  | 1:13:A:THR:HG21 | 1:6:A:3FB:HD1   | 7        | 0.83          |
| (2,13)  | 1:25:A:GLN:HG3  | 1:26:A:GLN:H    | 5        | 0.83          |
| (2,13)  | 1:25:A:GLN:HG3  | 1:26:A:GLN:H    | 8        | 0.83          |
| (2,13)  | 1:25:A:GLN:HG3  | 1:26:A:GLN:H    | 10       | 0.83          |
| (2,7)   | 1:8:A:ALA:HB3   | 1:10:A:PHE:H    | 5        | 0.83          |
| (1,323) | 1:28:A:LEU:HD12 | 1:28:A:LEU:HA   | 9        | 0.83          |
| (1,264) | 1:20:A:LEU:HG   | 1:17:A:PHE:HD1  | 4        | 0.83          |
| (1,9)   | 1:34:A:LEU:HD11 | 1:34:A:LEU:H    | 2        | 0.83          |
| (2,100) | 1:8:A:ALA:HB1   | 1:9:A:VAL:HA    | 6        | 0.82          |
| (2,23)  | 1:27:A:ASN:HB2  | 1:23:A:TRP:HZ3  | 10       | 0.82          |
| (2,13)  | 1:25:A:GLN:HG3  | 1:26:A:GLN:H    | 9        | 0.82          |
| (1,327) | 1:20:A:LEU:HD11 | 1:24:A:LYS:HA   | 10       | 0.82          |
| (1,262) | 1:25:A:GLN:HG2  | 1:17:A:PHE:HE2  | 2        | 0.82          |
| (1,9)   | 1:34:A:LEU:HD13 | 1:34:A:LEU:H    | 3        | 0.82          |
| (3,29)  | 1:32:A:LYS:H    | 1:28:A:LEU:O    | 3        | 0.81          |
| (2,100) | 1:8:A:ALA:HB3   | 1:9:A:VAL:HA    | 1        | 0.81          |
| (2,13)  | 1:25:A:GLN:HG3  | 1:26:A:GLN:H    | 7        | 0.81          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,530) | 1:24:A:LYS:HB2  | 1:21:A:PRO:HD3  | 10       | 0.81          |
| (1,286) | 1:20:A:LEU:HD11 | 1:17:A:PHE:HE1  | 4        | 0.81          |
| (1,108) | 1:24:A:LYS:HE3  | 1:23:A:TRP:HH2  | 4        | 0.81          |
| (3,12)  | 1:17:A:PHE:N    | 1:13:A:THR:O    | 5        | 0.8           |
| (3,2)   | 1:7:A:LYS:N     | 1:3:A:ASP:O     | 2        | 0.8           |
| (2,33)  | 1:9:A:VAL:H     | 1:7:A:LYS:HA    | 10       | 0.8           |
| (2,12)  | 1:29:A:LYS:HD3  | 1:29:A:LYS:H    | 6        | 0.8           |
| (1,472) | 1:8:A:ALA:HB2   | 1:5:A:ASP:HA    | 3        | 0.8           |
| (1,265) | 1:28:A:LEU:HG   | 1:17:A:PHE:HD1  | 10       | 0.8           |
| (3,11)  | 1:17:A:PHE:H    | 1:13:A:THR:O    | 10       | 0.79          |
| (3,10)  | 1:16:A:ALA:N    | 1:12:A:NLE:O    | 4        | 0.79          |
| (3,7)   | 1:10:A:PHE:H    | 1:6:A:3FB:O     | 10       | 0.79          |
| (2,17)  | 1:7:A:LYS:HE2   | 1:14:A:ARG:H    | 4        | 0.79          |
| (1,427) | 1:1:A:LEU:HG    | 1:5:A:ASP:HB2   | 5        | 0.79          |
| (1,329) | 1:12:A:NLE:HE1  | 1:10:A:PHE:HB2  | 2        | 0.79          |
| (1,323) | 1:28:A:LEU:HD11 | 1:28:A:LEU:HA   | 4        | 0.79          |
| (1,319) | 1:22:A:LEU:HD13 | 1:22:A:LEU:HA   | 5        | 0.79          |
| (2,94)  | 1:35:A:PHE:HB3  | 1:32:A:LYS:HA   | 8        | 0.78          |
| (1,332) | 1:20:A:LEU:HD12 | 1:21:A:PRO:HD3  | 8        | 0.78          |
| (1,327) | 1:20:A:LEU:HD13 | 1:24:A:LYS:HA   | 4        | 0.78          |
| (1,265) | 1:28:A:LEU:HG   | 1:17:A:PHE:HD1  | 9        | 0.78          |
| (1,9)   | 1:34:A:LEU:HD12 | 1:34:A:LEU:H    | 1        | 0.78          |
| (2,13)  | 1:25:A:GLN:HG3  | 1:26:A:GLN:H    | 1        | 0.77          |
| (1,319) | 1:22:A:LEU:HD12 | 1:22:A:LEU:HA   | 6        | 0.77          |
| (1,266) | 1:1:A:LEU:HG    | 1:6:A:3FB:HE2   | 1        | 0.77          |
| (1,262) | 1:25:A:GLN:HG2  | 1:17:A:PHE:HE2  | 5        | 0.77          |
| (2,100) | 1:8:A:ALA:HB1   | 1:9:A:VAL:HA    | 2        | 0.76          |
| (2,100) | 1:8:A:ALA:HB3   | 1:9:A:VAL:HA    | 5        | 0.76          |
| (2,84)  | 1:20:A:LEU:HD12 | 1:16:A:ALA:HB2  | 4        | 0.76          |
| (1,323) | 1:28:A:LEU:HD12 | 1:28:A:LEU:HA   | 8        | 0.76          |
| (1,319) | 1:22:A:LEU:HD13 | 1:22:A:LEU:HA   | 2        | 0.76          |
| (1,319) | 1:22:A:LEU:HD11 | 1:22:A:LEU:HA   | 7        | 0.76          |
| (1,262) | 1:25:A:GLN:HG2  | 1:17:A:PHE:HE1  | 1        | 0.76          |
| (1,25)  | 1:14:A:ARG:HG2  | 1:15:A:SER:H    | 6        | 0.76          |
| (2,23)  | 1:27:A:ASN:HB2  | 1:23:A:TRP:HZ3  | 2        | 0.75          |
| (1,290) | 1:9:A:VAL:HG22  | 1:10:A:PHE:HD2  | 3        | 0.75          |
| (1,153) | 1:16:A:ALA:HA   | 1:19:A:ASN:HD22 | 9        | 0.75          |
| (2,86)  | 1:1:A:LEU:HD22  | 1:34:A:LEU:HB2  | 4        | 0.74          |
| (2,65)  | 1:22:A:LEU:HD11 | 1:23:A:TRP:HD1  | 2        | 0.74          |
| (2,13)  | 1:25:A:GLN:HG3  | 1:26:A:GLN:H    | 6        | 0.74          |
| (1,323) | 1:28:A:LEU:HD11 | 1:28:A:LEU:HA   | 3        | 0.74          |
| (1,323) | 1:28:A:LEU:HD13 | 1:28:A:LEU:HA   | 7        | 0.74          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (2,60)  | 1:18:A:ALA:HB3  | 1:20:A:LEU:H    | 3        | 0.73          |
| (1,554) | 1:23:A:TRP:HE3  | 1:27:A:ASN:HD22 | 3        | 0.73          |
| (1,427) | 1:1:A:LEU:HG    | 1:5:A:ASP:HB2   | 4        | 0.73          |
| (1,323) | 1:28:A:LEU:HD11 | 1:28:A:LEU:HA   | 6        | 0.73          |
| (1,323) | 1:28:A:LEU:HD12 | 1:28:A:LEU:HA   | 10       | 0.73          |
| (1,319) | 1:22:A:LEU:HD13 | 1:22:A:LEU:HA   | 8        | 0.73          |
| (1,319) | 1:22:A:LEU:HD13 | 1:22:A:LEU:HA   | 9        | 0.73          |
| (1,294) | 1:28:A:LEU:HD22 | 1:17:A:PHE:HD1  | 9        | 0.73          |
| (3,6)   | 1:9:A:VAL:N     | 1:5:A:ASP:O     | 3        | 0.72          |
| (2,100) | 1:8:A:ALA:HB2   | 1:9:A:VAL:HA    | 4        | 0.72          |
| (2,1)   | 1:28:A:LEU:HD13 | 1:17:A:PHE:H    | 7        | 0.72          |
| (1,530) | 1:24:A:LYS:HB2  | 1:21:A:PRO:HD3  | 2        | 0.72          |
| (1,323) | 1:28:A:LEU:HD12 | 1:28:A:LEU:HA   | 5        | 0.72          |
| (1,286) | 1:20:A:LEU:HD12 | 1:17:A:PHE:HE1  | 6        | 0.72          |
| (1,257) | 1:21:A:PRO:HG3  | 1:23:A:TRP:HZ2  | 3        | 0.72          |
| (1,257) | 1:21:A:PRO:HG3  | 1:23:A:TRP:HZ2  | 10       | 0.72          |
| (1,11)  | 1:1:A:LEU:HD12  | 1:2:A:SER:H     | 3        | 0.72          |
| (3,11)  | 1:17:A:PHE:H    | 1:13:A:THR:O    | 2        | 0.71          |
| (2,102) | 1:29:A:LYS:HB2  | 1:29:A:LYS:HE3  | 2        | 0.71          |
| (2,102) | 1:30:A:LYS:HB3  | 1:30:A:LYS:HE3  | 5        | 0.71          |
| (2,100) | 1:8:A:ALA:HB2   | 1:9:A:VAL:HA    | 7        | 0.71          |
| (2,20)  | 1:10:A:PHE:HB3  | 1:13:A:THR:H    | 2        | 0.71          |
| (1,319) | 1:22:A:LEU:HD11 | 1:22:A:LEU:HA   | 3        | 0.71          |
| (1,18)  | 1:14:A:ARG:HG3  | 1:14:A:ARG:H    | 1        | 0.71          |
| (1,16)  | 1:22:A:LEU:HG   | 1:22:A:LEU:H    | 4        | 0.71          |
| (2,102) | 1:30:A:LYS:HB3  | 1:30:A:LYS:HE3  | 10       | 0.7           |
| (2,63)  | 1:13:A:THR:HG22 | 1:6:A:3FB:HD1   | 3        | 0.7           |
| (2,52)  | 1:28:A:LEU:HG   | 1:17:A:PHE:HE1  | 5        | 0.7           |
| (2,24)  | 1:6:A:3FB:HB2   | 1:10:A:PHE:HD2  | 8        | 0.7           |
| (2,1)   | 1:28:A:LEU:HD12 | 1:17:A:PHE:H    | 2        | 0.7           |
| (1,332) | 1:20:A:LEU:HD13 | 1:21:A:PRO:HD3  | 5        | 0.7           |
| (1,262) | 1:25:A:GLN:HG2  | 1:17:A:PHE:HE1  | 9        | 0.7           |
| (1,73)  | 1:31:A:GLU:HG2  | 1:31:A:GLU:H    | 5        | 0.7           |
| (1,42)  | 1:32:A:LYS:HB3  | 1:33:A:GLY:H    | 7        | 0.7           |
| (3,25)  | 1:30:A:LYS:H    | 1:26:A:GLN:O    | 6        | 0.69          |
| (2,100) | 1:8:A:ALA:HB2   | 1:9:A:VAL:HA    | 9        | 0.69          |
| (2,85)  | 1:24:A:LYS:HG2  | 1:12:A:NLE:HD2  | 3        | 0.69          |
| (1,360) | 1:28:A:LEU:HD23 | 1:20:A:LEU:HD11 | 2        | 0.69          |
| (1,323) | 1:28:A:LEU:HD13 | 1:28:A:LEU:HA   | 1        | 0.69          |
| (1,323) | 1:28:A:LEU:HD11 | 1:28:A:LEU:HA   | 2        | 0.69          |
| (1,16)  | 1:22:A:LEU:HG   | 1:22:A:LEU:H    | 1        | 0.69          |
| (3,12)  | 1:17:A:PHE:N    | 1:13:A:THR:O    | 8        | 0.68          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (2,9)   | 1:30:A:LYS:HG2  | 1:30:A:LYS:H    | 10       | 0.68          |
| (1,373) | 1:1:A:LEU:HG    | 1:5:A:ASP:HB3   | 1        | 0.68          |
| (1,264) | 1:20:A:LEU:HG   | 1:17:A:PHE:HD1  | 7        | 0.68          |
| (3,12)  | 1:17:A:PHE:N    | 1:13:A:THR:O    | 1        | 0.67          |
| (2,100) | 1:8:A:ALA:HB3   | 1:9:A:VAL:HA    | 10       | 0.67          |
| (2,94)  | 1:35:A:PHE:HB3  | 1:32:A:LYS:HA   | 3        | 0.67          |
| (2,60)  | 1:18:A:ALA:HB3  | 1:20:A:LEU:H    | 7        | 0.67          |
| (2,60)  | 1:18:A:ALA:HB3  | 1:20:A:LEU:H    | 9        | 0.67          |
| (2,33)  | 1:9:A:VAL:H     | 1:7:A:LYS:HA    | 7        | 0.67          |
| (1,265) | 1:28:A:LEU:HG   | 1:17:A:PHE:HD1  | 4        | 0.67          |
| (2,102) | 1:30:A:LYS:HB3  | 1:30:A:LYS:HE3  | 1        | 0.66          |
| (2,86)  | 1:1:A:LEU:HD23  | 1:34:A:LEU:HB2  | 6        | 0.66          |
| (2,33)  | 1:9:A:VAL:H     | 1:7:A:LYS:HA    | 5        | 0.66          |
| (2,12)  | 1:29:A:LYS:HD3  | 1:29:A:LYS:H    | 4        | 0.66          |
| (1,533) | 1:22:A:LEU:HD23 | 1:26:A:GLN:HG2  | 4        | 0.66          |
| (1,530) | 1:24:A:LYS:HB2  | 1:21:A:PRO:HD3  | 4        | 0.66          |
| (1,329) | 1:12:A:NLE:HE2  | 1:10:A:PHE:HB2  | 4        | 0.66          |
| (1,286) | 1:20:A:LEU:HD11 | 1:17:A:PHE:HE1  | 7        | 0.66          |
| (1,130) | 1:17:A:PHE:HB2  | 1:17:A:PHE:HE1  | 8        | 0.66          |
| (2,100) | 1:8:A:ALA:HB1   | 1:9:A:VAL:HA    | 8        | 0.65          |
| (2,85)  | 1:24:A:LYS:HG2  | 1:12:A:NLE:HD2  | 8        | 0.65          |
| (2,65)  | 1:22:A:LEU:HD11 | 1:23:A:TRP:HD1  | 8        | 0.65          |
| (2,33)  | 1:9:A:VAL:H     | 1:7:A:LYS:HA    | 9        | 0.65          |
| (2,23)  | 1:27:A:ASN:HB2  | 1:23:A:TRP:HZ3  | 6        | 0.65          |
| (1,294) | 1:28:A:LEU:HD23 | 1:17:A:PHE:HD1  | 5        | 0.65          |
| (1,156) | 1:24:A:LYS:HA   | 1:27:A:ASN:HD22 | 2        | 0.65          |
| (1,130) | 1:17:A:PHE:HB2  | 1:17:A:PHE:HE1  | 9        | 0.65          |
| (1,130) | 1:17:A:PHE:HB2  | 1:17:A:PHE:HE1  | 10       | 0.65          |
| (2,24)  | 1:6:A:3FB:HB2   | 1:10:A:PHE:HD2  | 4        | 0.64          |
| (1,493) | 1:7:A:LYS:HD3   | 1:7:A:LYS:HA    | 6        | 0.64          |
| (1,331) | 1:24:A:LYS:HG2  | 1:21:A:PRO:HD3  | 1        | 0.64          |
| (1,130) | 1:17:A:PHE:HB2  | 1:17:A:PHE:HE1  | 4        | 0.64          |
| (1,130) | 1:17:A:PHE:HB2  | 1:17:A:PHE:HE1  | 7        | 0.64          |
| (1,42)  | 1:32:A:LYS:HB3  | 1:33:A:GLY:H    | 9        | 0.64          |
| (1,35)  | 1:32:A:LYS:HG3  | 1:32:A:LYS:H    | 6        | 0.64          |
| (1,16)  | 1:22:A:LEU:HG   | 1:22:A:LEU:H    | 10       | 0.64          |
| (3,11)  | 1:17:A:PHE:H    | 1:13:A:THR:O    | 3        | 0.63          |
| (2,65)  | 1:22:A:LEU:HD11 | 1:23:A:TRP:HD1  | 5        | 0.63          |
| (2,65)  | 1:22:A:LEU:HD11 | 1:23:A:TRP:HD1  | 9        | 0.63          |
| (2,12)  | 1:29:A:LYS:HD2  | 1:29:A:LYS:H    | 3        | 0.63          |
| (2,12)  | 1:29:A:LYS:HD3  | 1:29:A:LYS:H    | 7        | 0.63          |
| (1,574) | 1:23:A:TRP:HZ3  | 1:27:A:ASN:HD22 | 5        | 0.63          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,290) | 1:9:A:VAL:HG21  | 1:10:A:PHE:HD2  | 8        | 0.63          |
| (1,130) | 1:17:A:PHE:HB2  | 1:17:A:PHE:HE1  | 1        | 0.63          |
| (3,25)  | 1:30:A:LYS:H    | 1:26:A:GLN:O    | 4        | 0.62          |
| (2,60)  | 1:18:A:ALA:HB1  | 1:20:A:LEU:H    | 2        | 0.62          |
| (2,60)  | 1:16:A:ALA:HB2  | 1:20:A:LEU:H    | 6        | 0.62          |
| (2,60)  | 1:18:A:ALA:HB2  | 1:20:A:LEU:H    | 10       | 0.62          |
| (1,529) | 1:12:A:NLE:HG3  | 1:10:A:PHE:HB2  | 10       | 0.62          |
| (1,513) | 1:32:A:LYS:HB2  | 1:35:A:PHE:HB3  | 5        | 0.62          |
| (1,426) | 1:22:A:LEU:HG   | 1:22:A:LEU:HB3  | 10       | 0.62          |
| (1,257) | 1:21:A:PRO:HG3  | 1:23:A:TRP:HZ2  | 2        | 0.62          |
| (1,130) | 1:17:A:PHE:HB2  | 1:17:A:PHE:HE1  | 5        | 0.62          |
| (2,60)  | 1:18:A:ALA:HB3  | 1:20:A:LEU:H    | 1        | 0.61          |
| (2,33)  | 1:9:A:VAL:H     | 1:7:A:LYS:HA    | 2        | 0.61          |
| (2,10)  | 1:32:A:LYS:HD2  | 1:33:A:GLY:H    | 4        | 0.61          |
| (1,426) | 1:22:A:LEU:HG   | 1:22:A:LEU:HB3  | 1        | 0.61          |
| (1,254) | 1:20:A:LEU:HB2  | 1:25:A:GLN:HE22 | 4        | 0.61          |
| (1,130) | 1:17:A:PHE:HB2  | 1:17:A:PHE:HE1  | 2        | 0.61          |
| (1,130) | 1:17:A:PHE:HB2  | 1:17:A:PHE:HE1  | 3        | 0.61          |
| (1,130) | 1:17:A:PHE:HB2  | 1:17:A:PHE:HE1  | 6        | 0.61          |
| (2,60)  | 1:18:A:ALA:HB1  | 1:20:A:LEU:H    | 5        | 0.6           |
| (1,467) | 1:22:A:LEU:HB2  | 1:21:A:PRO:HA   | 1        | 0.6           |
| (1,426) | 1:22:A:LEU:HG   | 1:22:A:LEU:HB2  | 5        | 0.6           |
| (1,356) | 1:28:A:LEU:HD22 | 1:13:A:THR:HG23 | 2        | 0.6           |
| (1,17)  | 1:14:A:ARG:HB3  | 1:14:A:ARG:H    | 6        | 0.6           |
| (3,13)  | 1:18:A:ALA:H    | 1:14:A:ARG:O    | 5        | 0.59          |
| (3,7)   | 1:10:A:PHE:H    | 1:6:A:3FB:O     | 8        | 0.59          |
| (2,9)   | 1:30:A:LYS:HG2  | 1:30:A:LYS:H    | 1        | 0.59          |
| (1,581) | 1:34:A:LEU:H    | 1:35:A:PHE:H    | 2        | 0.59          |
| (1,426) | 1:22:A:LEU:HG   | 1:22:A:LEU:HB2  | 6        | 0.59          |
| (1,360) | 1:28:A:LEU:HD22 | 1:20:A:LEU:HD11 | 3        | 0.59          |
| (1,332) | 1:20:A:LEU:HD13 | 1:21:A:PRO:HD3  | 4        | 0.59          |
| (1,27)  | 1:7:A:LYS:HG3   | 1:8:A:ALA:H     | 8        | 0.59          |
| (1,8)   | 1:28:A:LEU:HD12 | 1:29:A:LYS:H    | 6        | 0.59          |
| (2,84)  | 1:20:A:LEU:HD12 | 1:16:A:ALA:HB2  | 7        | 0.58          |
| (2,78)  | 1:9:A:VAL:HG23  | 1:8:A:ALA:HA    | 10       | 0.58          |
| (1,533) | 1:22:A:LEU:HD22 | 1:26:A:GLN:HG2  | 1        | 0.58          |
| (1,493) | 1:7:A:LYS:HD3   | 1:7:A:LYS:HA    | 7        | 0.58          |
| (1,426) | 1:22:A:LEU:HG   | 1:22:A:LEU:HB2  | 2        | 0.58          |
| (1,426) | 1:22:A:LEU:HG   | 1:22:A:LEU:HB3  | 4        | 0.58          |
| (1,426) | 1:22:A:LEU:HG   | 1:22:A:LEU:HB2  | 7        | 0.58          |
| (1,360) | 1:28:A:LEU:HD21 | 1:20:A:LEU:HD13 | 4        | 0.58          |
| (1,17)  | 1:14:A:ARG:HB3  | 1:14:A:ARG:H    | 5        | 0.58          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (3,16)  | 1:19:A:ASN:N    | 1:15:A:SER:O    | 1        | 0.57          |
| (3,12)  | 1:17:A:PHE:N    | 1:13:A:THR:O    | 2        | 0.57          |
| (2,52)  | 1:1:A:LEU:HG    | 1:6:A:3FB:HD2   | 7        | 0.57          |
| (2,24)  | 1:6:A:3FB:HB2   | 1:10:A:PHE:HD2  | 7        | 0.57          |
| (1,426) | 1:22:A:LEU:HG   | 1:22:A:LEU:HB2  | 8        | 0.57          |
| (1,373) | 1:1:A:LEU:HG    | 1:5:A:ASP:HB3   | 6        | 0.57          |
| (1,327) | 1:20:A:LEU:HD11 | 1:24:A:LYS:HA   | 1        | 0.57          |
| (1,264) | 1:20:A:LEU:HG   | 1:17:A:PHE:HD1  | 3        | 0.57          |
| (1,257) | 1:21:A:PRO:HG3  | 1:23:A:TRP:HZ2  | 4        | 0.57          |
| (1,217) | 1:2:A:SER:HB2   | 1:3:A:ASP:H     | 2        | 0.57          |
| (1,165) | 1:13:A:THR:H    | 1:11:A:GLY:HA3  | 5        | 0.57          |
| (1,156) | 1:24:A:LYS:HA   | 1:27:A:ASN:HD22 | 4        | 0.57          |
| (1,107) | 1:24:A:LYS:HE2  | 1:23:A:TRP:HH2  | 2        | 0.57          |
| (2,86)  | 1:1:A:LEU:HD22  | 1:34:A:LEU:HB3  | 9        | 0.56          |
| (2,78)  | 1:9:A:VAL:HG21  | 1:8:A:ALA:HA    | 4        | 0.56          |
| (1,467) | 1:22:A:LEU:HB2  | 1:21:A:PRO:HA   | 10       | 0.56          |
| (1,426) | 1:22:A:LEU:HG   | 1:22:A:LEU:HB2  | 3        | 0.56          |
| (1,426) | 1:22:A:LEU:HG   | 1:22:A:LEU:HB2  | 9        | 0.56          |
| (1,415) | 1:19:A:ASN:HB3  | 1:16:A:ALA:HA   | 6        | 0.56          |
| (1,266) | 1:1:A:LEU:HG    | 1:6:A:3FB:HE1   | 4        | 0.56          |
| (1,264) | 1:20:A:LEU:HG   | 1:17:A:PHE:HD1  | 2        | 0.56          |
| (1,17)  | 1:14:A:ARG:HB3  | 1:14:A:ARG:H    | 8        | 0.56          |
| (1,17)  | 1:14:A:ARG:HB3  | 1:14:A:ARG:H    | 10       | 0.56          |
| (3,13)  | 1:18:A:ALA:H    | 1:14:A:ARG:O    | 1        | 0.55          |
| (2,33)  | 1:9:A:VAL:H     | 1:7:A:LYS:HA    | 1        | 0.55          |
| (2,25)  | 1:21:A:PRO:HD3  | 1:23:A:TRP:HH2  | 9        | 0.55          |
| (1,332) | 1:20:A:LEU:HD11 | 1:21:A:PRO:HD3  | 3        | 0.55          |
| (1,107) | 1:24:A:LYS:HE2  | 1:23:A:TRP:HH2  | 5        | 0.55          |
| (1,17)  | 1:14:A:ARG:HB3  | 1:14:A:ARG:H    | 2        | 0.55          |
| (3,27)  | 1:31:A:GLU:H    | 1:27:A:ASN:O    | 6        | 0.54          |
| (3,16)  | 1:19:A:ASN:N    | 1:15:A:SER:O    | 7        | 0.54          |
| (3,15)  | 1:19:A:ASN:H    | 1:15:A:SER:O    | 2        | 0.54          |
| (2,78)  | 1:34:A:LEU:HD11 | 1:1:A:LEU:HA    | 8        | 0.54          |
| (2,75)  | 1:28:A:LEU:HD23 | 1:14:A:ARG:HH21 | 5        | 0.54          |
| (2,55)  | 1:32:A:LYS:HD3  | 1:10:A:PHE:HD2  | 1        | 0.54          |
| (2,30)  | 1:26:A:GLN:HA   | 1:17:A:PHE:HE1  | 8        | 0.54          |
| (2,25)  | 1:21:A:PRO:HD3  | 1:23:A:TRP:HH2  | 7        | 0.54          |
| (2,17)  | 1:7:A:LYS:HE2   | 1:14:A:ARG:H    | 3        | 0.54          |
| (2,12)  | 1:29:A:LYS:HD2  | 1:29:A:LYS:H    | 5        | 0.54          |
| (2,10)  | 1:32:A:LYS:HD2  | 1:33:A:GLY:H    | 3        | 0.54          |
| (1,581) | 1:34:A:LEU:H    | 1:35:A:PHE:H    | 6        | 0.54          |
| (1,530) | 1:24:A:LYS:HB2  | 1:21:A:PRO:HD3  | 7        | 0.54          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,351) | 1:20:A:LEU:HD12 | 1:12:A:NLE:HD2  | 5        | 0.54          |
| (1,327) | 1:20:A:LEU:HD12 | 1:24:A:LYS:HA   | 9        | 0.54          |
| (1,264) | 1:20:A:LEU:HG   | 1:17:A:PHE:HD1  | 10       | 0.54          |
| (1,134) | 1:17:A:PHE:HB2  | 1:14:A:ARG:HH22 | 7        | 0.54          |
| (1,109) | 1:19:A:ASN:HB3  | 1:19:A:ASN:HD22 | 4        | 0.54          |
| (3,15)  | 1:19:A:ASN:H    | 1:15:A:SER:O    | 8        | 0.53          |
| (2,94)  | 1:35:A:PHE:HB3  | 1:32:A:LYS:HA   | 7        | 0.53          |
| (2,10)  | 1:32:A:LYS:HD2  | 1:33:A:GLY:H    | 2        | 0.53          |
| (1,467) | 1:22:A:LEU:HB2  | 1:21:A:PRO:HA   | 4        | 0.53          |
| (1,332) | 1:20:A:LEU:HD11 | 1:21:A:PRO:HD3  | 2        | 0.53          |
| (1,254) | 1:20:A:LEU:HB2  | 1:25:A:GLN:HE22 | 10       | 0.53          |
| (1,165) | 1:13:A:THR:H    | 1:11:A:GLY:HA3  | 2        | 0.53          |
| (1,109) | 1:19:A:ASN:HB3  | 1:19:A:ASN:HD22 | 2        | 0.53          |
| (1,109) | 1:19:A:ASN:HB3  | 1:19:A:ASN:HD22 | 10       | 0.53          |
| (1,89)  | 1:10:A:PHE:HB3  | 1:10:A:PHE:H    | 8        | 0.53          |
| (1,17)  | 1:14:A:ARG:HB3  | 1:14:A:ARG:H    | 3        | 0.53          |
| (3,12)  | 1:17:A:PHE:N    | 1:13:A:THR:O    | 10       | 0.52          |
| (3,8)   | 1:10:A:PHE:N    | 1:6:A:3FB:O     | 10       | 0.52          |
| (2,4)   | 1:1:A:LEU:HD23  | 1:33:A:GLY:H    | 5        | 0.52          |
| (1,265) | 1:28:A:LEU:HG   | 1:17:A:PHE:HD1  | 8        | 0.52          |
| (1,109) | 1:19:A:ASN:HB3  | 1:19:A:ASN:HD22 | 1        | 0.52          |
| (1,109) | 1:19:A:ASN:HB3  | 1:19:A:ASN:HD22 | 3        | 0.52          |
| (1,109) | 1:19:A:ASN:HB3  | 1:19:A:ASN:HD22 | 5        | 0.52          |
| (1,109) | 1:19:A:ASN:HB3  | 1:19:A:ASN:HD22 | 6        | 0.52          |
| (1,109) | 1:19:A:ASN:HB3  | 1:19:A:ASN:HD22 | 7        | 0.52          |
| (1,109) | 1:19:A:ASN:HB3  | 1:19:A:ASN:HD22 | 8        | 0.52          |
| (2,78)  | 1:9:A:VAL:HG22  | 1:8:A:ALA:HA    | 6        | 0.51          |
| (2,58)  | 1:18:A:ALA:HB2  | 1:25:A:GLN:HE22 | 9        | 0.51          |
| (1,332) | 1:20:A:LEU:HD11 | 1:21:A:PRO:HD3  | 1        | 0.51          |
| (1,332) | 1:20:A:LEU:HD11 | 1:21:A:PRO:HD3  | 6        | 0.51          |
| (1,290) | 1:9:A:VAL:HG22  | 1:10:A:PHE:HD2  | 5        | 0.51          |
| (1,89)  | 1:10:A:PHE:HB3  | 1:10:A:PHE:H    | 5        | 0.51          |
| (2,95)  | 1:6:A:3FB:HB1   | 1:32:A:LYS:HA   | 5        | 0.5           |
| (2,75)  | 1:28:A:LEU:HD21 | 1:6:A:3FB:HE2   | 8        | 0.5           |
| (2,60)  | 1:18:A:ALA:HB1  | 1:20:A:LEU:H    | 8        | 0.5           |
| (2,41)  | 1:12:A:NLE:HA   | 1:13:A:THR:H    | 6        | 0.5           |
| (2,16)  | 1:20:A:LEU:HB2  | 1:18:A:ALA:H    | 3        | 0.5           |
| (1,530) | 1:24:A:LYS:HB2  | 1:21:A:PRO:HD3  | 8        | 0.5           |
| (1,329) | 1:12:A:NLE:HE2  | 1:10:A:PHE:HB2  | 8        | 0.5           |
| (1,165) | 1:13:A:THR:H    | 1:11:A:GLY:HA3  | 3        | 0.5           |
| (1,107) | 1:24:A:LYS:HE2  | 1:23:A:TRP:HH2  | 6        | 0.5           |
| (1,35)  | 1:32:A:LYS:HG2  | 1:32:A:LYS:H    | 5        | 0.5           |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (2,24)  | 1:35:A:PHE:HB3  | 1:14:A:ARG:HH21 | 6        | 0.49          |
| (1,530) | 1:24:A:LYS:HB2  | 1:21:A:PRO:HD3  | 3        | 0.49          |
| (1,376) | 1:12:A:NLE:HD2  | 1:12:A:NLE:HB3  | 9        | 0.49          |
| (1,360) | 1:28:A:LEU:HD22 | 1:20:A:LEU:HD13 | 7        | 0.49          |
| (3,16)  | 1:19:A:ASN:N    | 1:15:A:SER:O    | 10       | 0.48          |
| (3,10)  | 1:16:A:ALA:N    | 1:12:A:NLE:O    | 7        | 0.48          |
| (3,10)  | 1:16:A:ALA:N    | 1:12:A:NLE:O    | 9        | 0.48          |
| (3,8)   | 1:10:A:PHE:N    | 1:6:A:3FB:O     | 5        | 0.48          |
| (3,1)   | 1:7:A:LYS:H     | 1:3:A:ASP:O     | 8        | 0.48          |
| (2,41)  | 1:12:A:NLE:HA   | 1:13:A:THR:H    | 7        | 0.48          |
| (2,16)  | 1:20:A:LEU:HB2  | 1:18:A:ALA:H    | 4        | 0.48          |
| (2,4)   | 1:12:A:NLE:HE2  | 1:13:A:THR:H    | 9        | 0.48          |
| (1,530) | 1:24:A:LYS:HB2  | 1:21:A:PRO:HD3  | 9        | 0.48          |
| (1,529) | 1:12:A:NLE:HG3  | 1:10:A:PHE:HB2  | 6        | 0.48          |
| (1,332) | 1:20:A:LEU:HD13 | 1:21:A:PRO:HD3  | 7        | 0.48          |
| (1,332) | 1:20:A:LEU:HD11 | 1:21:A:PRO:HD3  | 10       | 0.48          |
| (1,294) | 1:28:A:LEU:HD21 | 1:17:A:PHE:HD1  | 7        | 0.48          |
| (1,265) | 1:28:A:LEU:HG   | 1:17:A:PHE:HD1  | 6        | 0.48          |
| (1,191) | 1:34:A:LEU:HA   | 1:35:A:PHE:H    | 7        | 0.48          |
| (1,89)  | 1:10:A:PHE:HB3  | 1:10:A:PHE:H    | 1        | 0.48          |
| (1,89)  | 1:10:A:PHE:HB3  | 1:10:A:PHE:H    | 2        | 0.48          |
| (1,89)  | 1:10:A:PHE:HB3  | 1:10:A:PHE:H    | 6        | 0.48          |
| (1,35)  | 1:32:A:LYS:HG3  | 1:32:A:LYS:H    | 2        | 0.48          |
| (3,26)  | 1:30:A:LYS:N    | 1:26:A:GLN:O    | 1        | 0.47          |
| (3,16)  | 1:19:A:ASN:N    | 1:15:A:SER:O    | 5        | 0.47          |
| (2,41)  | 1:12:A:NLE:HA   | 1:13:A:THR:H    | 9        | 0.47          |
| (2,10)  | 1:32:A:LYS:HD2  | 1:33:A:GLY:H    | 6        | 0.47          |
| (1,533) | 1:22:A:LEU:HD22 | 1:26:A:GLN:HG2  | 7        | 0.47          |
| (1,254) | 1:20:A:LEU:HB2  | 1:25:A:GLN:HE22 | 5        | 0.47          |
| (1,254) | 1:20:A:LEU:HB2  | 1:25:A:GLN:HE22 | 6        | 0.47          |
| (3,12)  | 1:17:A:PHE:N    | 1:13:A:THR:O    | 3        | 0.46          |
| (2,78)  | 1:9:A:VAL:HG23  | 1:8:A:ALA:HA    | 9        | 0.46          |
| (2,58)  | 1:18:A:ALA:HB2  | 1:25:A:GLN:HE22 | 7        | 0.46          |
| (2,8)   | 1:16:A:ALA:HB1  | 1:13:A:THR:H    | 1        | 0.46          |
| (1,535) | 1:22:A:LEU:HD21 | 1:26:A:GLN:HG3  | 8        | 0.46          |
| (1,530) | 1:24:A:LYS:HB2  | 1:21:A:PRO:HD3  | 5        | 0.46          |
| (1,452) | 1:26:A:GLN:HG2  | 1:23:A:TRP:HA   | 6        | 0.46          |
| (1,329) | 1:12:A:NLE:HE1  | 1:10:A:PHE:HB2  | 3        | 0.46          |
| (1,329) | 1:12:A:NLE:HE2  | 1:10:A:PHE:HB2  | 7        | 0.46          |
| (1,254) | 1:20:A:LEU:HB2  | 1:25:A:GLN:HE22 | 7        | 0.46          |
| (1,217) | 1:2:A:SER:HB2   | 1:3:A:ASP:H     | 7        | 0.46          |
| (1,92)  | 1:17:A:PHE:HB2  | 1:18:A:ALA:H    | 9        | 0.46          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,89)  | 1:10:A:PHE:HB3  | 1:10:A:PHE:H   | 4        | 0.46          |
| (1,89)  | 1:10:A:PHE:HB3  | 1:10:A:PHE:H   | 10       | 0.46          |
| (1,82)  | 1:6:A:3FB:HB1   | 1:7:A:LYS:H    | 10       | 0.46          |
| (1,61)  | 1:31:A:GLU:HB2  | 1:30:A:LYS:H   | 7        | 0.46          |
| (2,105) | 1:23:A:TRP:HH2  | 1:23:A:TRP:HE3 | 2        | 0.45          |
| (2,105) | 1:23:A:TRP:HH2  | 1:23:A:TRP:HE3 | 4        | 0.45          |
| (2,105) | 1:23:A:TRP:HH2  | 1:23:A:TRP:HE3 | 5        | 0.45          |
| (2,105) | 1:23:A:TRP:HH2  | 1:23:A:TRP:HE3 | 7        | 0.45          |
| (2,105) | 1:23:A:TRP:HH2  | 1:23:A:TRP:HE3 | 9        | 0.45          |
| (2,78)  | 1:9:A:VAL:HG23  | 1:8:A:ALA:HA   | 2        | 0.45          |
| (1,332) | 1:20:A:LEU:HD12 | 1:21:A:PRO:HD3 | 9        | 0.45          |
| (1,327) | 1:20:A:LEU:HD11 | 1:24:A:LYS:HA  | 3        | 0.45          |
| (1,165) | 1:13:A:THR:H    | 1:11:A:GLY:HA3 | 1        | 0.45          |
| (1,165) | 1:13:A:THR:H    | 1:11:A:GLY:HA3 | 9        | 0.45          |
| (1,89)  | 1:10:A:PHE:HB3  | 1:10:A:PHE:H   | 3        | 0.45          |
| (1,89)  | 1:10:A:PHE:HB3  | 1:10:A:PHE:H   | 9        | 0.45          |
| (1,8)   | 1:28:A:LEU:HD11 | 1:29:A:LYS:H   | 1        | 0.45          |
| (3,25)  | 1:30:A:LYS:H    | 1:26:A:GLN:O   | 8        | 0.44          |
| (3,3)   | 1:8:A:ALA:H     | 1:4:A:GLU:O    | 8        | 0.44          |
| (2,25)  | 1:21:A:PRO:HD3  | 1:23:A:TRP:HH2 | 5        | 0.44          |
| (2,20)  | 1:10:A:PHE:HB3  | 1:13:A:THR:H   | 5        | 0.44          |
| (2,8)   | 1:16:A:ALA:HB3  | 1:13:A:THR:H   | 5        | 0.44          |
| (2,8)   | 1:16:A:ALA:HB1  | 1:13:A:THR:H   | 8        | 0.44          |
| (1,493) | 1:7:A:LYS:HD2   | 1:7:A:LYS:HA   | 10       | 0.44          |
| (1,217) | 1:2:A:SER:HB2   | 1:3:A:ASP:H    | 4        | 0.44          |
| (1,165) | 1:13:A:THR:H    | 1:11:A:GLY:HA3 | 8        | 0.44          |
| (1,82)  | 1:6:A:3FB:HB1   | 1:7:A:LYS:H    | 2        | 0.44          |
| (1,82)  | 1:6:A:3FB:HB1   | 1:7:A:LYS:H    | 7        | 0.44          |
| (1,67)  | 1:3:A:ASP:H     | 1:3:A:ASP:HB3  | 9        | 0.44          |
| (1,35)  | 1:32:A:LYS:HG3  | 1:32:A:LYS:H   | 4        | 0.44          |
| (3,2)   | 1:7:A:LYS:N     | 1:3:A:ASP:O    | 9        | 0.43          |
| (2,88)  | 1:12:A:NLE:HE2  | 1:12:A:NLE:HB3 | 10       | 0.43          |
| (2,58)  | 1:29:A:LYS:HG3  | 1:35:A:PHE:HE1 | 8        | 0.43          |
| (2,16)  | 1:20:A:LEU:HB2  | 1:18:A:ALA:H   | 6        | 0.43          |
| (1,535) | 1:22:A:LEU:HD23 | 1:26:A:GLN:HG3 | 4        | 0.43          |
| (1,376) | 1:12:A:NLE:HD2  | 1:12:A:NLE:HB3 | 8        | 0.43          |
| (1,327) | 1:20:A:LEU:HD11 | 1:24:A:LYS:HA  | 6        | 0.43          |
| (1,290) | 1:9:A:VAL:HG21  | 1:10:A:PHE:HD2 | 6        | 0.43          |
| (1,265) | 1:28:A:LEU:HG   | 1:17:A:PHE:HD1 | 3        | 0.43          |
| (1,107) | 1:24:A:LYS:HE2  | 1:23:A:TRP:HH2 | 1        | 0.43          |
| (1,63)  | 1:5:A:ASP:HB3   | 1:2:A:SER:H    | 7        | 0.43          |
| (1,23)  | 1:16:A:ALA:HB3  | 1:17:A:PHE:H   | 6        | 0.43          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (2,97)  | 1:26:A:GLN:HA   | 1:29:A:LYS:HD2  | 8        | 0.42          |
| (2,94)  | 1:6:A:3FB:HB2   | 1:32:A:LYS:HA   | 5        | 0.42          |
| (2,78)  | 1:9:A:VAL:HG23  | 1:8:A:ALA:HA    | 5        | 0.42          |
| (2,16)  | 1:20:A:LEU:HB2  | 1:18:A:ALA:H    | 10       | 0.42          |
| (2,9)   | 1:32:A:LYS:HG3  | 1:33:A:GLY:H    | 3        | 0.42          |
| (1,360) | 1:28:A:LEU:HD21 | 1:20:A:LEU:HD13 | 5        | 0.42          |
| (1,351) | 1:20:A:LEU:HD13 | 1:12:A:NLE:HD2  | 6        | 0.42          |
| (1,290) | 1:9:A:VAL:HG23  | 1:10:A:PHE:HD2  | 4        | 0.42          |
| (1,257) | 1:21:A:PRO:HG3  | 1:23:A:TRP:HZ2  | 7        | 0.42          |
| (1,254) | 1:20:A:LEU:HB2  | 1:25:A:GLN:HE22 | 2        | 0.42          |
| (1,89)  | 1:10:A:PHE:HB3  | 1:10:A:PHE:H    | 7        | 0.42          |
| (1,82)  | 1:6:A:3FB:HB1   | 1:7:A:LYS:H     | 6        | 0.42          |
| (2,105) | 1:27:A:ASN:HD21 | 1:23:A:TRP:HE3  | 3        | 0.41          |
| (2,88)  | 1:12:A:NLE:HE3  | 1:12:A:NLE:HB3  | 6        | 0.41          |
| (2,16)  | 1:20:A:LEU:HB2  | 1:18:A:ALA:H    | 1        | 0.41          |
| (2,8)   | 1:16:A:ALA:HB1  | 1:13:A:THR:H    | 2        | 0.41          |
| (1,82)  | 1:6:A:3FB:HB1   | 1:7:A:LYS:H     | 8        | 0.41          |
| (1,42)  | 1:32:A:LYS:HB3  | 1:33:A:GLY:H    | 3        | 0.41          |
| (3,30)  | 1:32:A:LYS:N    | 1:28:A:LEU:O    | 3        | 0.4           |
| (3,28)  | 1:31:A:GLU:N    | 1:27:A:ASN:O    | 6        | 0.4           |
| (2,16)  | 1:20:A:LEU:HB2  | 1:18:A:ALA:H    | 7        | 0.4           |
| (2,16)  | 1:20:A:LEU:HB2  | 1:18:A:ALA:H    | 9        | 0.4           |
| (1,554) | 1:23:A:TRP:HE3  | 1:27:A:ASN:HD22 | 6        | 0.4           |
| (1,545) | 1:14:A:ARG:HH21 | 1:35:A:PHE:HD1  | 5        | 0.4           |
| (1,376) | 1:12:A:NLE:HD2  | 1:12:A:NLE:HB3  | 4        | 0.4           |
| (1,360) | 1:28:A:LEU:HD22 | 1:20:A:LEU:HD12 | 8        | 0.4           |
| (1,351) | 1:20:A:LEU:HD13 | 1:12:A:NLE:HD2  | 10       | 0.4           |
| (1,331) | 1:24:A:LYS:HG2  | 1:21:A:PRO:HD3  | 6        | 0.4           |
| (1,288) | 1:9:A:VAL:HG23  | 1:6:A:3FB:HD1   | 4        | 0.4           |
| (1,264) | 1:20:A:LEU:HG   | 1:17:A:PHE:HD1  | 5        | 0.4           |
| (1,217) | 1:2:A:SER:HB2   | 1:3:A:ASP:H     | 10       | 0.4           |
| (1,165) | 1:13:A:THR:H    | 1:11:A:GLY:HA3  | 10       | 0.4           |
| (1,82)  | 1:6:A:3FB:HB1   | 1:7:A:LYS:H     | 3        | 0.4           |
| (1,18)  | 1:14:A:ARG:HG3  | 1:14:A:ARG:H    | 9        | 0.4           |
| (3,13)  | 1:18:A:ALA:H    | 1:14:A:ARG:O    | 3        | 0.39          |
| (3,5)   | 1:9:A:VAL:H     | 1:5:A:ASP:O     | 1        | 0.39          |
| (2,25)  | 1:21:A:PRO:HD3  | 1:23:A:TRP:HH2  | 8        | 0.39          |
| (2,8)   | 1:16:A:ALA:HB2  | 1:13:A:THR:H    | 10       | 0.39          |
| (1,559) | 1:36:A:NH2:HN2  | 1:35:A:PHE:H    | 7        | 0.39          |
| (1,552) | 1:35:A:PHE:HD1  | 1:35:A:PHE:HE1  | 1        | 0.39          |
| (1,552) | 1:35:A:PHE:HD2  | 1:35:A:PHE:HE2  | 2        | 0.39          |
| (1,552) | 1:35:A:PHE:HD2  | 1:35:A:PHE:HE2  | 3        | 0.39          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,552) | 1:35:A:PHE:HD2  | 1:35:A:PHE:HE2  | 4        | 0.39          |
| (1,552) | 1:35:A:PHE:HD2  | 1:35:A:PHE:HE2  | 5        | 0.39          |
| (1,552) | 1:35:A:PHE:HD2  | 1:35:A:PHE:HE2  | 6        | 0.39          |
| (1,552) | 1:35:A:PHE:HD2  | 1:35:A:PHE:HE2  | 7        | 0.39          |
| (1,552) | 1:35:A:PHE:HD2  | 1:35:A:PHE:HE2  | 8        | 0.39          |
| (1,552) | 1:35:A:PHE:HD2  | 1:35:A:PHE:HE2  | 9        | 0.39          |
| (1,552) | 1:35:A:PHE:HD1  | 1:35:A:PHE:HE1  | 10       | 0.39          |
| (1,493) | 1:7:A:LYS:HD3   | 1:7:A:LYS:HA    | 4        | 0.39          |
| (1,351) | 1:20:A:LEU:HD11 | 1:12:A:NLE:HD2  | 9        | 0.39          |
| (1,286) | 1:20:A:LEU:HD12 | 1:17:A:PHE:HE1  | 2        | 0.39          |
| (1,286) | 1:20:A:LEU:HD12 | 1:17:A:PHE:HE1  | 10       | 0.39          |
| (1,107) | 1:24:A:LYS:HE2  | 1:23:A:TRP:HH2  | 9        | 0.39          |
| (1,82)  | 1:6:A:3FB:HB1   | 1:7:A:LYS:H     | 1        | 0.39          |
| (1,82)  | 1:6:A:3FB:HB1   | 1:7:A:LYS:H     | 5        | 0.39          |
| (1,75)  | 1:6:A:3FB:HC1   | 1:7:A:LYS:H     | 9        | 0.39          |
| (2,16)  | 1:20:A:LEU:HB2  | 1:18:A:ALA:H    | 2        | 0.38          |
| (2,9)   | 1:32:A:LYS:HG2  | 1:33:A:GLY:H    | 7        | 0.38          |
| (2,8)   | 1:16:A:ALA:HB1  | 1:13:A:THR:H    | 3        | 0.38          |
| (1,493) | 1:7:A:LYS:HD3   | 1:7:A:LYS:HA    | 5        | 0.38          |
| (1,452) | 1:26:A:GLN:HG2  | 1:23:A:TRP:HA   | 7        | 0.38          |
| (1,415) | 1:19:A:ASN:HB3  | 1:16:A:ALA:HA   | 3        | 0.38          |
| (1,294) | 1:28:A:LEU:HD21 | 1:17:A:PHE:HD1  | 1        | 0.38          |
| (1,294) | 1:28:A:LEU:HD21 | 1:17:A:PHE:HD1  | 3        | 0.38          |
| (1,294) | 1:28:A:LEU:HD23 | 1:17:A:PHE:HD1  | 4        | 0.38          |
| (1,254) | 1:20:A:LEU:HB2  | 1:25:A:GLN:HE22 | 9        | 0.38          |
| (1,156) | 1:24:A:LYS:HA   | 1:27:A:ASN:HD22 | 7        | 0.38          |
| (1,108) | 1:24:A:LYS:HE3  | 1:23:A:TRP:HH2  | 3        | 0.38          |
| (1,92)  | 1:17:A:PHE:HB2  | 1:18:A:ALA:H    | 3        | 0.38          |
| (1,75)  | 1:6:A:3FB:HC1   | 1:7:A:LYS:H     | 5        | 0.38          |
| (3,14)  | 1:18:A:ALA:N    | 1:14:A:ARG:O    | 5        | 0.37          |
| (2,99)  | 1:6:A:3FB:HA    | 1:13:A:THR:HG21 | 2        | 0.37          |
| (2,99)  | 1:6:A:3FB:HA    | 1:13:A:THR:HG22 | 9        | 0.37          |
| (2,84)  | 1:20:A:LEU:HD13 | 1:16:A:ALA:HB3  | 6        | 0.37          |
| (2,72)  | 1:28:A:LEU:HD13 | 1:35:A:PHE:HE1  | 5        | 0.37          |
| (2,55)  | 1:32:A:LYS:HD3  | 1:14:A:ARG:HH21 | 2        | 0.37          |
| (2,16)  | 1:20:A:LEU:HB2  | 1:18:A:ALA:H    | 5        | 0.37          |
| (2,4)   | 1:28:A:LEU:HD11 | 1:13:A:THR:H    | 2        | 0.37          |
| (1,535) | 1:22:A:LEU:HD21 | 1:26:A:GLN:HG3  | 6        | 0.37          |
| (1,517) | 1:28:A:LEU:HG   | 1:27:A:ASN:HB2  | 1        | 0.37          |
| (1,376) | 1:12:A:NLE:HD2  | 1:12:A:NLE:HB3  | 3        | 0.37          |
| (1,352) | 1:20:A:LEU:HD11 | 1:13:A:THR:HG23 | 7        | 0.37          |
| (1,298) | 1:18:A:ALA:HB2  | 1:25:A:GLN:HE21 | 3        | 0.37          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,108) | 1:24:A:LYS:HE3  | 1:23:A:TRP:HH2  | 10       | 0.37          |
| (1,92)  | 1:17:A:PHE:HB2  | 1:18:A:ALA:H    | 1        | 0.37          |
| (1,92)  | 1:17:A:PHE:HB2  | 1:18:A:ALA:H    | 6        | 0.37          |
| (3,16)  | 1:19:A:ASN:N    | 1:15:A:SER:O    | 3        | 0.36          |
| (3,14)  | 1:18:A:ALA:N    | 1:14:A:ARG:O    | 1        | 0.36          |
| (3,8)   | 1:10:A:PHE:N    | 1:6:A:3FB:O     | 8        | 0.36          |
| (2,20)  | 1:10:A:PHE:HB3  | 1:13:A:THR:H    | 1        | 0.36          |
| (1,581) | 1:34:A:LEU:H    | 1:35:A:PHE:H    | 10       | 0.36          |
| (1,529) | 1:12:A:NLE:HG3  | 1:10:A:PHE:HB2  | 4        | 0.36          |
| (1,377) | 1:12:A:NLE:HD2  | 1:12:A:NLE:HG2  | 7        | 0.36          |
| (1,376) | 1:12:A:NLE:HD2  | 1:12:A:NLE:HB3  | 1        | 0.36          |
| (1,376) | 1:12:A:NLE:HD2  | 1:12:A:NLE:HB3  | 10       | 0.36          |
| (1,352) | 1:20:A:LEU:HD13 | 1:13:A:THR:HG21 | 1        | 0.36          |
| (1,298) | 1:18:A:ALA:HB3  | 1:25:A:GLN:HE21 | 8        | 0.36          |
| (1,107) | 1:24:A:LYS:HE2  | 1:23:A:TRP:HH2  | 4        | 0.36          |
| (1,92)  | 1:17:A:PHE:HB2  | 1:18:A:ALA:H    | 4        | 0.36          |
| (1,92)  | 1:17:A:PHE:HB2  | 1:18:A:ALA:H    | 5        | 0.36          |
| (1,75)  | 1:6:A:3FB:HC1   | 1:7:A:LYS:H     | 1        | 0.36          |
| (1,61)  | 1:31:A:GLU:HB2  | 1:30:A:LYS:H    | 4        | 0.36          |
| (3,29)  | 1:32:A:LYS:H    | 1:28:A:LEU:O    | 8        | 0.35          |
| (2,88)  | 1:28:A:LEU:HD13 | 1:25:A:GLN:HG2  | 9        | 0.35          |
| (1,376) | 1:12:A:NLE:HD2  | 1:12:A:NLE:HB3  | 5        | 0.35          |
| (1,327) | 1:20:A:LEU:HD13 | 1:24:A:LYS:HA   | 7        | 0.35          |
| (1,165) | 1:13:A:THR:H    | 1:11:A:GLY:HA3  | 7        | 0.35          |
| (1,92)  | 1:17:A:PHE:HB2  | 1:18:A:ALA:H    | 2        | 0.35          |
| (1,82)  | 1:6:A:3FB:HB1   | 1:7:A:LYS:H     | 9        | 0.35          |
| (3,27)  | 1:31:A:GLU:H    | 1:27:A:ASN:O    | 10       | 0.34          |
| (2,94)  | 1:35:A:PHE:HB3  | 1:32:A:LYS:HA   | 9        | 0.34          |
| (2,85)  | 1:24:A:LYS:HG2  | 1:12:A:NLE:HD2  | 1        | 0.34          |
| (2,78)  | 1:9:A:VAL:HG23  | 1:8:A:ALA:HA    | 3        | 0.34          |
| (2,59)  | 1:16:A:ALA:HB3  | 1:19:A:ASN:HD22 | 9        | 0.34          |
| (2,41)  | 1:12:A:NLE:HA   | 1:13:A:THR:H    | 4        | 0.34          |
| (2,18)  | 1:6:A:3FB:HB2   | 1:7:A:LYS:H     | 7        | 0.34          |
| (1,550) | 1:23:A:TRP:HZ3  | 1:23:A:TRP:HZ2  | 1        | 0.34          |
| (1,550) | 1:23:A:TRP:HZ3  | 1:23:A:TRP:HZ2  | 2        | 0.34          |
| (1,550) | 1:23:A:TRP:HZ3  | 1:23:A:TRP:HZ2  | 3        | 0.34          |
| (1,550) | 1:23:A:TRP:HZ3  | 1:23:A:TRP:HZ2  | 4        | 0.34          |
| (1,550) | 1:23:A:TRP:HZ3  | 1:23:A:TRP:HZ2  | 5        | 0.34          |
| (1,550) | 1:23:A:TRP:HZ3  | 1:23:A:TRP:HZ2  | 6        | 0.34          |
| (1,550) | 1:23:A:TRP:HZ3  | 1:23:A:TRP:HZ2  | 7        | 0.34          |
| (1,535) | 1:22:A:LEU:HD22 | 1:26:A:GLN:HG3  | 2        | 0.34          |
| (1,377) | 1:12:A:NLE:HD2  | 1:12:A:NLE:HG2  | 2        | 0.34          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,194) | 1:28:A:LEU:HA   | 1:30:A:LYS:H    | 7        | 0.34          |
| (1,107) | 1:24:A:LYS:HE2  | 1:23:A:TRP:HH2  | 8        | 0.34          |
| (1,92)  | 1:17:A:PHE:HB2  | 1:18:A:ALA:H    | 7        | 0.34          |
| (1,18)  | 1:14:A:ARG:HG3  | 1:14:A:ARG:H    | 4        | 0.34          |
| (3,7)   | 1:10:A:PHE:H    | 1:6:A:3FB:O     | 7        | 0.33          |
| (2,90)  | 1:12:A:NLE:HD3  | 1:12:A:NLE:HB2  | 2        | 0.33          |
| (2,71)  | 1:24:A:LYS:HG2  | 1:23:A:TRP:HZ2  | 5        | 0.33          |
| (2,63)  | 1:13:A:THR:HG23 | 1:6:A:3FB:HD2   | 4        | 0.33          |
| (2,60)  | 1:16:A:ALA:HB1  | 1:20:A:LEU:H    | 4        | 0.33          |
| (2,46)  | 1:21:A:PRO:HA   | 1:23:A:TRP:HD1  | 5        | 0.33          |
| (1,550) | 1:23:A:TRP:HZ3  | 1:23:A:TRP:HZ2  | 8        | 0.33          |
| (1,550) | 1:23:A:TRP:HZ3  | 1:23:A:TRP:HZ2  | 9        | 0.33          |
| (1,550) | 1:23:A:TRP:HZ3  | 1:23:A:TRP:HZ2  | 10       | 0.33          |
| (1,535) | 1:22:A:LEU:HD23 | 1:26:A:GLN:HG3  | 9        | 0.33          |
| (1,415) | 1:19:A:ASN:HB3  | 1:16:A:ALA:HA   | 8        | 0.33          |
| (1,329) | 1:12:A:NLE:HE3  | 1:10:A:PHE:HB2  | 5        | 0.33          |
| (1,264) | 1:20:A:LEU:HG   | 1:17:A:PHE:HD1  | 1        | 0.33          |
| (1,75)  | 1:6:A:3FB:HC1   | 1:7:A:LYS:H     | 2        | 0.33          |
| (1,75)  | 1:6:A:3FB:HC1   | 1:7:A:LYS:H     | 10       | 0.33          |
| (1,72)  | 1:31:A:GLU:HG3  | 1:31:A:GLU:H    | 5        | 0.33          |
| (1,42)  | 1:32:A:LYS:HB3  | 1:33:A:GLY:H    | 10       | 0.33          |
| (2,80)  | 1:20:A:LEU:HD12 | 1:28:A:LEU:HG   | 9        | 0.32          |
| (1,559) | 1:36:A:NH2:HN2  | 1:35:A:PHE:H    | 8        | 0.32          |
| (1,558) | 1:23:A:TRP:HE3  | 1:27:A:ASN:H    | 7        | 0.32          |
| (1,298) | 1:18:A:ALA:HB2  | 1:25:A:GLN:HE21 | 7        | 0.32          |
| (1,92)  | 1:17:A:PHE:HB2  | 1:18:A:ALA:H    | 8        | 0.32          |
| (1,92)  | 1:17:A:PHE:HB2  | 1:18:A:ALA:H    | 10       | 0.32          |
| (1,27)  | 1:7:A:LYS:HG3   | 1:8:A:ALA:H     | 9        | 0.32          |
| (1,25)  | 1:14:A:ARG:HG2  | 1:15:A:SER:H    | 5        | 0.32          |
| (3,23)  | 1:29:A:LYS:H    | 1:25:A:GLN:O    | 3        | 0.31          |
| (3,23)  | 1:29:A:LYS:H    | 1:25:A:GLN:O    | 8        | 0.31          |
| (2,52)  | 1:1:A:LEU:HG    | 1:6:A:3FB:HD1   | 2        | 0.31          |
| (2,46)  | 1:21:A:PRO:HA   | 1:23:A:TRP:HD1  | 7        | 0.31          |
| (2,46)  | 1:21:A:PRO:HA   | 1:23:A:TRP:HD1  | 8        | 0.31          |
| (1,518) | 1:14:A:ARG:HB3  | 1:14:A:ARG:HD3  | 1        | 0.31          |
| (1,452) | 1:26:A:GLN:HG2  | 1:23:A:TRP:HA   | 3        | 0.31          |
| (1,415) | 1:19:A:ASN:HB3  | 1:16:A:ALA:HA   | 2        | 0.31          |
| (1,376) | 1:12:A:NLE:HD2  | 1:12:A:NLE:HB3  | 6        | 0.31          |
| (1,288) | 1:9:A:VAL:HG22  | 1:6:A:3FB:HD2   | 9        | 0.31          |
| (1,254) | 1:20:A:LEU:HB2  | 1:25:A:GLN:HE22 | 3        | 0.31          |
| (1,194) | 1:28:A:LEU:HA   | 1:30:A:LYS:H    | 3        | 0.31          |
| (3,5)   | 1:9:A:VAL:H     | 1:5:A:ASP:O     | 6        | 0.3           |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (3,1)   | 1:7:A:LYS:H     | 1:3:A:ASP:O     | 3        | 0.3           |
| (2,90)  | 1:12:A:NLE:HD3  | 1:12:A:NLE:HB2  | 7        | 0.3           |
| (1,558) | 1:23:A:TRP:HE3  | 1:27:A:ASN:H    | 5        | 0.3           |
| (1,377) | 1:12:A:NLE:HD2  | 1:12:A:NLE:HG3  | 1        | 0.3           |
| (1,278) | 1:24:A:LYS:HB3  | 1:23:A:TRP:HZ2  | 5        | 0.3           |
| (1,266) | 1:1:A:LEU:HG    | 1:6:A:3FB:HE1   | 5        | 0.3           |
| (1,254) | 1:20:A:LEU:HB2  | 1:25:A:GLN:HE22 | 1        | 0.3           |
| (1,61)  | 1:31:A:GLU:HB2  | 1:30:A:LYS:H    | 2        | 0.3           |
| (1,41)  | 1:28:A:LEU:HG   | 1:27:A:ASN:H    | 1        | 0.3           |
| (3,26)  | 1:30:A:LYS:N    | 1:26:A:GLN:O    | 4        | 0.29          |
| (3,13)  | 1:18:A:ALA:H    | 1:14:A:ARG:O    | 2        | 0.29          |
| (2,45)  | 1:5:A:ASP:HA    | 1:9:A:VAL:H     | 1        | 0.29          |
| (2,33)  | 1:9:A:VAL:H     | 1:7:A:LYS:HA    | 3        | 0.29          |
| (1,535) | 1:22:A:LEU:HD22 | 1:26:A:GLN:HG3  | 1        | 0.29          |
| (1,493) | 1:7:A:LYS:HD3   | 1:7:A:LYS:HA    | 2        | 0.29          |
| (1,452) | 1:26:A:GLN:HG2  | 1:23:A:TRP:HA   | 10       | 0.29          |
| (1,415) | 1:19:A:ASN:HB3  | 1:16:A:ALA:HA   | 5        | 0.29          |
| (1,377) | 1:12:A:NLE:HD2  | 1:12:A:NLE:HG3  | 4        | 0.29          |
| (1,356) | 1:28:A:LEU:HD21 | 1:13:A:THR:HG21 | 3        | 0.29          |
| (1,165) | 1:13:A:THR:H    | 1:11:A:GLY:HA3  | 4        | 0.29          |
| (1,61)  | 1:31:A:GLU:HB2  | 1:30:A:LYS:H    | 3        | 0.29          |
| (1,9)   | 1:34:A:LEU:HD12 | 1:34:A:LEU:H    | 8        | 0.29          |
| (1,8)   | 1:28:A:LEU:HD12 | 1:29:A:LYS:H    | 3        | 0.29          |
| (3,25)  | 1:30:A:LYS:H    | 1:26:A:GLN:O    | 2        | 0.28          |
| (3,25)  | 1:30:A:LYS:H    | 1:26:A:GLN:O    | 10       | 0.28          |
| (2,53)  | 1:28:A:LEU:HB3  | 1:17:A:PHE:HE1  | 8        | 0.28          |
| (2,20)  | 1:10:A:PHE:HB3  | 1:13:A:THR:H    | 8        | 0.28          |
| (2,16)  | 1:20:A:LEU:HB2  | 1:18:A:ALA:H    | 8        | 0.28          |
| (1,377) | 1:12:A:NLE:HD2  | 1:12:A:NLE:HG3  | 3        | 0.28          |
| (1,377) | 1:12:A:NLE:HD2  | 1:12:A:NLE:HG3  | 5        | 0.28          |
| (1,377) | 1:12:A:NLE:HD2  | 1:12:A:NLE:HG3  | 6        | 0.28          |
| (1,377) | 1:12:A:NLE:HD2  | 1:12:A:NLE:HG3  | 8        | 0.28          |
| (1,377) | 1:12:A:NLE:HD2  | 1:12:A:NLE:HG3  | 10       | 0.28          |
| (1,352) | 1:20:A:LEU:HD13 | 1:13:A:THR:HG23 | 6        | 0.28          |
| (1,182) | 1:15:A:SER:HB2  | 1:15:A:SER:H    | 7        | 0.28          |
| (1,156) | 1:24:A:LYS:HA   | 1:27:A:ASN:HD22 | 9        | 0.28          |
| (1,75)  | 1:6:A:3FB:HC1   | 1:7:A:LYS:H     | 6        | 0.28          |
| (1,27)  | 1:7:A:LYS:HG3   | 1:8:A:ALA:H     | 1        | 0.28          |
| (3,25)  | 1:30:A:LYS:H    | 1:26:A:GLN:O    | 3        | 0.27          |
| (3,19)  | 1:27:A:ASN:H    | 1:23:A:TRP:O    | 7        | 0.27          |
| (1,493) | 1:7:A:LYS:HD3   | 1:7:A:LYS:HA    | 3        | 0.27          |
| (1,331) | 1:24:A:LYS:HG2  | 1:21:A:PRO:HD3  | 10       | 0.27          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,327) | 1:20:A:LEU:HD13 | 1:24:A:LYS:HA   | 5        | 0.27          |
| (1,327) | 1:20:A:LEU:HD12 | 1:24:A:LYS:HA   | 8        | 0.27          |
| (1,298) | 1:18:A:ALA:HB2  | 1:25:A:GLN:HE21 | 9        | 0.27          |
| (1,286) | 1:20:A:LEU:HD12 | 1:17:A:PHE:HE1  | 3        | 0.27          |
| (1,279) | 1:20:A:LEU:HD23 | 1:19:A:ASN:H    | 8        | 0.27          |
| (1,262) | 1:25:A:GLN:HG2  | 1:17:A:PHE:HE1  | 8        | 0.27          |
| (1,150) | 1:16:A:ALA:HA   | 1:19:A:ASN:HD21 | 4        | 0.27          |
| (1,107) | 1:24:A:LYS:HE2  | 1:23:A:TRP:HH2  | 7        | 0.27          |
| (1,82)  | 1:6:A:3FB:HB1   | 1:7:A:LYS:H     | 4        | 0.27          |
| (1,75)  | 1:6:A:3FB:HC1   | 1:7:A:LYS:H     | 4        | 0.27          |
| (1,75)  | 1:6:A:3FB:HC1   | 1:7:A:LYS:H     | 8        | 0.27          |
| (1,50)  | 1:30:A:LYS:HB3  | 1:31:A:GLU:H    | 5        | 0.27          |
| (1,30)  | 1:13:A:THR:HG22 | 1:13:A:THR:H    | 5        | 0.27          |
| (2,97)  | 1:26:A:GLN:HA   | 1:29:A:LYS:HD3  | 1        | 0.26          |
| (2,46)  | 1:21:A:PRO:HA   | 1:23:A:TRP:HD1  | 9        | 0.26          |
| (1,581) | 1:34:A:LEU:H    | 1:35:A:PHE:H    | 3        | 0.26          |
| (1,452) | 1:26:A:GLN:HG2  | 1:23:A:TRP:HA   | 2        | 0.26          |
| (1,401) | 1:6:A:3FB:HC2   | 1:6:A:3FB:HB1   | 3        | 0.26          |
| (1,377) | 1:12:A:NLE:HD2  | 1:12:A:NLE:HG3  | 9        | 0.26          |
| (1,327) | 1:20:A:LEU:HD11 | 1:24:A:LYS:HA   | 2        | 0.26          |
| (1,265) | 1:28:A:LEU:HG   | 1:17:A:PHE:HD1  | 1        | 0.26          |
| (1,257) | 1:21:A:PRO:HG3  | 1:23:A:TRP:HZ2  | 5        | 0.26          |
| (1,61)  | 1:31:A:GLU:HB2  | 1:30:A:LYS:H    | 6        | 0.26          |
| (1,26)  | 1:12:A:NLE:HG3  | 1:11:A:GLY:H    | 4        | 0.26          |
| (3,25)  | 1:30:A:LYS:H    | 1:26:A:GLN:O    | 9        | 0.25          |
| (3,7)   | 1:10:A:PHE:H    | 1:6:A:3FB:O     | 6        | 0.25          |
| (2,33)  | 1:9:A:VAL:H     | 1:7:A:LYS:HA    | 6        | 0.25          |
| (1,582) | 1:24:A:LYS:HZ2  | 1:27:A:ASN:HD22 | 8        | 0.25          |
| (1,569) | 1:17:A:PHE:HD1  | 1:17:A:PHE:H    | 9        | 0.25          |
| (1,541) | 1:17:A:PHE:HD2  | 1:17:A:PHE:HE2  | 1        | 0.25          |
| (1,541) | 1:17:A:PHE:HD2  | 1:17:A:PHE:HE2  | 2        | 0.25          |
| (1,541) | 1:17:A:PHE:HD1  | 1:17:A:PHE:HE1  | 3        | 0.25          |
| (1,541) | 1:17:A:PHE:HD2  | 1:17:A:PHE:HE2  | 4        | 0.25          |
| (1,541) | 1:17:A:PHE:HD2  | 1:17:A:PHE:HE2  | 5        | 0.25          |
| (1,541) | 1:17:A:PHE:HD1  | 1:17:A:PHE:HE1  | 6        | 0.25          |
| (1,541) | 1:17:A:PHE:HD2  | 1:17:A:PHE:HE2  | 7        | 0.25          |
| (1,541) | 1:17:A:PHE:HD2  | 1:17:A:PHE:HE2  | 8        | 0.25          |
| (1,541) | 1:17:A:PHE:HD2  | 1:17:A:PHE:HE2  | 9        | 0.25          |
| (1,541) | 1:17:A:PHE:HD1  | 1:17:A:PHE:HE1  | 10       | 0.25          |
| (1,513) | 1:32:A:LYS:HB2  | 1:35:A:PHE:HB3  | 6        | 0.25          |
| (1,503) | 1:7:A:LYS:HG3   | 1:7:A:LYS:HA    | 8        | 0.25          |
| (1,349) | 1:34:A:LEU:HD12 | 1:34:A:LEU:HB3  | 10       | 0.25          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,298) | 1:18:A:ALA:HB3  | 1:25:A:GLN:HE21 | 5        | 0.25          |
| (1,165) | 1:13:A:THR:H    | 1:11:A:GLY:HA3  | 6        | 0.25          |
| (1,156) | 1:24:A:LYS:HA   | 1:27:A:ASN:HD22 | 3        | 0.25          |
| (1,122) | 1:6:A:3FB:HC1   | 1:6:A:3FB:HD1   | 3        | 0.25          |
| (1,101) | 1:6:A:3FB:HB1   | 1:6:A:3FB:H     | 3        | 0.25          |
| (1,97)  | 1:27:A:ASN:HB2  | 1:27:A:ASN:HD22 | 2        | 0.25          |
| (1,75)  | 1:6:A:3FB:HC1   | 1:7:A:LYS:H     | 7        | 0.25          |
| (3,26)  | 1:30:A:LYS:N    | 1:26:A:GLN:O    | 6        | 0.24          |
| (3,23)  | 1:29:A:LYS:H    | 1:25:A:GLN:O    | 6        | 0.24          |
| (3,2)   | 1:7:A:LYS:N     | 1:3:A:ASP:O     | 8        | 0.24          |
| (2,46)  | 1:21:A:PRO:HA   | 1:23:A:TRP:HD1  | 3        | 0.24          |
| (1,569) | 1:17:A:PHE:HD2  | 1:17:A:PHE:H    | 1        | 0.24          |
| (1,569) | 1:17:A:PHE:HD2  | 1:17:A:PHE:H    | 2        | 0.24          |
| (1,569) | 1:17:A:PHE:HD2  | 1:17:A:PHE:H    | 3        | 0.24          |
| (1,569) | 1:17:A:PHE:HD2  | 1:17:A:PHE:H    | 10       | 0.24          |
| (1,415) | 1:19:A:ASN:HB3  | 1:16:A:ALA:HA   | 7        | 0.24          |
| (1,286) | 1:20:A:LEU:HD11 | 1:17:A:PHE:HE1  | 5        | 0.24          |
| (1,265) | 1:28:A:LEU:HG   | 1:17:A:PHE:HD1  | 7        | 0.24          |
| (1,38)  | 1:28:A:LEU:HB3  | 1:28:A:LEU:H    | 6        | 0.24          |
| (1,9)   | 1:34:A:LEU:HD12 | 1:34:A:LEU:H    | 5        | 0.24          |
| (3,17)  | 1:26:A:GLN:H    | 1:22:A:LEU:O    | 10       | 0.23          |
| (3,1)   | 1:7:A:LYS:H     | 1:3:A:ASP:O     | 10       | 0.23          |
| (2,99)  | 1:6:A:3FB:HA    | 1:13:A:THR:HG22 | 6        | 0.23          |
| (1,534) | 1:1:A:LEU:HD23  | 1:5:A:ASP:HB3   | 3        | 0.23          |
| (1,534) | 1:1:A:LEU:HD12  | 1:5:A:ASP:HB3   | 7        | 0.23          |
| (1,527) | 1:13:A:THR:HG22 | 1:10:A:PHE:HB3  | 2        | 0.23          |
| (1,503) | 1:7:A:LYS:HG3   | 1:7:A:LYS:HA    | 1        | 0.23          |
| (1,374) | 1:8:A:ALA:HB2   | 1:5:A:ASP:HB3   | 4        | 0.23          |
| (1,286) | 1:20:A:LEU:HD12 | 1:17:A:PHE:HE1  | 1        | 0.23          |
| (1,61)  | 1:31:A:GLU:HB2  | 1:30:A:LYS:H    | 10       | 0.23          |
| (1,38)  | 1:28:A:LEU:HB3  | 1:28:A:LEU:H    | 2        | 0.23          |
| (1,38)  | 1:28:A:LEU:HB3  | 1:28:A:LEU:H    | 5        | 0.23          |
| (1,25)  | 1:14:A:ARG:HG2  | 1:15:A:SER:H    | 10       | 0.23          |
| (1,23)  | 1:16:A:ALA:HB1  | 1:17:A:PHE:H    | 9        | 0.23          |
| (1,17)  | 1:14:A:ARG:HB3  | 1:14:A:ARG:H    | 7        | 0.23          |
| (3,1)   | 1:7:A:LYS:H     | 1:3:A:ASP:O     | 6        | 0.22          |
| (2,88)  | 1:28:A:LEU:HD11 | 1:25:A:GLN:HG2  | 1        | 0.22          |
| (2,46)  | 1:21:A:PRO:HA   | 1:23:A:TRP:HD1  | 4        | 0.22          |
| (1,569) | 1:17:A:PHE:HD1  | 1:17:A:PHE:H    | 4        | 0.22          |
| (1,569) | 1:17:A:PHE:HD1  | 1:17:A:PHE:H    | 5        | 0.22          |
| (1,569) | 1:17:A:PHE:HD1  | 1:17:A:PHE:H    | 8        | 0.22          |
| (1,529) | 1:12:A:NLE:HG3  | 1:10:A:PHE:HB2  | 8        | 0.22          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,415) | 1:19:A:ASN:HB3  | 1:16:A:ALA:HA   | 10       | 0.22          |
| (1,349) | 1:34:A:LEU:HD12 | 1:34:A:LEU:HB3  | 4        | 0.22          |
| (1,170) | 1:9:A:VAL:HA    | 1:10:A:PHE:H    | 7        | 0.22          |
| (1,170) | 1:9:A:VAL:HA    | 1:10:A:PHE:H    | 9        | 0.22          |
| (1,122) | 1:6:A:3FB:HC1   | 1:6:A:3FB:HD2   | 5        | 0.22          |
| (1,117) | 1:6:A:3FB:HC1   | 1:6:A:3FB:H     | 4        | 0.22          |
| (1,76)  | 1:26:A:GLN:HG2  | 1:26:A:GLN:H    | 3        | 0.22          |
| (1,38)  | 1:28:A:LEU:HB3  | 1:28:A:LEU:H    | 1        | 0.22          |
| (1,38)  | 1:28:A:LEU:HB3  | 1:28:A:LEU:H    | 7        | 0.22          |
| (1,38)  | 1:28:A:LEU:HB3  | 1:28:A:LEU:H    | 8        | 0.22          |
| (1,38)  | 1:28:A:LEU:HB3  | 1:28:A:LEU:H    | 10       | 0.22          |
| (2,27)  | 1:25:A:GLN:HA   | 1:25:A:GLN:HE22 | 5        | 0.21          |
| (2,27)  | 1:25:A:GLN:HA   | 1:25:A:GLN:HE22 | 8        | 0.21          |
| (1,569) | 1:17:A:PHE:HD1  | 1:17:A:PHE:H    | 7        | 0.21          |
| (1,457) | 1:21:A:PRO:HG2  | 1:21:A:PRO:HA   | 8        | 0.21          |
| (1,265) | 1:28:A:LEU:HG   | 1:17:A:PHE:HD1  | 5        | 0.21          |
| (1,257) | 1:21:A:PRO:HG3  | 1:23:A:TRP:HZ2  | 9        | 0.21          |
| (1,183) | 1:15:A:SER:HB3  | 1:15:A:SER:H    | 1        | 0.21          |
| (1,183) | 1:15:A:SER:HB3  | 1:15:A:SER:H    | 5        | 0.21          |
| (1,170) | 1:9:A:VAL:HA    | 1:10:A:PHE:H    | 1        | 0.21          |
| (1,170) | 1:9:A:VAL:HA    | 1:10:A:PHE:H    | 2        | 0.21          |
| (1,101) | 1:6:A:3FB:HB1   | 1:6:A:3FB:H     | 1        | 0.21          |
| (1,38)  | 1:28:A:LEU:HB3  | 1:28:A:LEU:H    | 3        | 0.21          |
| (1,25)  | 1:14:A:ARG:HG2  | 1:15:A:SER:H    | 7        | 0.21          |
| (1,25)  | 1:14:A:ARG:HG2  | 1:15:A:SER:H    | 8        | 0.21          |
| (3,16)  | 1:19:A:ASN:N    | 1:15:A:SER:O    | 8        | 0.2           |
| (3,13)  | 1:18:A:ALA:H    | 1:14:A:ARG:O    | 8        | 0.2           |
| (3,3)   | 1:8:A:ALA:H     | 1:4:A:GLU:O     | 4        | 0.2           |
| (2,80)  | 1:20:A:LEU:HD11 | 1:28:A:LEU:HG   | 10       | 0.2           |
| (2,45)  | 1:5:A:ASP:HA    | 1:9:A:VAL:H     | 6        | 0.2           |
| (2,27)  | 1:25:A:GLN:HA   | 1:25:A:GLN:HE22 | 4        | 0.2           |
| (2,20)  | 1:10:A:PHE:HB3  | 1:13:A:THR:H    | 3        | 0.2           |
| (2,17)  | 1:7:A:LYS:HE3   | 1:14:A:ARG:H    | 7        | 0.2           |
| (1,457) | 1:21:A:PRO:HG2  | 1:21:A:PRO:HA   | 1        | 0.2           |
| (1,457) | 1:21:A:PRO:HG2  | 1:21:A:PRO:HA   | 2        | 0.2           |
| (1,457) | 1:21:A:PRO:HG2  | 1:21:A:PRO:HA   | 7        | 0.2           |
| (1,457) | 1:21:A:PRO:HG2  | 1:21:A:PRO:HA   | 9        | 0.2           |
| (1,375) | 1:8:A:ALA:HB3   | 1:4:A:GLU:HG2   | 3        | 0.2           |
| (1,351) | 1:20:A:LEU:HD13 | 1:12:A:NLE:HD2  | 1        | 0.2           |
| (1,288) | 1:9:A:VAL:HG23  | 1:6:A:3FB:HD1   | 7        | 0.2           |
| (1,288) | 1:9:A:VAL:HG21  | 1:6:A:3FB:HD2   | 8        | 0.2           |
| (1,278) | 1:24:A:LYS:HB3  | 1:23:A:TRP:HZ2  | 3        | 0.2           |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,278) | 1:24:A:LYS:HB3  | 1:23:A:TRP:HZ2  | 8        | 0.2           |
| (1,257) | 1:21:A:PRO:HG3  | 1:23:A:TRP:HZ2  | 8        | 0.2           |
| (1,238) | 1:23:A:TRP:HA   | 1:23:A:TRP:HE3  | 5        | 0.2           |
| (1,191) | 1:34:A:LEU:HA   | 1:35:A:PHE:H    | 8        | 0.2           |
| (1,183) | 1:15:A:SER:HB3  | 1:15:A:SER:H    | 3        | 0.2           |
| (1,171) | 1:29:A:LYS:HA   | 1:30:A:LYS:H    | 2        | 0.2           |
| (1,171) | 1:29:A:LYS:HA   | 1:30:A:LYS:H    | 7        | 0.2           |
| (1,170) | 1:9:A:VAL:HA    | 1:10:A:PHE:H    | 4        | 0.2           |
| (1,170) | 1:9:A:VAL:HA    | 1:10:A:PHE:H    | 6        | 0.2           |
| (1,122) | 1:6:A:3FB:HC1   | 1:6:A:3FB:HD1   | 10       | 0.2           |
| (1,101) | 1:6:A:3FB:HB1   | 1:6:A:3FB:H     | 5        | 0.2           |
| (1,38)  | 1:28:A:LEU:HB3  | 1:28:A:LEU:H    | 4        | 0.2           |
| (1,38)  | 1:28:A:LEU:HB3  | 1:28:A:LEU:H    | 9        | 0.2           |
| (1,26)  | 1:12:A:NLE:HG3  | 1:11:A:GLY:H    | 10       | 0.2           |
| (1,23)  | 1:16:A:ALA:HB2  | 1:17:A:PHE:H    | 4        | 0.2           |
| (1,9)   | 1:34:A:LEU:HD11 | 1:34:A:LEU:H    | 10       | 0.2           |
| (3,3)   | 1:8:A:ALA:H     | 1:4:A:GLU:O     | 2        | 0.19          |
| (2,86)  | 1:1:A:LEU:HD21  | 1:34:A:LEU:HB2  | 10       | 0.19          |
| (2,70)  | 1:20:A:LEU:HD11 | 1:25:A:GLN:H    | 4        | 0.19          |
| (2,55)  | 1:32:A:LYS:HD3  | 1:14:A:ARG:HH21 | 5        | 0.19          |
| (2,27)  | 1:25:A:GLN:HA   | 1:25:A:GLN:HE22 | 3        | 0.19          |
| (1,457) | 1:21:A:PRO:HG2  | 1:21:A:PRO:HA   | 3        | 0.19          |
| (1,457) | 1:21:A:PRO:HG2  | 1:21:A:PRO:HA   | 5        | 0.19          |
| (1,457) | 1:21:A:PRO:HG2  | 1:21:A:PRO:HA   | 6        | 0.19          |
| (1,183) | 1:15:A:SER:HB3  | 1:15:A:SER:H    | 2        | 0.19          |
| (1,170) | 1:9:A:VAL:HA    | 1:10:A:PHE:H    | 3        | 0.19          |
| (1,170) | 1:9:A:VAL:HA    | 1:10:A:PHE:H    | 8        | 0.19          |
| (1,170) | 1:9:A:VAL:HA    | 1:10:A:PHE:H    | 10       | 0.19          |
| (3,27)  | 1:31:A:GLU:H    | 1:27:A:ASN:O    | 4        | 0.18          |
| (3,25)  | 1:30:A:LYS:H    | 1:26:A:GLN:O    | 7        | 0.18          |
| (3,19)  | 1:27:A:ASN:H    | 1:23:A:TRP:O    | 5        | 0.18          |
| (3,14)  | 1:18:A:ALA:N    | 1:14:A:ARG:O    | 3        | 0.18          |
| (2,87)  | 1:1:A:LEU:HD22  | 1:34:A:LEU:HD13 | 1        | 0.18          |
| (2,37)  | 1:31:A:GLU:HA   | 1:32:A:LYS:H    | 5        | 0.18          |
| (2,37)  | 1:31:A:GLU:HA   | 1:32:A:LYS:H    | 7        | 0.18          |
| (1,518) | 1:14:A:ARG:HB3  | 1:14:A:ARG:HD2  | 9        | 0.18          |
| (1,513) | 1:32:A:LYS:HB2  | 1:35:A:PHE:HB3  | 4        | 0.18          |
| (1,401) | 1:6:A:3FB:HC2   | 1:6:A:3FB:HB1   | 5        | 0.18          |
| (1,331) | 1:24:A:LYS:HG2  | 1:21:A:PRO:HD3  | 2        | 0.18          |
| (1,298) | 1:18:A:ALA:HB3  | 1:25:A:GLN:HE21 | 2        | 0.18          |
| (1,194) | 1:28:A:LEU:HA   | 1:30:A:LYS:H    | 5        | 0.18          |
| (1,171) | 1:29:A:LYS:HA   | 1:30:A:LYS:H    | 3        | 0.18          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,171) | 1:29:A:LYS:HA   | 1:30:A:LYS:H    | 5        | 0.18          |
| (1,171) | 1:29:A:LYS:HA   | 1:30:A:LYS:H    | 10       | 0.18          |
| (1,101) | 1:6:A:3FB:HB1   | 1:6:A:3FB:H     | 10       | 0.18          |
| (1,25)  | 1:14:A:ARG:HG2  | 1:15:A:SER:H    | 2        | 0.18          |
| (1,17)  | 1:14:A:ARG:HB3  | 1:14:A:ARG:H    | 1        | 0.18          |
| (2,46)  | 1:21:A:PRO:HA   | 1:23:A:TRP:HD1  | 2        | 0.17          |
| (2,18)  | 1:6:A:3FB:HB2   | 1:7:A:LYS:H     | 5        | 0.17          |
| (1,581) | 1:34:A:LEU:H    | 1:35:A:PHE:H    | 5        | 0.17          |
| (1,569) | 1:17:A:PHE:HD1  | 1:17:A:PHE:H    | 6        | 0.17          |
| (1,558) | 1:23:A:TRP:HE3  | 1:27:A:ASN:H    | 2        | 0.17          |
| (1,535) | 1:22:A:LEU:HD21 | 1:26:A:GLN:HG3  | 3        | 0.17          |
| (1,518) | 1:14:A:ARG:HB3  | 1:14:A:ARG:HD2  | 4        | 0.17          |
| (1,349) | 1:34:A:LEU:HD12 | 1:34:A:LEU:HB2  | 3        | 0.17          |
| (1,278) | 1:24:A:LYS:HB3  | 1:23:A:TRP:HZ2  | 4        | 0.17          |
| (1,194) | 1:28:A:LEU:HA   | 1:30:A:LYS:H    | 2        | 0.17          |
| (1,175) | 1:15:A:SER:HA   | 1:18:A:ALA:H    | 4        | 0.17          |
| (1,170) | 1:9:A:VAL:HA    | 1:10:A:PHE:H    | 5        | 0.17          |
| (1,134) | 1:17:A:PHE:HB2  | 1:14:A:ARG:HH22 | 8        | 0.17          |
| (1,2)   | 1:9:A:VAL:HG13  | 1:9:A:VAL:H     | 9        | 0.17          |
| (3,28)  | 1:31:A:GLU:N    | 1:27:A:ASN:O    | 10       | 0.16          |
| (2,71)  | 1:24:A:LYS:HG2  | 1:23:A:TRP:HZ2  | 8        | 0.16          |
| (2,46)  | 1:21:A:PRO:HA   | 1:23:A:TRP:HD1  | 6        | 0.16          |
| (2,37)  | 1:31:A:GLU:HA   | 1:32:A:LYS:H    | 9        | 0.16          |
| (1,529) | 1:12:A:NLE:HG3  | 1:10:A:PHE:HB2  | 3        | 0.16          |
| (1,518) | 1:14:A:ARG:HB3  | 1:14:A:ARG:HD2  | 6        | 0.16          |
| (1,515) | 1:14:A:ARG:HB2  | 1:14:A:ARG:HD2  | 10       | 0.16          |
| (1,457) | 1:21:A:PRO:HG2  | 1:21:A:PRO:HA   | 4        | 0.16          |
| (1,401) | 1:6:A:3FB:HC2   | 1:6:A:3FB:HB1   | 10       | 0.16          |
| (1,238) | 1:23:A:TRP:HA   | 1:23:A:TRP:HE3  | 2        | 0.16          |
| (1,238) | 1:23:A:TRP:HA   | 1:23:A:TRP:HE3  | 8        | 0.16          |
| (1,208) | 1:27:A:ASN:HA   | 1:29:A:LYS:H    | 10       | 0.16          |
| (1,156) | 1:24:A:LYS:HA   | 1:27:A:ASN:HD22 | 6        | 0.16          |
| (1,101) | 1:6:A:3FB:HB1   | 1:6:A:3FB:H     | 9        | 0.16          |
| (1,76)  | 1:26:A:GLN:HG2  | 1:26:A:GLN:H    | 5        | 0.16          |
| (1,61)  | 1:31:A:GLU:HB2  | 1:30:A:LYS:H    | 9        | 0.16          |
| (1,41)  | 1:28:A:LEU:HG   | 1:27:A:ASN:H    | 10       | 0.16          |
| (1,40)  | 1:14:A:ARG:HB3  | 1:15:A:SER:H    | 1        | 0.16          |
| (1,2)   | 1:9:A:VAL:HG12  | 1:9:A:VAL:H     | 2        | 0.16          |
| (1,2)   | 1:9:A:VAL:HG13  | 1:9:A:VAL:H     | 7        | 0.16          |
| (1,2)   | 1:9:A:VAL:HG13  | 1:9:A:VAL:H     | 8        | 0.16          |
| (3,7)   | 1:10:A:PHE:H    | 1:6:A:3FB:O     | 2        | 0.15          |
| (3,7)   | 1:10:A:PHE:H    | 1:6:A:3FB:O     | 3        | 0.15          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (2,86)  | 1:1:A:LEU:HD23  | 1:34:A:LEU:HB2  | 5        | 0.15          |
| (2,37)  | 1:31:A:GLU:HA   | 1:32:A:LYS:H    | 2        | 0.15          |
| (1,574) | 1:23:A:TRP:HZ3  | 1:27:A:ASN:HD22 | 3        | 0.15          |
| (1,457) | 1:21:A:PRO:HG2  | 1:21:A:PRO:HA   | 10       | 0.15          |
| (1,452) | 1:26:A:GLN:HG2  | 1:23:A:TRP:HA   | 9        | 0.15          |
| (1,278) | 1:24:A:LYS:HB3  | 1:23:A:TRP:HZ2  | 9        | 0.15          |
| (1,219) | 1:13:A:THR:HA   | 1:14:A:ARG:H    | 4        | 0.15          |
| (1,171) | 1:29:A:LYS:HA   | 1:30:A:LYS:H    | 4        | 0.15          |
| (1,167) | 1:34:A:LEU:H    | 1:33:A:GLY:HA3  | 1        | 0.15          |
| (1,156) | 1:24:A:LYS:HA   | 1:27:A:ASN:HD22 | 5        | 0.15          |
| (1,101) | 1:6:A:3FB:HB1   | 1:6:A:3FB:H     | 2        | 0.15          |
| (1,2)   | 1:9:A:VAL:HG13  | 1:9:A:VAL:H     | 4        | 0.15          |
| (1,2)   | 1:9:A:VAL:HG12  | 1:9:A:VAL:H     | 5        | 0.15          |
| (3,29)  | 1:32:A:LYS:H    | 1:28:A:LEU:O    | 10       | 0.14          |
| (3,19)  | 1:27:A:ASN:H    | 1:23:A:TRP:O    | 1        | 0.14          |
| (3,16)  | 1:19:A:ASN:N    | 1:15:A:SER:O    | 2        | 0.14          |
| (3,4)   | 1:8:A:ALA:N     | 1:4:A:GLU:O     | 8        | 0.14          |
| (2,97)  | 1:26:A:GLN:HA   | 1:29:A:LYS:HD3  | 10       | 0.14          |
| (2,88)  | 1:28:A:LEU:HD13 | 1:25:A:GLN:HG2  | 5        | 0.14          |
| (1,529) | 1:12:A:NLE:HG3  | 1:10:A:PHE:HB2  | 5        | 0.14          |
| (1,469) | 1:32:A:LYS:HD3  | 1:32:A:LYS:HA   | 8        | 0.14          |
| (1,429) | 1:21:A:PRO:HD2  | 1:20:A:LEU:HA   | 7        | 0.14          |
| (1,349) | 1:34:A:LEU:HD13 | 1:34:A:LEU:HB2  | 2        | 0.14          |
| (1,290) | 1:9:A:VAL:HG23  | 1:10:A:PHE:HD2  | 7        | 0.14          |
| (1,235) | 1:23:A:TRP:HA   | 1:23:A:TRP:HD1  | 1        | 0.14          |
| (1,208) | 1:27:A:ASN:HA   | 1:29:A:LYS:H    | 7        | 0.14          |
| (1,194) | 1:28:A:LEU:HA   | 1:30:A:LYS:H    | 10       | 0.14          |
| (1,171) | 1:29:A:LYS:HA   | 1:30:A:LYS:H    | 9        | 0.14          |
| (1,125) | 1:14:A:ARG:HD2  | 1:14:A:ARG:HH22 | 4        | 0.14          |
| (1,125) | 1:14:A:ARG:HD3  | 1:14:A:ARG:HH22 | 5        | 0.14          |
| (1,125) | 1:14:A:ARG:HD3  | 1:14:A:ARG:HH22 | 6        | 0.14          |
| (1,125) | 1:14:A:ARG:HD3  | 1:14:A:ARG:HH22 | 7        | 0.14          |
| (1,101) | 1:6:A:3FB:HB1   | 1:6:A:3FB:H     | 6        | 0.14          |
| (1,101) | 1:6:A:3FB:HB1   | 1:6:A:3FB:H     | 7        | 0.14          |
| (1,50)  | 1:30:A:LYS:HB3  | 1:31:A:GLU:H    | 8        | 0.14          |
| (1,36)  | 1:28:A:LEU:HB3  | 1:29:A:LYS:H    | 6        | 0.14          |
| (1,9)   | 1:34:A:LEU:HD12 | 1:34:A:LEU:H    | 9        | 0.14          |
| (2,70)  | 1:20:A:LEU:HD12 | 1:25:A:GLN:H    | 1        | 0.13          |
| (1,558) | 1:23:A:TRP:HE3  | 1:27:A:ASN:H    | 6        | 0.13          |
| (1,351) | 1:20:A:LEU:HD13 | 1:12:A:NLE:HD2  | 3        | 0.13          |
| (1,349) | 1:34:A:LEU:HD11 | 1:34:A:LEU:HB3  | 1        | 0.13          |
| (1,278) | 1:24:A:LYS:HB3  | 1:23:A:TRP:HZ2  | 10       | 0.13          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,252) | 1:25:A:GLN:HG3  | 1:25:A:GLN:HE22 | 2        | 0.13          |
| (1,252) | 1:25:A:GLN:HG3  | 1:25:A:GLN:HE22 | 7        | 0.13          |
| (1,252) | 1:25:A:GLN:HG3  | 1:25:A:GLN:HE22 | 8        | 0.13          |
| (1,238) | 1:23:A:TRP:HA   | 1:23:A:TRP:HE3  | 4        | 0.13          |
| (1,238) | 1:23:A:TRP:HA   | 1:23:A:TRP:HE3  | 9        | 0.13          |
| (1,125) | 1:14:A:ARG:HD3  | 1:14:A:ARG:HH22 | 2        | 0.13          |
| (1,125) | 1:14:A:ARG:HD2  | 1:14:A:ARG:HH22 | 3        | 0.13          |
| (1,125) | 1:14:A:ARG:HD3  | 1:14:A:ARG:HH22 | 8        | 0.13          |
| (1,125) | 1:14:A:ARG:HD2  | 1:14:A:ARG:HH22 | 9        | 0.13          |
| (1,76)  | 1:26:A:GLN:HG2  | 1:26:A:GLN:H    | 10       | 0.13          |
| (1,2)   | 1:9:A:VAL:HG12  | 1:9:A:VAL:H     | 6        | 0.13          |
| (3,27)  | 1:31:A:GLU:H    | 1:27:A:ASN:O    | 2        | 0.12          |
| (2,80)  | 1:20:A:LEU:HD12 | 1:12:A:NLE:HB2  | 4        | 0.12          |
| (2,37)  | 1:31:A:GLU:HA   | 1:32:A:LYS:H    | 8        | 0.12          |
| (1,542) | 1:23:A:TRP:HZ3  | 1:23:A:TRP:HH2  | 1        | 0.12          |
| (1,542) | 1:23:A:TRP:HZ3  | 1:23:A:TRP:HH2  | 2        | 0.12          |
| (1,542) | 1:23:A:TRP:HZ3  | 1:23:A:TRP:HH2  | 3        | 0.12          |
| (1,542) | 1:23:A:TRP:HZ3  | 1:23:A:TRP:HH2  | 4        | 0.12          |
| (1,542) | 1:23:A:TRP:HZ3  | 1:23:A:TRP:HH2  | 5        | 0.12          |
| (1,542) | 1:23:A:TRP:HZ3  | 1:23:A:TRP:HH2  | 6        | 0.12          |
| (1,542) | 1:23:A:TRP:HZ3  | 1:23:A:TRP:HH2  | 7        | 0.12          |
| (1,542) | 1:23:A:TRP:HZ3  | 1:23:A:TRP:HH2  | 8        | 0.12          |
| (1,542) | 1:23:A:TRP:HZ3  | 1:23:A:TRP:HH2  | 9        | 0.12          |
| (1,542) | 1:23:A:TRP:HZ3  | 1:23:A:TRP:HH2  | 10       | 0.12          |
| (1,518) | 1:14:A:ARG:HB3  | 1:14:A:ARG:HD2  | 5        | 0.12          |
| (1,415) | 1:19:A:ASN:HB3  | 1:16:A:ALA:HA   | 1        | 0.12          |
| (1,349) | 1:34:A:LEU:HD12 | 1:34:A:LEU:HB2  | 5        | 0.12          |
| (1,349) | 1:34:A:LEU:HD11 | 1:34:A:LEU:HB3  | 8        | 0.12          |
| (1,252) | 1:25:A:GLN:HG2  | 1:25:A:GLN:HE22 | 1        | 0.12          |
| (1,252) | 1:25:A:GLN:HG3  | 1:25:A:GLN:HE22 | 3        | 0.12          |
| (1,252) | 1:25:A:GLN:HG3  | 1:25:A:GLN:HE22 | 4        | 0.12          |
| (1,252) | 1:25:A:GLN:HG3  | 1:25:A:GLN:HE22 | 5        | 0.12          |
| (1,252) | 1:25:A:GLN:HG2  | 1:25:A:GLN:HE22 | 6        | 0.12          |
| (1,252) | 1:25:A:GLN:HG3  | 1:25:A:GLN:HE22 | 9        | 0.12          |
| (1,252) | 1:25:A:GLN:HG3  | 1:25:A:GLN:HE22 | 10       | 0.12          |
| (1,240) | 1:35:A:PHE:HA   | 1:35:A:PHE:HE2  | 1        | 0.12          |
| (1,235) | 1:23:A:TRP:HA   | 1:23:A:TRP:HD1  | 6        | 0.12          |
| (1,235) | 1:23:A:TRP:HA   | 1:23:A:TRP:HD1  | 7        | 0.12          |
| (1,171) | 1:29:A:LYS:HA   | 1:30:A:LYS:H    | 1        | 0.12          |
| (1,154) | 1:8:A:ALA:HA    | 1:9:A:VAL:H     | 7        | 0.12          |
| (1,154) | 1:8:A:ALA:HA    | 1:9:A:VAL:H     | 8        | 0.12          |
| (1,154) | 1:8:A:ALA:HA    | 1:9:A:VAL:H     | 10       | 0.12          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,125) | 1:14:A:ARG:HD3  | 1:14:A:ARG:HH22 | 1        | 0.12          |
| (1,125) | 1:14:A:ARG:HD2  | 1:14:A:ARG:HH22 | 10       | 0.12          |
| (1,117) | 1:6:A:3FB:HC1   | 1:6:A:3FB:H     | 2        | 0.12          |
| (1,101) | 1:6:A:3FB:HB1   | 1:6:A:3FB:H     | 8        | 0.12          |
| (1,62)  | 1:31:A:GLU:HB3  | 1:32:A:LYS:H    | 6        | 0.12          |
| (1,50)  | 1:30:A:LYS:HB3  | 1:31:A:GLU:H    | 9        | 0.12          |
| (1,2)   | 1:9:A:VAL:HG11  | 1:9:A:VAL:H     | 10       | 0.12          |
| (3,30)  | 1:32:A:LYS:N    | 1:28:A:LEU:O    | 8        | 0.11          |
| (3,19)  | 1:27:A:ASN:H    | 1:23:A:TRP:O    | 2        | 0.11          |
| (3,2)   | 1:7:A:LYS:N     | 1:3:A:ASP:O     | 3        | 0.11          |
| (2,14)  | 1:28:A:LEU:HB2  | 1:29:A:LYS:H    | 6        | 0.11          |
| (1,582) | 1:24:A:LYS:HZ1  | 1:27:A:ASN:HD22 | 3        | 0.11          |
| (1,582) | 1:24:A:LYS:HZ1  | 1:27:A:ASN:HD22 | 4        | 0.11          |
| (1,558) | 1:23:A:TRP:HE3  | 1:27:A:ASN:H    | 8        | 0.11          |
| (1,430) | 1:15:A:SER:HB2  | 1:15:A:SER:HA   | 1        | 0.11          |
| (1,430) | 1:15:A:SER:HB2  | 1:15:A:SER:HA   | 2        | 0.11          |
| (1,430) | 1:15:A:SER:HB2  | 1:15:A:SER:HA   | 3        | 0.11          |
| (1,430) | 1:15:A:SER:HB2  | 1:15:A:SER:HA   | 5        | 0.11          |
| (1,403) | 1:5:A:ASP:HB2   | 1:6:A:3FB:HB2   | 5        | 0.11          |
| (1,403) | 1:5:A:ASP:HB2   | 1:6:A:3FB:HB2   | 10       | 0.11          |
| (1,351) | 1:20:A:LEU:HD12 | 1:12:A:NLE:HD2  | 4        | 0.11          |
| (1,272) | 1:18:A:ALA:HB2  | 1:17:A:PHE:HD2  | 8        | 0.11          |
| (1,238) | 1:23:A:TRP:HA   | 1:23:A:TRP:HE3  | 7        | 0.11          |
| (1,238) | 1:23:A:TRP:HA   | 1:23:A:TRP:HE3  | 10       | 0.11          |
| (1,235) | 1:23:A:TRP:HA   | 1:23:A:TRP:HD1  | 3        | 0.11          |
| (1,235) | 1:23:A:TRP:HA   | 1:23:A:TRP:HD1  | 10       | 0.11          |
| (1,203) | 1:27:A:ASN:HA   | 1:31:A:GLU:H    | 6        | 0.11          |
| (1,171) | 1:29:A:LYS:HA   | 1:30:A:LYS:H    | 8        | 0.11          |
| (1,154) | 1:8:A:ALA:HA    | 1:9:A:VAL:H     | 4        | 0.11          |
| (1,154) | 1:8:A:ALA:HA    | 1:9:A:VAL:H     | 5        | 0.11          |
| (1,154) | 1:8:A:ALA:HA    | 1:9:A:VAL:H     | 9        | 0.11          |
| (1,90)  | 1:27:A:ASN:HB3  | 1:29:A:LYS:H    | 5        | 0.11          |
| (1,26)  | 1:12:A:NLE:HG3  | 1:11:A:GLY:H    | 3        | 0.11          |
| (3,24)  | 1:29:A:LYS:N    | 1:25:A:GLN:O    | 8        | 0.1           |
| (3,21)  | 1:28:A:LEU:H    | 1:24:A:LYS:O    | 5        | 0.1           |
| (3,19)  | 1:27:A:ASN:H    | 1:23:A:TRP:O    | 4        | 0.1           |
| (3,19)  | 1:27:A:ASN:H    | 1:23:A:TRP:O    | 8        | 0.1           |
| (3,6)   | 1:9:A:VAL:N     | 1:5:A:ASP:O     | 1        | 0.1           |
| (2,99)  | 1:10:A:PHE:HA   | 1:13:A:THR:HG22 | 7        | 0.1           |
| (2,71)  | 1:24:A:LYS:HG2  | 1:23:A:TRP:HZ2  | 9        | 0.1           |
| (2,37)  | 1:31:A:GLU:HA   | 1:32:A:LYS:H    | 1        | 0.1           |
| (1,254) | 1:20:A:LEU:HB2  | 1:25:A:GLN:HE22 | 8        | 0.1           |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,238) | 1:23:A:TRP:HA  | 1:23:A:TRP:HE3 | 3        | 0.1           |
| (1,227) | 1:23:A:TRP:HB2 | 1:23:A:TRP:H   | 10       | 0.1           |
| (1,154) | 1:8:A:ALA:HA   | 1:9:A:VAL:H    | 1        | 0.1           |
| (1,154) | 1:8:A:ALA:HA   | 1:9:A:VAL:H    | 2        | 0.1           |
| (1,2)   | 1:9:A:VAL:HG13 | 1:9:A:VAL:H    | 1        | 0.1           |

## 10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found