



# Full wwPDB NMR Structure Validation Report ⓘ

Mar 6, 2026 – 09:45 AM UTC

PDB ID : 6SAB / pdb\_00006sab  
BMRB ID : 34418  
Title : M-BUTX-Ptr1a (Parabuthus transvaalicus)  
Authors : Meudal, H.; Landon, C.; Delmas, A.F.  
Deposited on : 2019-07-16

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

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

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with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

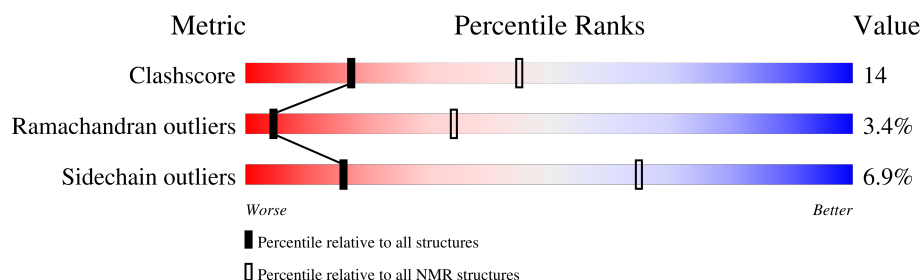
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 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     | 34     | <br>65% 32% .    |

## 2 Ensemble composition and analysis

This entry contains 10 models. Model 6 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

| Well-defined (core) protein residues |                       |                   |              |
|--------------------------------------|-----------------------|-------------------|--------------|
| Well-defined core                    | Residue range (total) | Backbone RMSD (Å) | Medoid model |
| 1                                    | A:2-A:34 (33)         | 0.70              | 6            |

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

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

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

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

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

There is only 1 type of molecule in this entry. The entry contains 527 atoms, of which 271 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called M-BUTX-Ptr1a.

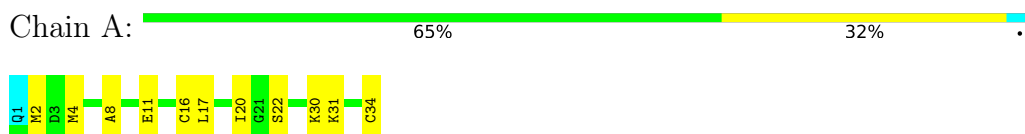
| Mol | Chain | Residues | Atoms |     |     |    |    |   | Trace |
|-----|-------|----------|-------|-----|-----|----|----|---|-------|
| 1   | A     | 34       | Total | C   | H   | N  | O  | S | 0     |
|     |       |          | 527   | 155 | 271 | 47 | 45 | 9 |       |

## 4 Residue-property plots

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

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

- Molecule 1: M-BUTX-Ptr1a

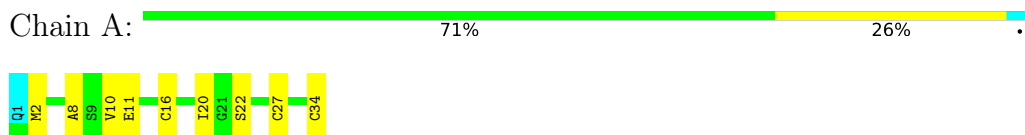


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

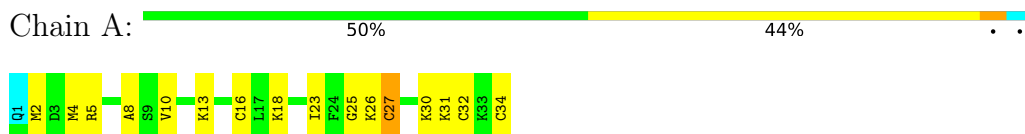
#### 4.2.1 Score per residue for model 1

- Molecule 1: M-BUTX-Ptr1a



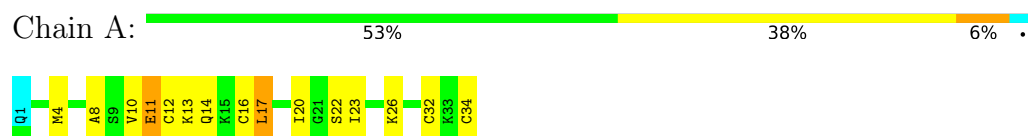
#### 4.2.2 Score per residue for model 2

- Molecule 1: M-BUTX-Ptr1a



### 4.2.3 Score per residue for model 3

- Molecule 1: M-BUTX-Ptr1a



### 4.2.4 Score per residue for model 4

- Molecule 1: M-BUTX-Ptr1a



### 4.2.5 Score per residue for model 5

- Molecule 1: M-BUTX-Ptr1a



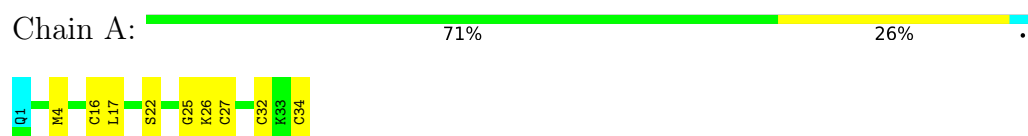
### 4.2.6 Score per residue for model 6 (medoid)

- Molecule 1: M-BUTX-Ptr1a



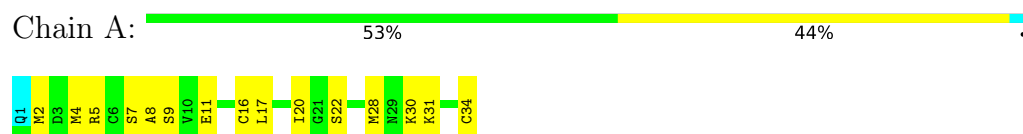
### 4.2.7 Score per residue for model 7

- Molecule 1: M-BUTX-Ptr1a



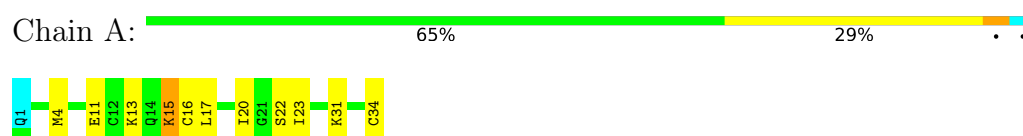
#### 4.2.8 Score per residue for model 8

- Molecule 1: M-BUTX-Ptr1a



#### 4.2.9 Score per residue for model 9

- Molecule 1: M-BUTX-Ptr1a



#### 4.2.10 Score per residue for model 10

- Molecule 1: M-BUTX-Ptr1a



## 5 Refinement protocol and experimental data overview

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

Of the 25 calculated structures, 10 were deposited, based on the following criterion: *total energies and restraint violation statistics*.

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

| Software name | Classification        | Version |
|---------------|-----------------------|---------|
| CNS           | refinement            |         |
| 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                       | 235            |
| Number of shifts mapped to atoms             | 235            |
| 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](#)

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     | 247   | 261      | 261      | 7±2     |
| All | All   | 2470  | 2610     | 2610     | 69      |

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 14.

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:CYS:SG   | 1:A:22:SER:HB2 | 0.73     | 2.24        | 8      | 3     |
| 1:A:16:CYS:SG   | 1:A:25:GLY:HA2 | 0.68     | 2.27        | 2      | 2     |
| 1:A:20:ILE:HG12 | 1:A:34:CYS:SG  | 0.67     | 2.29        | 3      | 6     |
| 1:A:16:CYS:SG   | 1:A:22:SER:HB3 | 0.64     | 2.32        | 3      | 4     |
| 1:A:4:MET:HA    | 1:A:8:ALA:HB2  | 0.61     | 1.72        | 2      | 2     |
| 1:A:26:LYS:O    | 1:A:32:CYS:HA  | 0.61     | 1.96        | 3      | 4     |
| 1:A:2:MET:HG3   | 1:A:8:ALA:O    | 0.61     | 1.96        | 1      | 1     |
| 1:A:16:CYS:CB   | 1:A:34:CYS:SG  | 0.57     | 2.92        | 4      | 1     |
| 1:A:25:GLY:HA2  | 1:A:34:CYS:SG  | 0.54     | 2.42        | 2      | 3     |
| 1:A:13:LYS:HD3  | 1:A:23:ILE:O   | 0.53     | 2.02        | 3      | 3     |
| 1:A:4:MET:N     | 1:A:8:ALA:HB2  | 0.53     | 2.19        | 10     | 1     |
| 1:A:2:MET:CB    | 1:A:8:ALA:HA   | 0.52     | 2.35        | 4      | 2     |
| 1:A:16:CYS:SG   | 1:A:25:GLY:CA  | 0.50     | 2.99        | 2      | 2     |
| 1:A:13:LYS:O    | 1:A:17:LEU:HB2 | 0.50     | 2.07        | 3      | 2     |

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| Atom-1         | Atom-2         | Clash(Å) | Distance(Å) | Models |       |
|----------------|----------------|----------|-------------|--------|-------|
|                |                |          |             | Worst  | Total |
| 1:A:4:MET:H    | 1:A:8:ALA:HB2  | 0.50     | 1.65        | 10     | 1     |
| 1:A:2:MET:HB2  | 1:A:8:ALA:HA   | 0.49     | 1.84        | 6      | 3     |
| 1:A:30:LYS:C   | 1:A:31:LYS:HD3 | 0.49     | 2.32        | 6      | 2     |
| 1:A:4:MET:O    | 1:A:31:LYS:HB3 | 0.49     | 2.08        | 4      | 1     |
| 1:A:5:ARG:HA   | 1:A:30:LYS:O   | 0.48     | 2.08        | 4      | 3     |
| 1:A:2:MET:HA   | 1:A:8:ALA:CB   | 0.47     | 2.39        | 8      | 1     |
| 1:A:8:ALA:HB3  | 1:A:11:GLU:CD  | 0.47     | 2.35        | 10     | 3     |
| 1:A:12:CYS:HA  | 1:A:32:CYS:CB  | 0.47     | 2.39        | 3      | 3     |
| 1:A:8:ALA:HB3  | 1:A:11:GLU:HG3 | 0.47     | 1.86        | 3      | 1     |
| 1:A:30:LYS:C   | 1:A:31:LYS:HD2 | 0.47     | 2.35        | 10     | 1     |
| 1:A:11:GLU:O   | 1:A:15:LYS:HB2 | 0.45     | 2.12        | 9      | 1     |
| 1:A:16:CYS:HB3 | 1:A:22:SER:O   | 0.45     | 2.11        | 6      | 3     |
| 1:A:13:LYS:HD2 | 1:A:23:ILE:O   | 0.44     | 2.13        | 6      | 1     |
| 1:A:2:MET:HB3  | 1:A:7:SER:C    | 0.44     | 2.37        | 4      | 1     |
| 1:A:31:LYS:N   | 1:A:31:LYS:HD3 | 0.43     | 2.28        | 4      | 1     |
| 1:A:2:MET:HB3  | 1:A:7:SER:O    | 0.42     | 2.14        | 4      | 1     |
| 1:A:2:MET:HG2  | 1:A:8:ALA:O    | 0.42     | 2.15        | 10     | 1     |
| 1:A:10:VAL:O   | 1:A:14:GLN:HB2 | 0.41     | 2.15        | 3      | 1     |
| 1:A:16:CYS:HB2 | 1:A:34:CYS:SG  | 0.41     | 2.55        | 4      | 1     |
| 1:A:27:CYS:HA  | 1:A:31:LYS:O   | 0.41     | 2.16        | 2      | 1     |
| 1:A:8:ALA:HB3  | 1:A:11:GLU:CG  | 0.41     | 2.45        | 3      | 1     |
| 1:A:4:MET:HB2  | 1:A:31:LYS:NZ  | 0.40     | 2.31        | 8      | 1     |

## 6.3 Torsion angles

### 6.3.1 Protein backbone

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     | 32/34 (94%)   | 21±2 (66±6%) | 10±2 (31±7%) | 1±1 (3±3%) | <b>4</b>    | 34 |
| All | All   | 320/340 (94%) | 211 (66%)    | 98 (31%)     | 11 (3%)    | <b>4</b>    | 34 |

All 5 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     | 27  | CYS  | 4              |
| 1   | A     | 10  | VAL  | 3              |
| 1   | A     | 7   | SER  | 2              |
| 1   | A     | 9   | SER  | 1              |
| 1   | A     | 2   | MET  | 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     | 29/30 (97%)   | 27±1 (93±3%) | 2±1 (7±3%) | 16          | 65 |
| All | All   | 290/300 (97%) | 270 (93%)    | 20 (7%)    | 16          | 65 |

All 7 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     | 17  | LEU  | 6              |
| 1   | A     | 15  | LYS  | 4              |
| 1   | A     | 31  | LYS  | 3              |
| 1   | A     | 4   | MET  | 3              |
| 1   | A     | 11  | GLU  | 2              |
| 1   | A     | 18  | LYS  | 1              |
| 1   | A     | 28  | MET  | 1              |

### 6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.6 Ligand geometry

There are no ligands in this entry.

## 6.7 Other polymers

There are no such molecules in this entry.

## 6.8 Polymer linkage issues

There are no chain breaks in this entry.

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

The completeness of assignment taking into account all chemical shift lists is 53% for the well-defined parts and 53% 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                  | 235 |
| Number of shifts mapped to atoms        | 235 |
| 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. 228 atoms were assigned a chemical shift out of a possible 431. 0 out of 2 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total         | <sup>1</sup> H | <sup>13</sup> C | <sup>15</sup> N |
|-----------|---------------|----------------|-----------------|-----------------|
| Backbone  | 68/167 (41%)  | 68/68 (100%)   | 0/66 (0%)       | 0/33 (0%)       |
| Sidechain | 155/254 (61%) | 154/164 (94%)  | 1/78 (1%)       | 0/12 (0%)       |
| Aromatic  | 5/10 (50%)    | 5/5 (100%)     | 0/5 (0%)        | 0/0 (—%)        |
| Overall   | 228/431 (53%) | 227/237 (96%)  | 1/149 (1%)      | 0/45 (0%)       |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 53%, i.e. 235 atoms were assigned a chemical shift out of a possible 446. 0 out of 2 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total         | $^1\text{H}$  | $^{13}\text{C}$ | $^{15}\text{N}$ |
|-----------|---------------|---------------|-----------------|-----------------|
| Backbone  | 69/172 (40%)  | 69/70 (99%)   | 0/68 (0%)       | 0/34 (0%)       |
| Sidechain | 161/264 (61%) | 160/170 (94%) | 1/81 (1%)       | 0/13 (0%)       |
| Aromatic  | 5/10 (50%)    | 5/5 (100%)    | 0/5 (0%)        | 0/0 (—%)        |
| Overall   | 235/446 (53%) | 234/245 (96%) | 1/154 (1%)      | 0/47 (0%)       |

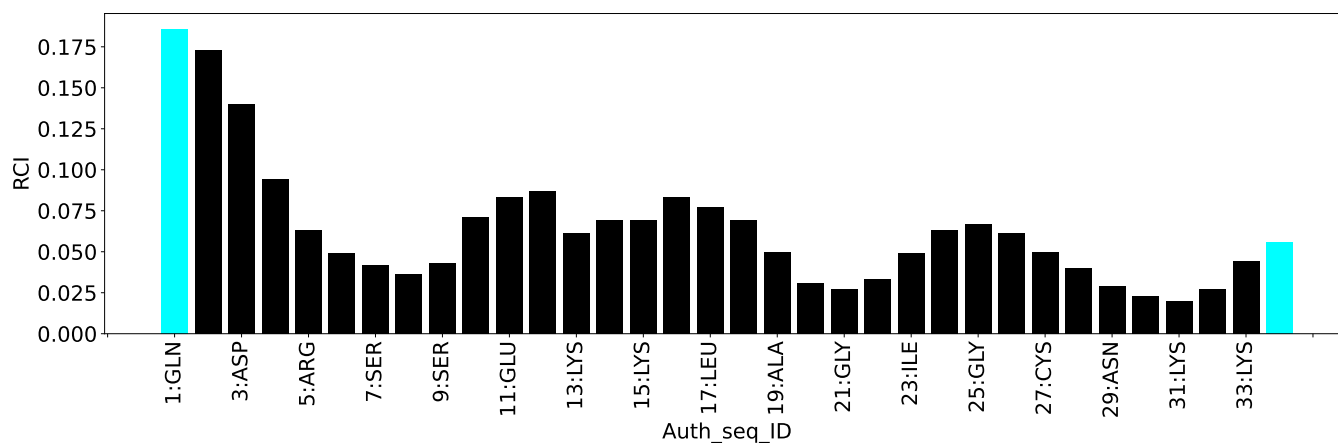
### 7.1.4 Statistically unusual chemical shifts [i](#)

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                                | 847   |
| Intra-residue ( $ i-j =0$ )                              | 290   |
| Sequential ( $ i-j =1$ )                                 | 229   |
| Medium range ( $ i-j >1$ and $ i-j <5$ )                 | 163   |
| Long range ( $ i-j \geq 5$ )                             | 157   |
| Inter-chain                                              | 0     |
| Hydrogen bond restraints                                 | 8     |
| Disulfide bond restraints                                | 0     |
| Total dihedral-angle restraints                          | 0     |
| Number of unmapped restraints                            | 0     |
| Number of restraints per residue                         | 24.9  |
| Number of long range restraints per residue <sup>1</sup> | 4.7   |

<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)  | 21.1                                   | 0.2     |
| 0.2-0.5 (Medium) | 38.1                                   | 0.5     |
| >0.5 (Large)     | 49.2                                   | 3.26    |

### 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 ⓘ

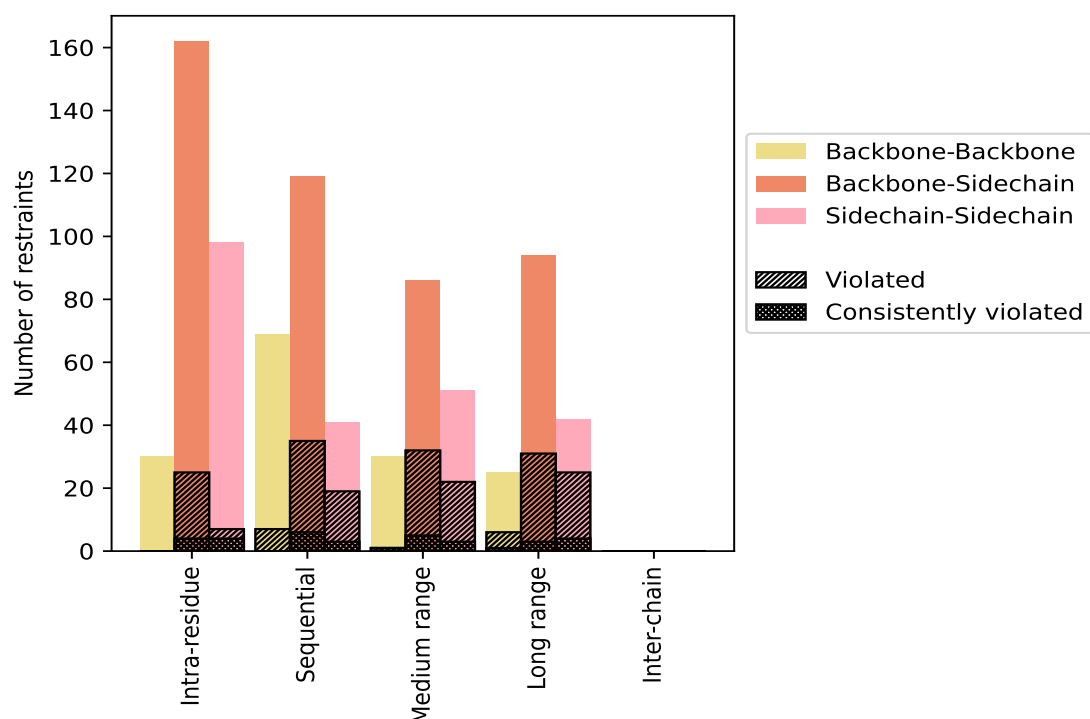
### 9.1 Summary of distance violations ⓘ

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="#">290</a> | <a href="#">34.2</a>  | <a href="#">32</a>    | <a href="#">11.0</a> | <a href="#">3.8</a>  | <a href="#">8</a>                  | <a href="#">2.8</a> | <a href="#">0.9</a> |
| Backbone-Backbone                                          | 30                  | 3.5                   | 0                     | 0.0                  | 0.0                  | 0                                  | 0.0                 | 0.0                 |
| Backbone-Sidechain                                         | 162                 | 19.1                  | 25                    | 15.4                 | 3.0                  | 4                                  | 2.5                 | 0.5                 |
| Sidechain-Sidechain                                        | 98                  | 11.6                  | 7                     | 7.1                  | 0.8                  | 4                                  | 4.1                 | 0.5                 |
| <a href="#">Sequential ( i-j =1)</a>                       | <a href="#">229</a> | <a href="#">27.0</a>  | <a href="#">61</a>    | <a href="#">26.6</a> | <a href="#">7.2</a>  | <a href="#">9</a>                  | <a href="#">3.9</a> | <a href="#">1.1</a> |
| Backbone-Backbone                                          | 69                  | 8.1                   | 7                     | 10.1                 | 0.8                  | 0                                  | 0.0                 | 0.0                 |
| Backbone-Sidechain                                         | 119                 | 14.0                  | 35                    | 29.4                 | 4.1                  | 6                                  | 5.0                 | 0.7                 |
| Sidechain-Sidechain                                        | 41                  | 4.8                   | 19                    | 46.3                 | 2.2                  | 3                                  | 7.3                 | 0.4                 |
| <a href="#">Medium range ( i-j &gt;1 &amp;  i-j &lt;5)</a> | <a href="#">163</a> | <a href="#">19.2</a>  | <a href="#">55</a>    | <a href="#">33.7</a> | <a href="#">6.5</a>  | <a href="#">9</a>                  | <a href="#">5.5</a> | <a href="#">1.1</a> |
| Backbone-Backbone                                          | 30                  | 3.5                   | 1                     | 3.3                  | 0.1                  | 1                                  | 3.3                 | 0.1                 |
| Backbone-Sidechain                                         | 82                  | 9.7                   | 32                    | 39.0                 | 3.8                  | 5                                  | 6.1                 | 0.6                 |
| Sidechain-Sidechain                                        | 51                  | 6.0                   | 22                    | 43.1                 | 2.6                  | 3                                  | 5.9                 | 0.4                 |
| <a href="#">Long range ( i-j ≥5)</a>                       | <a href="#">157</a> | <a href="#">18.5</a>  | <a href="#">62</a>    | <a href="#">39.5</a> | <a href="#">7.3</a>  | <a href="#">8</a>                  | <a href="#">5.1</a> | <a href="#">0.9</a> |
| Backbone-Backbone                                          | 25                  | 3.0                   | 6                     | 24.0                 | 0.7                  | 1                                  | 4.0                 | 0.1                 |
| Backbone-Sidechain                                         | 90                  | 10.6                  | 31                    | 34.4                 | 3.7                  | 3                                  | 3.3                 | 0.4                 |
| Sidechain-Sidechain                                        | 42                  | 5.0                   | 25                    | 59.5                 | 3.0                  | 4                                  | 9.5                 | 0.5                 |
| <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="#">8</a>   | <a href="#">0.9</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="#">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="#">847</a> | <a href="#">100.0</a> | <a href="#">210</a>   | <a href="#">24.8</a> | <a href="#">24.8</a> | <a href="#">34</a>                 | <a href="#">4.0</a> | <a href="#">4.0</a> |
| Backbone-Backbone                                          | 154                 | 18.2                  | 14                    | 9.1                  | 1.7                  | 2                                  | 1.3                 | 0.2                 |
| Backbone-Sidechain                                         | 461                 | 54.4                  | 123                   | 26.7                 | 14.5                 | 18                                 | 3.9                 | 2.1                 |
| Sidechain-Sidechain                                        | 232                 | 27.4                  | 73                    | 31.5                 | 8.6                  | 14                                 | 6.0                 | 1.7                 |

<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 disulfide bonds are counted in their appropriate category on the x-axis

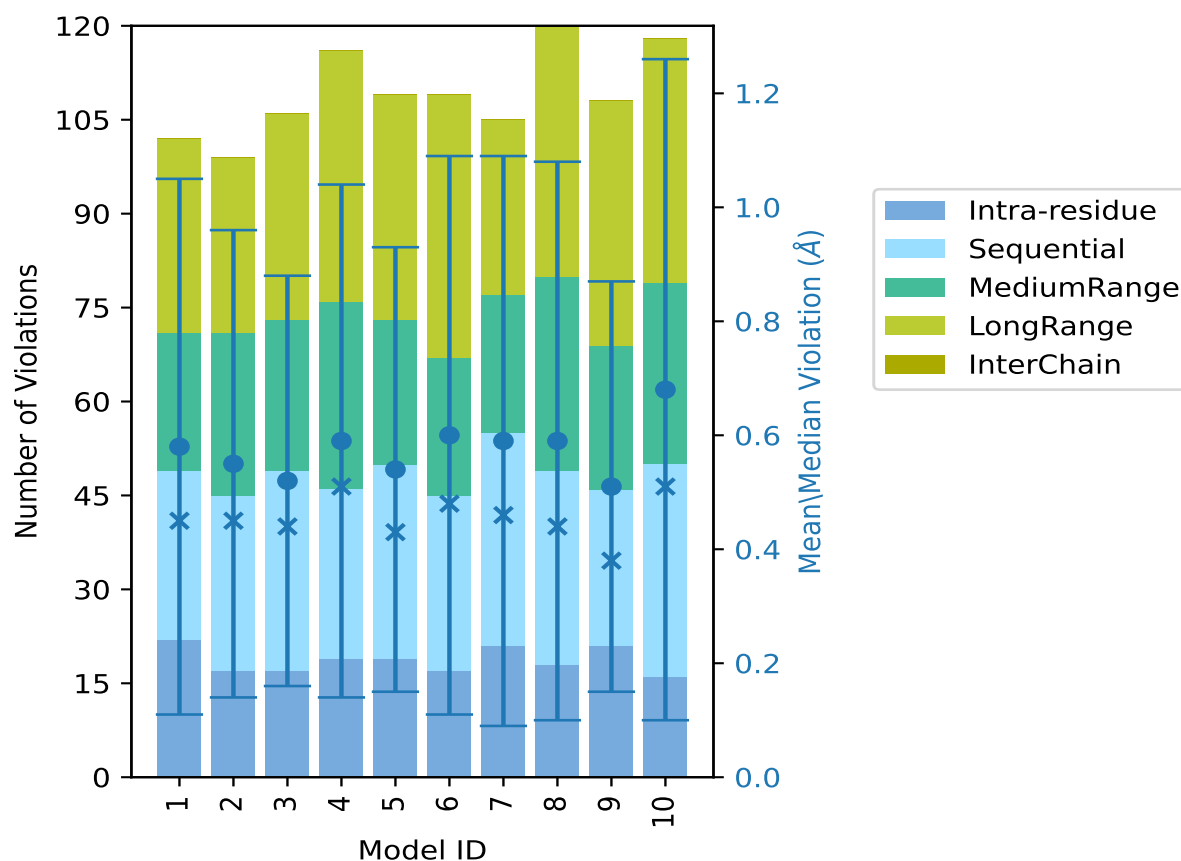
## 9.2 Distance violation statistics for each model [i](#)

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        | 22                   | 27              | 22              | 31              | 0               | 102   | 0.58     | 2.71    | 0.47                | 0.45       |
| 2        | 17                   | 28              | 26              | 28              | 0               | 99    | 0.55     | 2.16    | 0.41                | 0.45       |
| 3        | 17                   | 32              | 24              | 33              | 0               | 106   | 0.52     | 2.22    | 0.36                | 0.44       |
| 4        | 19                   | 27              | 30              | 40              | 0               | 116   | 0.59     | 2.73    | 0.45                | 0.51       |
| 5        | 19                   | 31              | 23              | 36              | 0               | 109   | 0.54     | 2.38    | 0.39                | 0.43       |
| 6        | 17                   | 28              | 22              | 42              | 0               | 109   | 0.6      | 3.05    | 0.49                | 0.48       |
| 7        | 21                   | 34              | 22              | 28              | 0               | 105   | 0.59     | 3.26    | 0.5                 | 0.46       |
| 8        | 18                   | 31              | 31              | 40              | 0               | 120   | 0.59     | 2.97    | 0.49                | 0.44       |
| 9        | 21                   | 25              | 23              | 39              | 0               | 108   | 0.51     | 1.85    | 0.36                | 0.38       |
| 10       | 16                   | 34              | 29              | 39              | 0               | 118   | 0.68     | 2.85    | 0.58                | 0.51       |

<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, 629(IR:258, SQ:168, MR:108, LR:95, 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>       | %    |
| 5                             | 13              | 11              | 10              | 0               | 39    | 1                        | 10.0 |
| 3                             | 2               | 9               | 6               | 0               | 20    | 2                        | 20.0 |
| 4                             | 8               | 6               | 1               | 0               | 19    | 3                        | 30.0 |

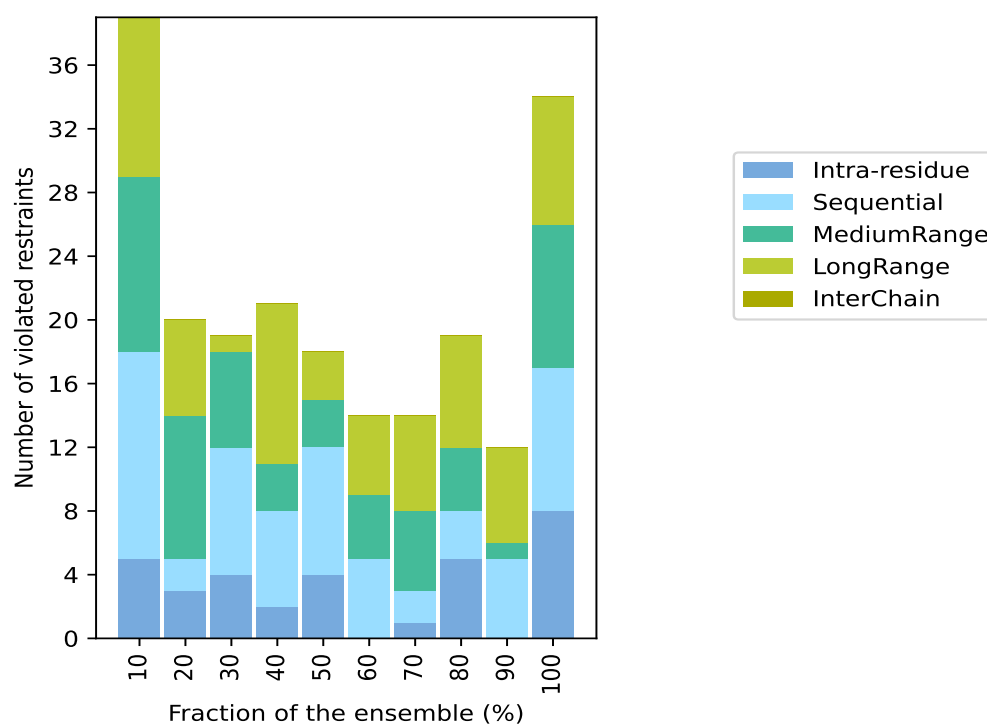
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| Number of violated restraints |                 |                 |                 |                 |       | Fraction of the ensemble |       |
|-------------------------------|-----------------|-----------------|-----------------|-----------------|-------|--------------------------|-------|
| 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>       | %     |
| 2                             | 6               | 3               | 10              | 0               | 21    | 4                        | 40.0  |
| 4                             | 8               | 3               | 3               | 0               | 18    | 5                        | 50.0  |
| 0                             | 5               | 4               | 5               | 0               | 14    | 6                        | 60.0  |
| 1                             | 2               | 5               | 6               | 0               | 14    | 7                        | 70.0  |
| 5                             | 3               | 4               | 7               | 0               | 19    | 8                        | 80.0  |
| 0                             | 5               | 1               | 6               | 0               | 12    | 9                        | 90.0  |
| 8                             | 9               | 9               | 8               | 0               | 34    | 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 [i](#)

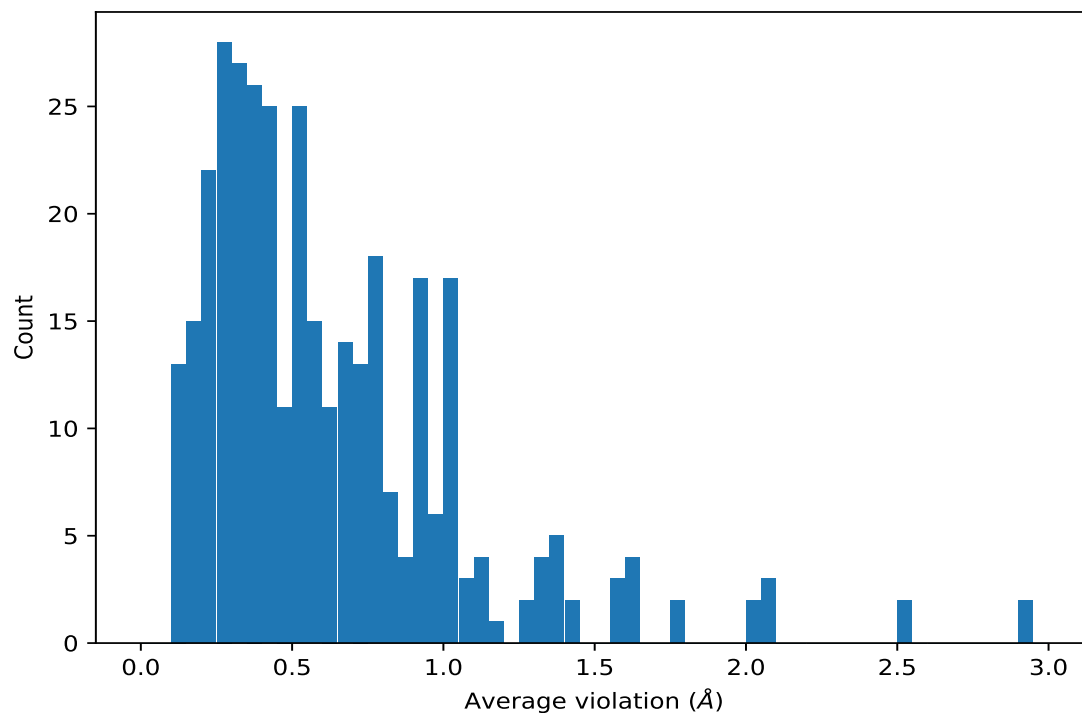


## 9.4 Most violated distance restraints in the ensemble [i](#)

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

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

in the ensemble



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

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

| Key     | Atom-1         | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|----------------|-----------------|---------------------|----------|---------------------|------------|
| (2,221) | 1:13:A:LYS:HE3 | 1:10:A:VAL:HG11 | 10                  | 1.65     | 0.93                | 1.6        |
| (2,221) | 1:13:A:LYS:HE3 | 1:10:A:VAL:HG13 | 10                  | 1.65     | 0.93                | 1.6        |
| (2,221) | 1:13:A:LYS:HE2 | 1:10:A:VAL:HG13 | 10                  | 1.65     | 0.93                | 1.6        |
| (2,221) | 1:13:A:LYS:HE3 | 1:10:A:VAL:HG12 | 10                  | 1.65     | 0.93                | 1.6        |
| (2,51)  | 1:24:A:PHE:HD2 | 1:13:A:LYS:HB3  | 10                  | 1.13     | 0.09                | 1.13       |
| (2,51)  | 1:24:A:PHE:HD1 | 1:13:A:LYS:HB3  | 10                  | 1.13     | 0.09                | 1.13       |
| (3,332) | 1:24:A:PHE:HD2 | 1:23:A:ILE:HD12 | 10                  | 1.03     | 0.2                 | 1.06       |
| (3,332) | 1:24:A:PHE:HD2 | 1:23:A:ILE:HD11 | 10                  | 1.03     | 0.2                 | 1.06       |
| (3,332) | 1:24:A:PHE:HD1 | 1:23:A:ILE:HD12 | 10                  | 1.03     | 0.2                 | 1.06       |
| (3,332) | 1:24:A:PHE:HD1 | 1:23:A:ILE:HD11 | 10                  | 1.03     | 0.2                 | 1.06       |
| (3,257) | 1:19:A:ALA:H   | 1:15:A:LYS:HB2  | 10                  | 0.99     | 0.1                 | 1.04       |
| (2,196) | 1:21:A:GLY:HA2 | 1:20:A:ILE:HD12 | 10                  | 0.99     | 0.24                | 0.95       |
| (2,196) | 1:21:A:GLY:HA2 | 1:20:A:ILE:HD11 | 10                  | 0.99     | 0.24                | 0.95       |
| (2,196) | 1:21:A:GLY:HA2 | 1:20:A:ILE:HG21 | 10                  | 0.99     | 0.24                | 0.95       |
| (2,196) | 1:21:A:GLY:HA2 | 1:20:A:ILE:HG23 | 10                  | 0.99     | 0.24                | 0.95       |

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| Key     | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (2,196) | 1:21:A:GLY:HA2  | 1:20:A:ILE:HG22 | 10                  | 0.99     | 0.24                | 0.95       |
| (2,258) | 1:19:A:ALA:HB3  | 1:20:A:ILE:HB   | 10                  | 0.92     | 0.07                | 0.94       |
| (2,258) | 1:15:A:LYS:HG3  | 1:14:A:GLN:HB3  | 10                  | 0.92     | 0.07                | 0.94       |
| (2,258) | 1:15:A:LYS:HG3  | 1:14:A:GLN:HB2  | 10                  | 0.92     | 0.07                | 0.94       |
| (2,258) | 1:19:A:ALA:HB2  | 1:20:A:ILE:HB   | 10                  | 0.92     | 0.07                | 0.94       |
| (2,89)  | 1:24:A:PHE:HE1  | 1:13:A:LYS:HD3  | 10                  | 0.91     | 0.31                | 1.02       |
| (2,89)  | 1:24:A:PHE:HE2  | 1:13:A:LYS:HD2  | 10                  | 0.91     | 0.31                | 1.02       |
| (2,89)  | 1:24:A:PHE:HE2  | 1:13:A:LYS:HD3  | 10                  | 0.91     | 0.31                | 1.02       |
| (2,89)  | 1:24:A:PHE:HE1  | 1:13:A:LYS:HD2  | 10                  | 0.91     | 0.31                | 1.02       |
| (2,116) | 1:16:A:CYS:H    | 1:20:A:ILE:HG23 | 10                  | 0.91     | 0.17                | 1.0        |
| (2,116) | 1:16:A:CYS:H    | 1:20:A:ILE:HD12 | 10                  | 0.91     | 0.17                | 1.0        |
| (2,116) | 1:16:A:CYS:H    | 1:20:A:ILE:HG21 | 10                  | 0.91     | 0.17                | 1.0        |
| (2,116) | 1:16:A:CYS:H    | 1:20:A:ILE:HD13 | 10                  | 0.91     | 0.17                | 1.0        |
| (2,116) | 1:16:A:CYS:H    | 1:20:A:ILE:HD11 | 10                  | 0.91     | 0.17                | 1.0        |
| (2,116) | 1:16:A:CYS:H    | 1:20:A:ILE:HG22 | 10                  | 0.91     | 0.17                | 1.0        |
| (3,281) | 1:25:A:GLY:H    | 1:13:A:LYS:HG3  | 10                  | 0.85     | 0.14                | 0.86       |
| (2,279) | 1:16:A:CYS:H    | 1:34:A:CYS:HA   | 10                  | 0.83     | 0.33                | 0.86       |
| (2,279) | 1:16:A:CYS:H    | 1:24:A:PHE:HA   | 10                  | 0.83     | 0.33                | 0.86       |
| (2,122) | 1:17:A:LEU:H    | 1:20:A:ILE:HG23 | 10                  | 0.79     | 0.15                | 0.82       |
| (2,122) | 1:17:A:LEU:H    | 1:20:A:ILE:HD12 | 10                  | 0.79     | 0.15                | 0.82       |
| (2,122) | 1:17:A:LEU:H    | 1:20:A:ILE:HG21 | 10                  | 0.79     | 0.15                | 0.82       |
| (2,122) | 1:17:A:LEU:H    | 1:20:A:ILE:HD13 | 10                  | 0.79     | 0.15                | 0.82       |
| (2,122) | 1:17:A:LEU:H    | 1:20:A:ILE:HD11 | 10                  | 0.79     | 0.15                | 0.82       |
| (3,409) | 1:23:A:ILE:HD11 | 1:23:A:ILE:HA   | 10                  | 0.75     | 0.02                | 0.76       |
| (3,409) | 1:23:A:ILE:HD13 | 1:23:A:ILE:HA   | 10                  | 0.75     | 0.02                | 0.76       |
| (3,409) | 1:23:A:ILE:HD12 | 1:23:A:ILE:HA   | 10                  | 0.75     | 0.02                | 0.76       |
| (2,94)  | 1:24:A:PHE:HD1  | 1:26:A:LYS:HG2  | 10                  | 0.74     | 0.32                | 0.76       |
| (2,94)  | 1:24:A:PHE:HD2  | 1:26:A:LYS:HG2  | 10                  | 0.74     | 0.32                | 0.76       |
| (3,299) | 1:25:A:GLY:H    | 1:23:A:ILE:HG23 | 10                  | 0.72     | 0.06                | 0.72       |
| (3,299) | 1:25:A:GLY:H    | 1:23:A:ILE:HG21 | 10                  | 0.72     | 0.06                | 0.72       |
| (3,299) | 1:25:A:GLY:H    | 1:23:A:ILE:HG22 | 10                  | 0.72     | 0.06                | 0.72       |
| (3,298) | 1:25:A:GLY:H    | 1:20:A:ILE:HD12 | 10                  | 0.69     | 0.06                | 0.7        |
| (3,298) | 1:25:A:GLY:H    | 1:20:A:ILE:HD11 | 10                  | 0.69     | 0.06                | 0.7        |
| (3,298) | 1:25:A:GLY:H    | 1:20:A:ILE:HD13 | 10                  | 0.69     | 0.06                | 0.7        |
| (3,329) | 1:24:A:PHE:HD2  | 1:23:A:ILE:HG22 | 10                  | 0.67     | 0.09                | 0.66       |
| (3,329) | 1:24:A:PHE:HD1  | 1:23:A:ILE:HG23 | 10                  | 0.67     | 0.09                | 0.66       |
| (3,329) | 1:24:A:PHE:HD1  | 1:23:A:ILE:HG22 | 10                  | 0.67     | 0.09                | 0.66       |
| (3,329) | 1:24:A:PHE:HD2  | 1:23:A:ILE:HG23 | 10                  | 0.67     | 0.09                | 0.66       |
| (3,329) | 1:24:A:PHE:HD2  | 1:23:A:ILE:HG21 | 10                  | 0.67     | 0.09                | 0.66       |
| (3,536) | 1:17:A:LEU:HD13 | 1:22:A:SER:HA   | 10                  | 0.67     | 0.15                | 0.68       |
| (3,536) | 1:17:A:LEU:HD11 | 1:22:A:SER:HA   | 10                  | 0.67     | 0.15                | 0.68       |
| (3,536) | 1:17:A:LEU:HD12 | 1:22:A:SER:HA   | 10                  | 0.67     | 0.15                | 0.68       |

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| Key     | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (3,320) | 1:24:A:PHE:HE2  | 1:20:A:ILE:HD12 | 10                  | 0.64     | 0.26                | 0.62       |
| (3,320) | 1:24:A:PHE:HE1  | 1:20:A:ILE:HD12 | 10                  | 0.64     | 0.26                | 0.62       |
| (3,320) | 1:24:A:PHE:HE1  | 1:20:A:ILE:HD11 | 10                  | 0.64     | 0.26                | 0.62       |
| (3,320) | 1:24:A:PHE:HE2  | 1:20:A:ILE:HD13 | 10                  | 0.64     | 0.26                | 0.62       |
| (3,320) | 1:24:A:PHE:HE2  | 1:20:A:ILE:HD11 | 10                  | 0.64     | 0.26                | 0.62       |
| (2,67)  | 1:28:A:MET:H    | 1:31:A:LYS:HD3  | 10                  | 0.6      | 0.15                | 0.52       |
| (2,67)  | 1:28:A:MET:H    | 1:31:A:LYS:HD2  | 10                  | 0.6      | 0.15                | 0.52       |
| (2,78)  | 1:6:A:CYS:H     | 1:5:A:ARG:HB2   | 10                  | 0.54     | 0.03                | 0.54       |
| (2,11)  | 1:6:A:CYS:H     | 1:8:A:ALA:HA    | 10                  | 0.52     | 0.06                | 0.54       |
| (2,11)  | 1:6:A:CYS:H     | 1:27:A:CYS:HA   | 10                  | 0.52     | 0.06                | 0.54       |
| (3,186) | 1:34:A:CYS:H    | 1:34:A:CYS:HB3  | 10                  | 0.48     | 0.16                | 0.47       |
| (3,164) | 1:32:A:CYS:H    | 1:32:A:CYS:HB3  | 10                  | 0.4      | 0.03                | 0.4        |
| (2,119) | 1:19:A:ALA:H    | 1:20:A:ILE:HG23 | 10                  | 0.38     | 0.08                | 0.37       |
| (2,119) | 1:19:A:ALA:H    | 1:20:A:ILE:HG22 | 10                  | 0.38     | 0.08                | 0.37       |
| (2,119) | 1:19:A:ALA:H    | 1:20:A:ILE:HG21 | 10                  | 0.38     | 0.08                | 0.37       |
| (2,111) | 1:27:A:CYS:H    | 1:26:A:LYS:HG2  | 10                  | 0.38     | 0.06                | 0.38       |
| (2,43)  | 1:24:A:PHE:HE1  | 1:13:A:LYS:HE2  | 10                  | 0.36     | 0.08                | 0.37       |
| (2,43)  | 1:24:A:PHE:HE2  | 1:13:A:LYS:HE2  | 10                  | 0.36     | 0.08                | 0.37       |
| (2,43)  | 1:24:A:PHE:HE1  | 1:13:A:LYS:HE3  | 10                  | 0.36     | 0.08                | 0.37       |
| (2,175) | 1:9:A:SER:HB2   | 1:2:A:MET:HG3   | 10                  | 0.34     | 0.15                | 0.3        |
| (2,175) | 1:9:A:SER:HB3   | 1:2:A:MET:HG3   | 10                  | 0.34     | 0.15                | 0.3        |
| (2,175) | 1:9:A:SER:HB2   | 1:2:A:MET:HG2   | 10                  | 0.34     | 0.15                | 0.3        |
| (2,175) | 1:9:A:SER:HB3   | 1:2:A:MET:HG2   | 10                  | 0.34     | 0.15                | 0.3        |
| (3,246) | 1:28:A:MET:H    | 1:28:A:MET:HB3  | 10                  | 0.31     | 0.03                | 0.32       |
| (2,40)  | 1:5:A:ARG:H     | 1:6:A:CYS:HB2   | 10                  | 0.28     | 0.17                | 0.23       |
| (2,40)  | 1:5:A:ARG:H     | 1:6:A:CYS:HB3   | 10                  | 0.28     | 0.17                | 0.23       |
| (3,31)  | 1:24:A:PHE:HD2  | 1:25:A:GLY:H    | 10                  | 0.24     | 0.07                | 0.24       |
| (3,31)  | 1:24:A:PHE:HD1  | 1:25:A:GLY:H    | 10                  | 0.24     | 0.07                | 0.24       |
| (2,250) | 1:18:A:LYS:HD3  | 1:18:A:LYS:HG2  | 10                  | 0.22     | 0.02                | 0.22       |
| (2,250) | 1:13:A:LYS:HD3  | 1:13:A:LYS:HG2  | 10                  | 0.22     | 0.02                | 0.22       |
| (2,5)   | 1:1:A:GLN:HE22  | 1:1:A:GLN:HE21  | 10                  | 0.19     | 0.0                 | 0.19       |
| (2,5)   | 1:29:A:ASN:HD22 | 1:29:A:ASN:HD21 | 10                  | 0.19     | 0.0                 | 0.19       |
| (2,239) | 1:5:A:ARG:HB2   | 1:5:A:ARG:HG3   | 10                  | 0.19     | 0.05                | 0.17       |
| (2,235) | 1:2:A:MET:HG2   | 1:2:A:MET:HB3   | 10                  | 0.18     | 0.04                | 0.18       |
| (2,235) | 1:2:A:MET:HG3   | 1:2:A:MET:HB2   | 10                  | 0.18     | 0.04                | 0.18       |
| (3,499) | 1:11:A:GLU:HG2  | 1:10:A:VAL:HG23 | 9                   | 2.06     | 0.86                | 2.03       |
| (3,499) | 1:11:A:GLU:HG2  | 1:10:A:VAL:HG21 | 9                   | 2.06     | 0.86                | 2.03       |
| (3,499) | 1:11:A:GLU:HG2  | 1:10:A:VAL:HG22 | 9                   | 2.06     | 0.86                | 2.03       |
| (2,19)  | 1:1:A:GLN:HE21  | 1:9:A:SER:HB2   | 9                   | 1.15     | 0.6                 | 1.54       |
| (2,19)  | 1:1:A:GLN:HE21  | 1:9:A:SER:HB3   | 9                   | 1.15     | 0.6                 | 1.54       |
| (2,265) | 1:34:A:CYS:H    | 1:15:A:LYS:HA   | 9                   | 0.76     | 0.13                | 0.77       |
| (2,265) | 1:34:A:CYS:H    | 1:17:A:LEU:HA   | 9                   | 0.76     | 0.13                | 0.77       |

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| Key     | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (2,121) | 1:18:A:LYS:H    | 1:17:A:LEU:HD12 | 9                   | 0.72     | 0.3                 | 0.75       |
| (2,121) | 1:23:A:ILE:H    | 1:17:A:LEU:HD13 | 9                   | 0.72     | 0.3                 | 0.75       |
| (2,121) | 1:18:A:LYS:H    | 1:17:A:LEU:HD13 | 9                   | 0.72     | 0.3                 | 0.75       |
| (2,121) | 1:23:A:ILE:H    | 1:17:A:LEU:HD12 | 9                   | 0.72     | 0.3                 | 0.75       |
| (2,121) | 1:18:A:LYS:H    | 1:17:A:LEU:HD11 | 9                   | 0.72     | 0.3                 | 0.75       |
| (3,309) | 1:24:A:PHE:H    | 1:23:A:ILE:HD11 | 9                   | 0.56     | 0.06                | 0.57       |
| (3,309) | 1:24:A:PHE:H    | 1:23:A:ILE:HD13 | 9                   | 0.56     | 0.06                | 0.57       |
| (2,198) | 1:21:A:GLY:HA3  | 1:20:A:ILE:HD11 | 9                   | 0.53     | 0.26                | 0.45       |
| (2,198) | 1:21:A:GLY:HA3  | 1:20:A:ILE:HD13 | 9                   | 0.53     | 0.26                | 0.45       |
| (2,198) | 1:17:A:LEU:HA   | 1:20:A:ILE:HD13 | 9                   | 0.53     | 0.26                | 0.45       |
| (2,240) | 1:15:A:LYS:HB3  | 1:31:A:LYS:HB3  | 9                   | 0.52     | 0.3                 | 0.47       |
| (2,240) | 1:15:A:LYS:HB3  | 1:31:A:LYS:HB2  | 9                   | 0.52     | 0.3                 | 0.47       |
| (3,304) | 1:24:A:PHE:H    | 1:23:A:ILE:HG22 | 9                   | 0.44     | 0.07                | 0.44       |
| (3,304) | 1:24:A:PHE:H    | 1:23:A:ILE:HG23 | 9                   | 0.44     | 0.07                | 0.44       |
| (3,304) | 1:24:A:PHE:H    | 1:23:A:ILE:HG21 | 9                   | 0.44     | 0.07                | 0.44       |
| (2,193) | 1:15:A:LYS:HA   | 1:31:A:LYS:HG3  | 9                   | 0.37     | 0.09                | 0.37       |
| (2,193) | 1:15:A:LYS:HA   | 1:31:A:LYS:HG2  | 9                   | 0.37     | 0.09                | 0.37       |
| (2,88)  | 1:24:A:PHE:HD1  | 1:13:A:LYS:HD3  | 9                   | 0.34     | 0.15                | 0.37       |
| (2,88)  | 1:24:A:PHE:HD2  | 1:13:A:LYS:HD3  | 9                   | 0.34     | 0.15                | 0.37       |
| (2,88)  | 1:24:A:PHE:HD1  | 1:13:A:LYS:HD2  | 9                   | 0.34     | 0.15                | 0.37       |
| (2,35)  | 1:26:A:LYS:H    | 1:12:A:CYS:HB3  | 9                   | 0.3      | 0.08                | 0.28       |
| (2,35)  | 1:26:A:LYS:H    | 1:16:A:CYS:HB3  | 9                   | 0.3      | 0.08                | 0.28       |
| (2,107) | 1:16:A:CYS:H    | 1:19:A:ALA:HB3  | 9                   | 0.24     | 0.1                 | 0.24       |
| (2,107) | 1:16:A:CYS:H    | 1:19:A:ALA:HB2  | 9                   | 0.24     | 0.1                 | 0.24       |
| (2,107) | 1:16:A:CYS:H    | 1:15:A:LYS:HG3  | 9                   | 0.24     | 0.1                 | 0.24       |
| (3,296) | 1:8:A:ALA:H     | 1:10:A:VAL:HG23 | 8                   | 1.55     | 0.86                | 2.12       |
| (3,296) | 1:8:A:ALA:H     | 1:10:A:VAL:HG21 | 8                   | 1.55     | 0.86                | 2.12       |
| (3,296) | 1:8:A:ALA:H     | 1:10:A:VAL:HG22 | 8                   | 1.55     | 0.86                | 2.12       |
| (2,93)  | 1:24:A:PHE:HE1  | 1:17:A:LEU:HG   | 8                   | 0.88     | 0.44                | 0.78       |
| (2,93)  | 1:24:A:PHE:HE2  | 1:17:A:LEU:HG   | 8                   | 0.88     | 0.44                | 0.78       |
| (2,93)  | 1:24:A:PHE:HE1  | 1:13:A:LYS:HG2  | 8                   | 0.88     | 0.44                | 0.78       |
| (2,92)  | 1:24:A:PHE:HD1  | 1:17:A:LEU:HG   | 8                   | 0.85     | 0.29                | 0.86       |
| (2,92)  | 1:24:A:PHE:HD2  | 1:17:A:LEU:HG   | 8                   | 0.85     | 0.29                | 0.86       |
| (2,92)  | 1:24:A:PHE:HD1  | 1:13:A:LYS:HG2  | 8                   | 0.85     | 0.29                | 0.86       |
| (3,295) | 1:19:A:ALA:H    | 1:17:A:LEU:HD12 | 8                   | 0.66     | 0.1                 | 0.65       |
| (3,295) | 1:19:A:ALA:H    | 1:17:A:LEU:HD13 | 8                   | 0.66     | 0.1                 | 0.65       |
| (3,295) | 1:19:A:ALA:H    | 1:17:A:LEU:HD11 | 8                   | 0.66     | 0.1                 | 0.65       |
| (2,49)  | 1:29:A:ASN:HD21 | 1:28:A:MET:HG2  | 8                   | 0.54     | 0.26                | 0.47       |
| (2,49)  | 1:12:A:CYS:H    | 1:14:A:GLN:HG3  | 8                   | 0.54     | 0.26                | 0.47       |
| (2,207) | 1:18:A:LYS:HE2  | 1:18:A:LYS:HB2  | 8                   | 0.5      | 0.04                | 0.52       |
| (2,207) | 1:18:A:LYS:HE3  | 1:18:A:LYS:HB3  | 8                   | 0.5      | 0.04                | 0.52       |
| (2,207) | 1:18:A:LYS:HE2  | 1:18:A:LYS:HB3  | 8                   | 0.5      | 0.04                | 0.52       |

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| Key     | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (2,207) | 1:18:A:LYS:HE3  | 1:18:A:LYS:HB2  | 8                   | 0.5      | 0.04                | 0.52       |
| (3,442) | 1:17:A:LEU:HA   | 1:17:A:LEU:HD12 | 8                   | 0.5      | 0.1                 | 0.44       |
| (3,442) | 1:17:A:LEU:HA   | 1:17:A:LEU:HD13 | 8                   | 0.5      | 0.1                 | 0.44       |
| (3,442) | 1:17:A:LEU:HA   | 1:17:A:LEU:HD11 | 8                   | 0.5      | 0.1                 | 0.44       |
| (3,380) | 1:11:A:GLU:HG2  | 1:11:A:GLU:HA   | 8                   | 0.46     | 0.21                | 0.41       |
| (2,224) | 1:13:A:LYS:HE2  | 1:23:A:ILE:HG21 | 8                   | 0.44     | 0.2                 | 0.4        |
| (2,224) | 1:13:A:LYS:HE2  | 1:23:A:ILE:HG22 | 8                   | 0.44     | 0.2                 | 0.4        |
| (2,224) | 1:13:A:LYS:HE3  | 1:23:A:ILE:HG23 | 8                   | 0.44     | 0.2                 | 0.4        |
| (2,224) | 1:13:A:LYS:HE3  | 1:23:A:ILE:HG22 | 8                   | 0.44     | 0.2                 | 0.4        |
| (2,224) | 1:13:A:LYS:HE2  | 1:23:A:ILE:HG23 | 8                   | 0.44     | 0.2                 | 0.4        |
| (2,64)  | 1:32:A:CYS:H    | 1:31:A:LYS:HD3  | 8                   | 0.42     | 0.15                | 0.44       |
| (2,64)  | 1:32:A:CYS:H    | 1:15:A:LYS:HD3  | 8                   | 0.42     | 0.15                | 0.44       |
| (2,110) | 1:4:A:MET:H     | 1:31:A:LYS:HG2  | 8                   | 0.42     | 0.14                | 0.36       |
| (2,110) | 1:4:A:MET:H     | 1:31:A:LYS:HG3  | 8                   | 0.42     | 0.14                | 0.36       |
| (2,82)  | 1:14:A:GLN:H    | 1:17:A:LEU:HB2  | 8                   | 0.4      | 0.17                | 0.41       |
| (2,82)  | 1:6:A:CYS:H     | 1:5:A:ARG:HG2   | 8                   | 0.4      | 0.17                | 0.41       |
| (2,82)  | 1:6:A:CYS:H     | 1:5:A:ARG:HG3   | 8                   | 0.4      | 0.17                | 0.41       |
| (2,216) | 1:24:A:PHE:HB2  | 1:26:A:LYS:HG2  | 8                   | 0.4      | 0.19                | 0.39       |
| (2,246) | 1:26:A:LYS:HB2  | 1:33:A:LYS:HG3  | 8                   | 0.38     | 0.08                | 0.37       |
| (2,246) | 1:26:A:LYS:HB2  | 1:33:A:LYS:HG2  | 8                   | 0.38     | 0.08                | 0.37       |
| (2,109) | 1:28:A:MET:H    | 1:31:A:LYS:HG3  | 8                   | 0.37     | 0.08                | 0.36       |
| (2,164) | 1:23:A:ILE:HD13 | 1:22:A:SER:HA   | 8                   | 0.36     | 0.07                | 0.37       |
| (2,164) | 1:23:A:ILE:HD11 | 1:24:A:PHE:HA   | 8                   | 0.36     | 0.07                | 0.37       |
| (2,164) | 1:23:A:ILE:HD12 | 1:22:A:SER:HA   | 8                   | 0.36     | 0.07                | 0.37       |
| (2,241) | 1:13:A:LYS:HB2  | 1:13:A:LYS:HG2  | 8                   | 0.2      | 0.03                | 0.19       |
| (3,387) | 1:13:A:LYS:HA   | 1:25:A:GLY:HA3  | 8                   | 0.18     | 0.03                | 0.18       |
| (3,436) | 1:13:A:LYS:HA   | 1:13:A:LYS:HG3  | 8                   | 0.13     | 0.01                | 0.12       |
| (3,383) | 1:22:A:SER:HB3  | 1:34:A:CYS:HB2  | 7                   | 1.3      | 0.4                 | 1.23       |
| (2,90)  | 1:14:A:GLN:HE22 | 1:13:A:LYS:HD2  | 7                   | 1.04     | 0.24                | 1.1        |
| (2,90)  | 1:14:A:GLN:HE22 | 1:18:A:LYS:HD2  | 7                   | 1.04     | 0.24                | 1.1        |
| (2,90)  | 1:11:A:GLU:H    | 1:13:A:LYS:HD3  | 7                   | 1.04     | 0.24                | 1.1        |
| (2,252) | 1:31:A:LYS:HB3  | 1:15:A:LYS:HG2  | 7                   | 0.73     | 0.32                | 0.72       |
| (2,252) | 1:31:A:LYS:HB2  | 1:15:A:LYS:HG2  | 7                   | 0.73     | 0.32                | 0.72       |
| (3,256) | 1:26:A:LYS:H    | 1:33:A:LYS:HB2  | 7                   | 0.71     | 0.27                | 0.76       |
| (2,261) | 1:8:A:ALA:HB3   | 1:2:A:MET:HG2   | 7                   | 0.62     | 0.24                | 0.68       |
| (2,261) | 1:8:A:ALA:HB2   | 1:2:A:MET:HG2   | 7                   | 0.62     | 0.24                | 0.68       |
| (2,261) | 1:8:A:ALA:HB1   | 1:2:A:MET:HG2   | 7                   | 0.62     | 0.24                | 0.68       |
| (3,231) | 1:8:A:ALA:H     | 1:11:A:GLU:HB3  | 7                   | 0.61     | 0.1                 | 0.65       |
| (2,98)  | 1:8:A:ALA:H     | 1:31:A:LYS:HD3  | 7                   | 0.55     | 0.21                | 0.43       |
| (2,98)  | 1:8:A:ALA:H     | 1:31:A:LYS:HD2  | 7                   | 0.55     | 0.21                | 0.43       |
| (3,302) | 1:21:A:GLY:H    | 1:17:A:LEU:HD11 | 7                   | 0.52     | 0.23                | 0.42       |
| (3,302) | 1:21:A:GLY:H    | 1:17:A:LEU:HD13 | 7                   | 0.52     | 0.23                | 0.42       |

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| Key     | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (3,302) | 1:21:A:GLY:H    | 1:17:A:LEU:HD12 | 7                   | 0.52     | 0.23                | 0.42       |
| (2,189) | 1:30:A:LYS:HA   | 1:31:A:LYS:HD2  | 7                   | 0.45     | 0.2                 | 0.56       |
| (2,189) | 1:30:A:LYS:HA   | 1:30:A:LYS:HD2  | 7                   | 0.45     | 0.2                 | 0.56       |
| (2,1)   | 1:6:A:CYS:H     | 1:32:A:CYS:H    | 7                   | 0.45     | 0.18                | 0.45       |
| (2,1)   | 1:14:A:GLN:H    | 1:32:A:CYS:H    | 7                   | 0.45     | 0.18                | 0.45       |
| (2,197) | 1:17:A:LEU:HA   | 1:20:A:ILE:HD12 | 7                   | 0.41     | 0.23                | 0.35       |
| (2,197) | 1:17:A:LEU:HA   | 1:20:A:ILE:HD13 | 7                   | 0.41     | 0.23                | 0.35       |
| (2,197) | 1:17:A:LEU:HA   | 1:20:A:ILE:HD11 | 7                   | 0.41     | 0.23                | 0.35       |
| (2,58)  | 1:3:A:ASP:H     | 1:1:A:GLN:HB3   | 7                   | 0.38     | 0.08                | 0.4        |
| (2,58)  | 1:3:A:ASP:H     | 1:1:A:GLN:HB2   | 7                   | 0.38     | 0.08                | 0.4        |
| (2,117) | 1:16:A:CYS:H    | 1:23:A:ILE:HG23 | 7                   | 0.28     | 0.16                | 0.21       |
| (2,117) | 1:16:A:CYS:H    | 1:23:A:ILE:HG21 | 7                   | 0.28     | 0.16                | 0.21       |
| (2,117) | 1:16:A:CYS:H    | 1:23:A:ILE:HG22 | 7                   | 0.28     | 0.16                | 0.21       |
| (2,277) | 1:16:A:CYS:HA   | 1:15:A:LYS:HA   | 7                   | 0.16     | 0.02                | 0.16       |
| (2,277) | 1:16:A:CYS:HA   | 1:17:A:LEU:HA   | 7                   | 0.16     | 0.02                | 0.16       |
| (2,195) | 1:9:A:SER:HB2   | 1:10:A:VAL:HG22 | 6                   | 1.38     | 0.44                | 1.51       |
| (2,195) | 1:9:A:SER:HB3   | 1:10:A:VAL:HG23 | 6                   | 1.38     | 0.44                | 1.51       |
| (2,195) | 1:9:A:SER:HB3   | 1:10:A:VAL:HG21 | 6                   | 1.38     | 0.44                | 1.51       |
| (2,195) | 1:9:A:SER:HB2   | 1:10:A:VAL:HG21 | 6                   | 1.38     | 0.44                | 1.51       |
| (3,425) | 1:19:A:ALA:HA   | 1:33:A:LYS:HB3  | 6                   | 1.32     | 0.31                | 1.42       |
| (3,240) | 1:27:A:CYS:H    | 1:33:A:LYS:HB2  | 6                   | 1.2      | 0.14                | 1.15       |
| (3,385) | 1:22:A:SER:HB2  | 1:34:A:CYS:HB2  | 6                   | 0.93     | 0.28                | 1.1        |
| (3,218) | 1:29:A:ASN:HD22 | 1:28:A:MET:HB2  | 6                   | 0.64     | 0.34                | 0.68       |
| (3,465) | 1:34:A:CYS:HB2  | 1:16:A:CYS:HB3  | 6                   | 0.61     | 0.23                | 0.68       |
| (2,191) | 1:22:A:SER:HB2  | 1:19:A:ALA:HB3  | 6                   | 0.57     | 0.27                | 0.5        |
| (2,191) | 1:7:A:SER:HB3   | 1:8:A:ALA:HB2   | 6                   | 0.57     | 0.27                | 0.5        |
| (2,191) | 1:7:A:SER:HB3   | 1:8:A:ALA:HB1   | 6                   | 0.57     | 0.27                | 0.5        |
| (3,433) | 1:7:A:SER:HB2   | 1:8:A:ALA:HB2   | 6                   | 0.46     | 0.15                | 0.42       |
| (3,433) | 1:7:A:SER:HB2   | 1:8:A:ALA:HB1   | 6                   | 0.46     | 0.15                | 0.42       |
| (3,433) | 1:7:A:SER:HB2   | 1:8:A:ALA:HB3   | 6                   | 0.46     | 0.15                | 0.42       |
| (2,200) | 1:14:A:GLN:HA   | 1:23:A:ILE:HG23 | 6                   | 0.37     | 0.17                | 0.41       |
| (2,200) | 1:14:A:GLN:HA   | 1:23:A:ILE:HG21 | 6                   | 0.37     | 0.17                | 0.41       |
| (2,200) | 1:14:A:GLN:HA   | 1:23:A:ILE:HG22 | 6                   | 0.37     | 0.17                | 0.41       |
| (2,27)  | 1:14:A:GLN:HE21 | 1:17:A:LEU:HA   | 6                   | 0.36     | 0.1                 | 0.39       |
| (3,328) | 1:24:A:PHE:HZ   | 1:23:A:ILE:HG22 | 6                   | 0.34     | 0.14                | 0.32       |
| (3,328) | 1:24:A:PHE:HZ   | 1:23:A:ILE:HG23 | 6                   | 0.34     | 0.14                | 0.32       |
| (3,328) | 1:24:A:PHE:HZ   | 1:23:A:ILE:HG21 | 6                   | 0.34     | 0.14                | 0.32       |
| (2,37)  | 1:8:A:ALA:H     | 1:2:A:MET:HG3   | 6                   | 0.31     | 0.08                | 0.34       |
| (2,37)  | 1:8:A:ALA:H     | 1:2:A:MET:HG2   | 6                   | 0.31     | 0.08                | 0.34       |
| (2,215) | 1:32:A:CYS:HB3  | 1:26:A:LYS:HG3  | 6                   | 0.26     | 0.12                | 0.2        |
| (2,215) | 1:32:A:CYS:HB3  | 1:31:A:LYS:HG2  | 6                   | 0.26     | 0.12                | 0.2        |
| (2,17)  | 1:11:A:GLU:H    | 1:9:A:SER:HB2   | 6                   | 0.21     | 0.04                | 0.21       |

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| Key     | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (2,17)  | 1:11:A:GLU:H    | 1:9:A:SER:HB3   | 6                   | 0.21     | 0.04                | 0.21       |
| (3,498) | 1:11:A:GLU:HG2  | 1:10:A:VAL:HG12 | 5                   | 2.0      | 0.65                | 2.25       |
| (3,498) | 1:11:A:GLU:HG2  | 1:10:A:VAL:HG11 | 5                   | 2.0      | 0.65                | 2.25       |
| (3,292) | 1:10:A:VAL:H    | 1:10:A:VAL:HG23 | 5                   | 1.08     | 0.03                | 1.09       |
| (3,292) | 1:10:A:VAL:H    | 1:10:A:VAL:HG21 | 5                   | 1.08     | 0.03                | 1.09       |
| (3,292) | 1:10:A:VAL:H    | 1:10:A:VAL:HG22 | 5                   | 1.08     | 0.03                | 1.09       |
| (2,255) | 1:13:A:LYS:HG2  | 1:10:A:VAL:HG13 | 5                   | 1.03     | 0.35                | 1.0        |
| (2,255) | 1:8:A:ALA:HB1   | 1:10:A:VAL:HG12 | 5                   | 1.03     | 0.35                | 1.0        |
| (2,255) | 1:13:A:LYS:HG2  | 1:10:A:VAL:HG12 | 5                   | 1.03     | 0.35                | 1.0        |
| (2,255) | 1:8:A:ALA:HB2   | 1:10:A:VAL:HG12 | 5                   | 1.03     | 0.35                | 1.0        |
| (3,443) | 1:10:A:VAL:HA   | 1:10:A:VAL:HG11 | 5                   | 1.01     | 0.02                | 1.02       |
| (3,443) | 1:10:A:VAL:HA   | 1:10:A:VAL:HG12 | 5                   | 1.01     | 0.02                | 1.02       |
| (3,443) | 1:10:A:VAL:HA   | 1:10:A:VAL:HG13 | 5                   | 1.01     | 0.02                | 1.02       |
| (3,460) | 1:5:A:ARG:HD2   | 1:4:A:MET:HE2   | 5                   | 0.9      | 0.27                | 1.02       |
| (3,460) | 1:5:A:ARG:HD2   | 1:4:A:MET:HE3   | 5                   | 0.9      | 0.27                | 1.02       |
| (2,153) | 1:5:A:ARG:HG2   | 1:6:A:CYS:HA    | 5                   | 0.78     | 0.15                | 0.81       |
| (2,153) | 1:5:A:ARG:HG3   | 1:6:A:CYS:HA    | 5                   | 0.78     | 0.15                | 0.81       |
| (3,500) | 1:11:A:GLU:HB3  | 1:10:A:VAL:HG23 | 5                   | 0.77     | 0.21                | 0.69       |
| (3,500) | 1:11:A:GLU:HB3  | 1:10:A:VAL:HG21 | 5                   | 0.77     | 0.21                | 0.69       |
| (3,500) | 1:11:A:GLU:HB3  | 1:10:A:VAL:HG22 | 5                   | 0.77     | 0.21                | 0.69       |
| (3,177) | 1:32:A:CYS:H    | 1:27:A:CYS:HB2  | 5                   | 0.76     | 0.11                | 0.83       |
| (3,554) | 1:5:A:ARG:H     | 1:5:A:ARG:HB3   | 5                   | 0.52     | 0.15                | 0.59       |
| (3,293) | 1:16:A:CYS:H    | 1:17:A:LEU:HD13 | 5                   | 0.4      | 0.33                | 0.16       |
| (3,293) | 1:16:A:CYS:H    | 1:17:A:LEU:HD12 | 5                   | 0.4      | 0.33                | 0.16       |
| (3,293) | 1:16:A:CYS:H    | 1:17:A:LEU:HD11 | 5                   | 0.4      | 0.33                | 0.16       |
| (2,162) | 1:20:A:ILE:HG22 | 1:16:A:CYS:HA   | 5                   | 0.32     | 0.11                | 0.36       |
| (2,162) | 1:20:A:ILE:HG21 | 1:16:A:CYS:HA   | 5                   | 0.32     | 0.11                | 0.36       |
| (2,162) | 1:20:A:ILE:HD11 | 1:16:A:CYS:HA   | 5                   | 0.32     | 0.11                | 0.36       |
| (2,162) | 1:20:A:ILE:HD12 | 1:16:A:CYS:HA   | 5                   | 0.32     | 0.11                | 0.36       |
| (2,44)  | 1:24:A:PHE:HD1  | 1:13:A:LYS:HE2  | 5                   | 0.32     | 0.18                | 0.3        |
| (2,44)  | 1:24:A:PHE:HD2  | 1:13:A:LYS:HE2  | 5                   | 0.32     | 0.18                | 0.3        |
| (2,44)  | 1:24:A:PHE:HD1  | 1:13:A:LYS:HE3  | 5                   | 0.32     | 0.18                | 0.3        |
| (2,102) | 1:5:A:ARG:H     | 1:31:A:LYS:HG2  | 5                   | 0.31     | 0.12                | 0.3        |
| (2,102) | 1:5:A:ARG:H     | 1:31:A:LYS:HG3  | 5                   | 0.31     | 0.12                | 0.3        |
| (3,219) | 1:24:A:PHE:HD1  | 1:23:A:ILE:HB   | 5                   | 0.29     | 0.11                | 0.3        |
| (3,219) | 1:24:A:PHE:HD2  | 1:23:A:ILE:HB   | 5                   | 0.29     | 0.11                | 0.3        |
| (2,66)  | 1:27:A:CYS:H    | 1:26:A:LYS:HD3  | 5                   | 0.25     | 0.18                | 0.18       |
| (2,66)  | 1:27:A:CYS:H    | 1:26:A:LYS:HD2  | 5                   | 0.25     | 0.18                | 0.18       |
| (3,445) | 1:21:A:GLY:HA3  | 1:17:A:LEU:HD21 | 5                   | 0.2      | 0.09                | 0.16       |
| (3,445) | 1:21:A:GLY:HA3  | 1:17:A:LEU:HD22 | 5                   | 0.2      | 0.09                | 0.16       |
| (3,445) | 1:21:A:GLY:HA3  | 1:17:A:LEU:HD23 | 5                   | 0.2      | 0.09                | 0.16       |
| (3,166) | 1:27:A:CYS:H    | 1:27:A:CYS:HB3  | 5                   | 0.17     | 0.01                | 0.18       |

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| Key     | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (3,13)  | 1:5:A:ARG:H     | 1:4:A:MET:H     | 5                   | 0.16     | 0.04                | 0.14       |
| (3,388) | 1:22:A:SER:HB3  | 1:16:A:CYS:HB3  | 4                   | 1.38     | 0.78                | 0.95       |
| (2,108) | 1:28:A:MET:H    | 1:33:A:LYS:HG2  | 4                   | 1.0      | 0.19                | 0.98       |
| (3,535) | 1:19:A:ALA:H    | 1:34:A:CYS:HB3  | 4                   | 0.82     | 0.51                | 0.78       |
| (3,473) | 1:34:A:CYS:HB3  | 1:19:A:ALA:HB3  | 4                   | 0.77     | 0.67                | 0.57       |
| (3,473) | 1:34:A:CYS:HB3  | 1:19:A:ALA:HB2  | 4                   | 0.77     | 0.67                | 0.57       |
| (3,297) | 1:8:A:ALA:H     | 1:10:A:VAL:HG11 | 4                   | 0.6      | 0.12                | 0.64       |
| (3,297) | 1:8:A:ALA:H     | 1:10:A:VAL:HG12 | 4                   | 0.6      | 0.12                | 0.64       |
| (2,218) | 1:12:A:CYS:HB3  | 1:13:A:LYS:HB2  | 4                   | 0.58     | 0.33                | 0.51       |
| (2,218) | 1:16:A:CYS:HB3  | 1:15:A:LYS:HB2  | 4                   | 0.58     | 0.33                | 0.51       |
| (2,218) | 1:16:A:CYS:HB3  | 1:13:A:LYS:HB3  | 4                   | 0.58     | 0.33                | 0.51       |
| (3,183) | 1:4:A:MET:H     | 1:4:A:MET:HG3   | 4                   | 0.54     | 0.3                 | 0.49       |
| (3,158) | 1:16:A:CYS:H    | 1:22:A:SER:HB3  | 4                   | 0.38     | 0.14                | 0.32       |
| (3,316) | 1:11:A:GLU:H    | 1:10:A:VAL:HG23 | 4                   | 0.33     | 0.18                | 0.32       |
| (3,316) | 1:11:A:GLU:H    | 1:10:A:VAL:HG22 | 4                   | 0.33     | 0.18                | 0.32       |
| (2,106) | 1:34:A:CYS:H    | 1:33:A:LYS:HG2  | 4                   | 0.31     | 0.07                | 0.33       |
| (3,252) | 1:16:A:CYS:H    | 1:15:A:LYS:HB3  | 4                   | 0.3      | 0.08                | 0.31       |
| (3,276) | 1:18:A:LYS:H    | 1:18:A:LYS:HG2  | 4                   | 0.26     | 0.12                | 0.22       |
| (3,533) | 1:24:A:PHE:HD1  | 1:13:A:LYS:HA   | 4                   | 0.21     | 0.08                | 0.18       |
| (3,533) | 1:24:A:PHE:HD2  | 1:13:A:LYS:HA   | 4                   | 0.21     | 0.08                | 0.18       |
| (2,41)  | 1:31:A:LYS:H    | 1:6:A:CYS:HB2   | 4                   | 0.2      | 0.01                | 0.2        |
| (3,415) | 1:22:A:SER:HB2  | 1:16:A:CYS:HB3  | 4                   | 0.2      | 0.12                | 0.14       |
| (2,57)  | 1:16:A:CYS:H    | 1:14:A:GLN:HB2  | 4                   | 0.19     | 0.07                | 0.18       |
| (3,47)  | 1:2:A:MET:H     | 1:8:A:ALA:HA    | 4                   | 0.16     | 0.06                | 0.15       |
| (3,24)  | 1:11:A:GLU:H    | 1:10:A:VAL:H    | 4                   | 0.16     | 0.02                | 0.16       |
| (3,56)  | 1:3:A:ASP:H     | 1:2:A:MET:HA    | 4                   | 0.15     | 0.04                | 0.14       |
| (2,254) | 1:17:A:LEU:HB2  | 1:17:A:LEU:HD22 | 4                   | 0.13     | 0.01                | 0.12       |
| (2,254) | 1:17:A:LEU:HB2  | 1:23:A:ILE:HG21 | 4                   | 0.13     | 0.01                | 0.12       |
| (2,254) | 1:17:A:LEU:HB2  | 1:17:A:LEU:HD23 | 4                   | 0.13     | 0.01                | 0.12       |
| (2,22)  | 1:18:A:LYS:H    | 1:18:A:LYS:HA   | 4                   | 0.12     | 0.01                | 0.12       |
| (3,335) | 1:14:A:GLN:HE21 | 1:17:A:LEU:HD12 | 3                   | 1.02     | 0.48                | 1.05       |
| (3,335) | 1:14:A:GLN:HE21 | 1:17:A:LEU:HD13 | 3                   | 1.02     | 0.48                | 1.05       |
| (3,228) | 1:29:A:ASN:HD21 | 1:28:A:MET:HB2  | 3                   | 0.87     | 0.54                | 0.98       |
| (2,231) | 1:28:A:MET:HG2  | 1:33:A:LYS:HD3  | 3                   | 0.59     | 0.31                | 0.7        |
| (3,247) | 1:4:A:MET:H     | 1:4:A:MET:HB3   | 3                   | 0.51     | 0.02                | 0.52       |
| (3,368) | 1:4:A:MET:HG3   | 1:4:A:MET:HA    | 3                   | 0.45     | 0.25                | 0.62       |
| (3,119) | 1:8:A:ALA:H     | 1:7:A:SER:HB3   | 3                   | 0.38     | 0.09                | 0.44       |
| (2,59)  | 1:3:A:ASP:H     | 1:2:A:MET:HB3   | 3                   | 0.38     | 0.09                | 0.34       |
| (3,476) | 1:12:A:CYS:HB3  | 1:15:A:LYS:HB3  | 3                   | 0.35     | 0.25                | 0.21       |
| (3,202) | 1:14:A:GLN:H    | 1:14:A:GLN:HG3  | 3                   | 0.31     | 0.13                | 0.25       |
| (2,24)  | 1:10:A:VAL:H    | 1:9:A:SER:HB2   | 3                   | 0.29     | 0.05                | 0.32       |
| (2,132) | 1:22:A:SER:HB3  | 1:16:A:CYS:HA   | 3                   | 0.27     | 0.08                | 0.22       |

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| Key     | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (2,132) | 1:22:A:SER:HB3  | 1:25:A:GLY:HA2  | 3                   | 0.27     | 0.08                | 0.22       |
| (2,120) | 1:21:A:GLY:H    | 1:20:A:ILE:HG22 | 3                   | 0.21     | 0.07                | 0.2        |
| (2,120) | 1:21:A:GLY:H    | 1:20:A:ILE:HG21 | 3                   | 0.21     | 0.07                | 0.2        |
| (2,120) | 1:21:A:GLY:H    | 1:20:A:ILE:HG23 | 3                   | 0.21     | 0.07                | 0.2        |
| (2,228) | 1:28:A:MET:HG3  | 1:26:A:LYS:HG3  | 3                   | 0.2      | 0.06                | 0.17       |
| (2,72)  | 1:30:A:LYS:H    | 1:30:A:LYS:HD3  | 3                   | 0.17     | 0.03                | 0.18       |
| (2,72)  | 1:30:A:LYS:H    | 1:31:A:LYS:HB2  | 3                   | 0.17     | 0.03                | 0.18       |
| (2,23)  | 1:8:A:ALA:H     | 1:9:A:SER:HB2   | 3                   | 0.15     | 0.03                | 0.14       |
| (2,76)  | 1:5:A:ARG:H     | 1:5:A:ARG:HG3   | 3                   | 0.14     | 0.02                | 0.15       |
| (3,205) | 1:31:A:LYS:H    | 1:32:A:CYS:HB3  | 3                   | 0.13     | 0.02                | 0.13       |
| (2,68)  | 1:28:A:MET:H    | 1:26:A:LYS:HB2  | 3                   | 0.12     | 0.02                | 0.12       |
| (3,85)  | 1:24:A:PHE:HE2  | 1:22:A:SER:HA   | 3                   | 0.12     | 0.01                | 0.12       |
| (3,509) | 1:23:A:ILE:HB   | 1:17:A:LEU:HD13 | 2                   | 2.91     | 0.06                | 2.91       |
| (3,509) | 1:23:A:ILE:HB   | 1:17:A:LEU:HD11 | 2                   | 2.91     | 0.06                | 2.91       |
| (3,412) | 1:17:A:LEU:HD11 | 1:23:A:ILE:HA   | 2                   | 2.54     | 0.08                | 2.54       |
| (3,412) | 1:17:A:LEU:HD12 | 1:23:A:ILE:HA   | 2                   | 2.54     | 0.08                | 2.54       |
| (3,307) | 1:14:A:GLN:H    | 1:17:A:LEU:HD12 | 2                   | 1.76     | 0.19                | 1.76       |
| (3,307) | 1:14:A:GLN:H    | 1:17:A:LEU:HD13 | 2                   | 1.76     | 0.19                | 1.76       |
| (3,529) | 1:14:A:GLN:HG3  | 1:17:A:LEU:HD12 | 2                   | 1.42     | 0.34                | 1.42       |
| (3,529) | 1:14:A:GLN:HG3  | 1:17:A:LEU:HD13 | 2                   | 1.42     | 0.34                | 1.42       |
| (3,441) | 1:14:A:GLN:HA   | 1:17:A:LEU:HD12 | 2                   | 1.33     | 0.22                | 1.33       |
| (3,441) | 1:14:A:GLN:HA   | 1:17:A:LEU:HD13 | 2                   | 1.33     | 0.22                | 1.33       |
| (3,528) | 1:14:A:GLN:HG2  | 1:17:A:LEU:HD12 | 2                   | 1.27     | 0.29                | 1.27       |
| (3,528) | 1:14:A:GLN:HG2  | 1:17:A:LEU:HD13 | 2                   | 1.27     | 0.29                | 1.27       |
| (2,86)  | 1:14:A:GLN:HE22 | 1:18:A:LYS:HB2  | 2                   | 0.5      | 0.28                | 0.5        |
| (2,86)  | 1:14:A:GLN:HE22 | 1:23:A:ILE:HB   | 2                   | 0.5      | 0.28                | 0.5        |
| (3,333) | 1:14:A:GLN:HE21 | 1:10:A:VAL:HG11 | 2                   | 0.47     | 0.22                | 0.47       |
| (2,32)  | 1:4:A:MET:H     | 1:3:A:ASP:HB2   | 2                   | 0.42     | 0.23                | 0.42       |
| (2,32)  | 1:4:A:MET:H     | 1:4:A:MET:HG2   | 2                   | 0.42     | 0.23                | 0.42       |
| (3,514) | 1:17:A:LEU:HB2  | 1:17:A:LEU:HD12 | 2                   | 0.38     | 0.0                 | 0.38       |
| (2,229) | 1:28:A:MET:HG2  | 1:26:A:LYS:HG3  | 2                   | 0.37     | 0.15                | 0.37       |
| (2,168) | 1:11:A:GLU:HA   | 1:31:A:LYS:HE2  | 2                   | 0.28     | 0.12                | 0.28       |
| (2,168) | 1:11:A:GLU:HA   | 1:15:A:LYS:HE3  | 2                   | 0.28     | 0.12                | 0.28       |
| (2,50)  | 1:14:A:GLN:HE21 | 1:18:A:LYS:HB3  | 2                   | 0.28     | 0.07                | 0.28       |
| (2,71)  | 1:30:A:LYS:H    | 1:31:A:LYS:HD2  | 2                   | 0.27     | 0.09                | 0.27       |
| (2,71)  | 1:30:A:LYS:H    | 1:30:A:LYS:HD2  | 2                   | 0.27     | 0.09                | 0.27       |
| (2,126) | 1:14:A:GLN:HE21 | 1:17:A:LEU:HD22 | 2                   | 0.27     | 0.09                | 0.27       |
| (2,126) | 1:14:A:GLN:HE21 | 1:17:A:LEU:HD23 | 2                   | 0.27     | 0.09                | 0.27       |
| (2,60)  | 1:10:A:VAL:H    | 1:2:A:MET:HB3   | 2                   | 0.26     | 0.14                | 0.26       |
| (3,322) | 1:22:A:SER:H    | 1:20:A:ILE:HD12 | 2                   | 0.26     | 0.09                | 0.26       |
| (3,322) | 1:22:A:SER:H    | 1:20:A:ILE:HD11 | 2                   | 0.26     | 0.09                | 0.26       |
| (2,274) | 1:23:A:ILE:HA   | 1:13:A:LYS:HG2  | 2                   | 0.24     | 0.08                | 0.24       |

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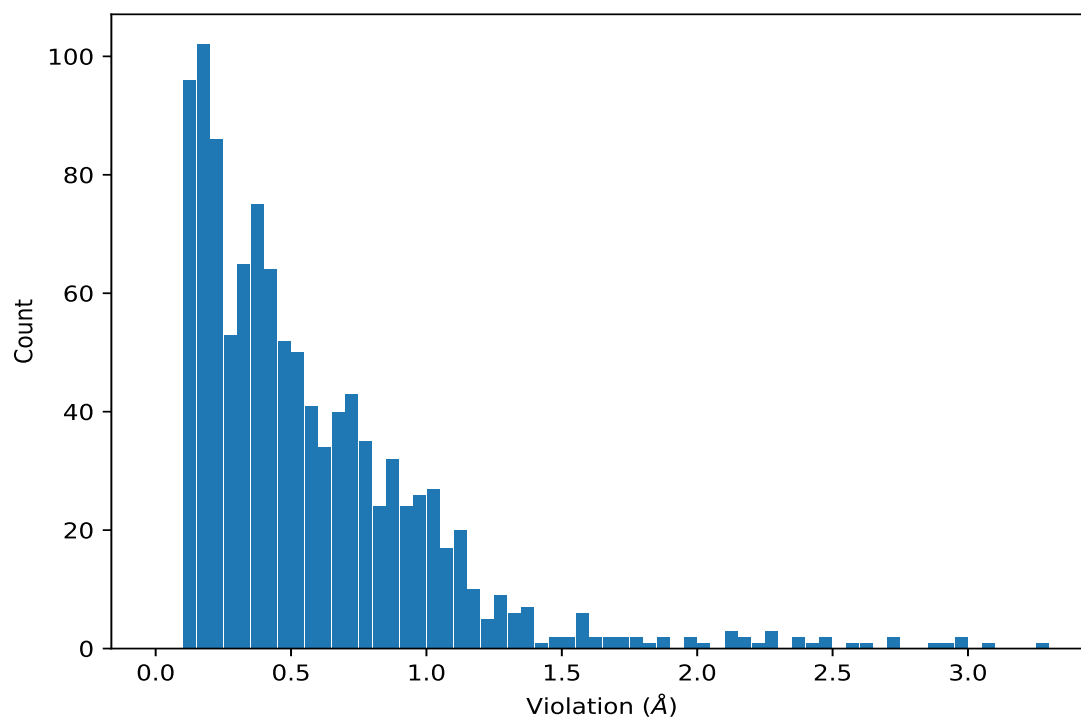
| Key     | Atom-1        | Atom-2       | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|---------------|--------------|---------------------|----------|---------------------|------------|
| (3,78)  | 1:6:A:CYS:H   | 1:5:A:ARG:HA | 2                   | 0.13     | 0.02                | 0.13       |
| (3,357) | 1:5:A:ARG:HD3 | 1:5:A:ARG:HA | 2                   | 0.11     | 0.0                 | 0.11       |

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

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

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

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



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

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

| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (3,499) | 1:11:A:GLU:HG2 | 1:10:A:VAL:HG22 | 7        | 3.26          |
| (3,499) | 1:11:A:GLU:HG2 | 1:10:A:VAL:HG22 | 6        | 3.05          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (2,221) | 1:13:A:LYS:HE2  | 1:10:A:VAL:HG13 | 6        | 2.98          |
| (3,509) | 1:23:A:ILE:HB   | 1:17:A:LEU:HD13 | 8        | 2.97          |
| (2,221) | 1:13:A:LYS:HE3  | 1:10:A:VAL:HG11 | 7        | 2.91          |
| (3,509) | 1:23:A:ILE:HB   | 1:17:A:LEU:HD11 | 10       | 2.85          |
| (3,388) | 1:22:A:SER:HB3  | 1:16:A:CYS:HB3  | 4        | 2.73          |
| (3,499) | 1:11:A:GLU:HG2  | 1:10:A:VAL:HG23 | 1        | 2.71          |
| (3,412) | 1:17:A:LEU:HD12 | 1:23:A:ILE:HA   | 10       | 2.62          |
| (3,499) | 1:11:A:GLU:HG2  | 1:10:A:VAL:HG22 | 10       | 2.55          |
| (3,498) | 1:11:A:GLU:HG2  | 1:10:A:VAL:HG11 | 8        | 2.45          |
| (3,412) | 1:17:A:LEU:HD11 | 1:23:A:ILE:HA   | 8        | 2.45          |
| (2,221) | 1:13:A:LYS:HE3  | 1:10:A:VAL:HG11 | 1        | 2.41          |
| (3,498) | 1:11:A:GLU:HG2  | 1:10:A:VAL:HG12 | 5        | 2.38          |
| (3,296) | 1:8:A:ALA:H     | 1:10:A:VAL:HG22 | 7        | 2.37          |
| (3,296) | 1:8:A:ALA:H     | 1:10:A:VAL:HG23 | 1        | 2.27          |
| (3,498) | 1:11:A:GLU:HG2  | 1:10:A:VAL:HG12 | 4        | 2.25          |
| (2,221) | 1:13:A:LYS:HE3  | 1:10:A:VAL:HG11 | 10       | 2.25          |
| (3,498) | 1:11:A:GLU:HG2  | 1:10:A:VAL:HG12 | 3        | 2.22          |
| (2,221) | 1:13:A:LYS:HE3  | 1:10:A:VAL:HG13 | 2        | 2.16          |
| (3,296) | 1:8:A:ALA:H     | 1:10:A:VAL:HG22 | 10       | 2.15          |
| (3,383) | 1:22:A:SER:HB3  | 1:34:A:CYS:HB2  | 5        | 2.13          |
| (3,296) | 1:8:A:ALA:H     | 1:10:A:VAL:HG22 | 6        | 2.12          |
| (3,296) | 1:8:A:ALA:H     | 1:10:A:VAL:HG21 | 2        | 2.11          |
| (3,499) | 1:11:A:GLU:HG2  | 1:10:A:VAL:HG22 | 4        | 2.03          |
| (3,499) | 1:11:A:GLU:HG2  | 1:10:A:VAL:HG21 | 3        | 1.98          |
| (3,307) | 1:14:A:GLN:H    | 1:17:A:LEU:HD13 | 10       | 1.95          |
| (2,195) | 1:9:A:SER:HB3   | 1:10:A:VAL:HG23 | 2        | 1.86          |
| (2,19)  | 1:1:A:GLN:HE21  | 1:9:A:SER:HB3   | 9        | 1.85          |
| (3,473) | 1:34:A:CYS:HB3  | 1:19:A:ALA:HB2  | 4        | 1.83          |
| (2,93)  | 1:24:A:PHE:HE1  | 1:13:A:LYS:HG2  | 10       | 1.78          |
| (3,529) | 1:14:A:GLN:HG3  | 1:17:A:LEU:HD13 | 10       | 1.76          |
| (2,19)  | 1:1:A:GLN:HE21  | 1:9:A:SER:HB2   | 2        | 1.72          |
| (2,19)  | 1:1:A:GLN:HE21  | 1:9:A:SER:HB3   | 5        | 1.7           |
| (2,195) | 1:9:A:SER:HB2   | 1:10:A:VAL:HG22 | 1        | 1.66          |
| (2,195) | 1:9:A:SER:HB2   | 1:10:A:VAL:HG21 | 10       | 1.65          |
| (3,425) | 1:19:A:ALA:HA   | 1:33:A:LYS:HB3  | 10       | 1.64          |
| (3,335) | 1:14:A:GLN:HE21 | 1:17:A:LEU:HD13 | 10       | 1.6           |
| (3,425) | 1:19:A:ALA:HA   | 1:33:A:LYS:HB3  | 9        | 1.58          |
| (3,425) | 1:19:A:ALA:HA   | 1:33:A:LYS:HB3  | 6        | 1.57          |
| (3,307) | 1:14:A:GLN:H    | 1:17:A:LEU:HD12 | 8        | 1.56          |
| (3,528) | 1:14:A:GLN:HG2  | 1:17:A:LEU:HD13 | 10       | 1.55          |
| (3,441) | 1:14:A:GLN:HA   | 1:17:A:LEU:HD13 | 10       | 1.55          |
| (2,19)  | 1:1:A:GLN:HE21  | 1:9:A:SER:HB3   | 8        | 1.55          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (2,19)  | 1:1:A:GLN:HE21  | 1:9:A:SER:HB2   | 10       | 1.54          |
| (3,535) | 1:19:A:ALA:H    | 1:34:A:CYS:HB3  | 4        | 1.52          |
| (3,228) | 1:29:A:ASN:HD21 | 1:28:A:MET:HB2  | 4        | 1.48          |
| (2,255) | 1:8:A:ALA:HB2   | 1:10:A:VAL:HG12 | 9        | 1.45          |
| (3,240) | 1:27:A:CYS:H    | 1:33:A:LYS:HB2  | 8        | 1.43          |
| (2,255) | 1:13:A:LYS:HG2  | 1:10:A:VAL:HG13 | 4        | 1.38          |
| (2,195) | 1:9:A:SER:HB3   | 1:10:A:VAL:HG21 | 7        | 1.37          |
| (2,90)  | 1:14:A:GLN:HE22 | 1:18:A:LYS:HD2  | 6        | 1.37          |
| (2,196) | 1:21:A:GLY:HA2  | 1:20:A:ILE:HG22 | 8        | 1.36          |
| (3,499) | 1:11:A:GLU:HG2  | 1:10:A:VAL:HG21 | 8        | 1.35          |
| (3,383) | 1:22:A:SER:HB3  | 1:34:A:CYS:HB2  | 7        | 1.35          |
| (2,252) | 1:31:A:LYS:HB2  | 1:15:A:LYS:HG2  | 4        | 1.35          |
| (2,92)  | 1:24:A:PHE:HD1  | 1:13:A:LYS:HG2  | 10       | 1.34          |
| (3,240) | 1:27:A:CYS:H    | 1:33:A:LYS:HB2  | 1        | 1.33          |
| (2,94)  | 1:24:A:PHE:HD1  | 1:26:A:LYS:HG2  | 3        | 1.33          |
| (2,93)  | 1:24:A:PHE:HE1  | 1:13:A:LYS:HG2  | 8        | 1.32          |
| (3,383) | 1:22:A:SER:HB3  | 1:34:A:CYS:HB2  | 9        | 1.3           |
| (2,89)  | 1:24:A:PHE:HE1  | 1:13:A:LYS:HD2  | 4        | 1.3           |
| (2,196) | 1:21:A:GLY:HA2  | 1:20:A:ILE:HG23 | 7        | 1.29          |
| (2,195) | 1:9:A:SER:HB3   | 1:10:A:VAL:HG21 | 6        | 1.28          |
| (3,425) | 1:19:A:ALA:HA   | 1:33:A:LYS:HB3  | 1        | 1.27          |
| (3,332) | 1:24:A:PHE:HD1  | 1:23:A:ILE:HD11 | 8        | 1.26          |
| (2,90)  | 1:11:A:GLU:H    | 1:13:A:LYS:HD3  | 10       | 1.26          |
| (2,51)  | 1:24:A:PHE:HD2  | 1:13:A:LYS:HB3  | 5        | 1.26          |
| (2,279) | 1:16:A:CYS:H    | 1:34:A:CYS:HA   | 10       | 1.25          |
| (2,108) | 1:28:A:MET:H    | 1:33:A:LYS:HG2  | 9        | 1.25          |
| (2,51)  | 1:24:A:PHE:HD1  | 1:13:A:LYS:HB3  | 6        | 1.25          |
| (2,279) | 1:16:A:CYS:H    | 1:24:A:PHE:HA   | 2        | 1.24          |
| (2,196) | 1:21:A:GLY:HA2  | 1:20:A:ILE:HG21 | 4        | 1.24          |
| (3,383) | 1:22:A:SER:HB3  | 1:34:A:CYS:HB2  | 3        | 1.23          |
| (3,383) | 1:22:A:SER:HB3  | 1:34:A:CYS:HB2  | 6        | 1.22          |
| (2,121) | 1:18:A:LYS:H    | 1:17:A:LEU:HD11 | 9        | 1.21          |
| (3,385) | 1:22:A:SER:HB2  | 1:34:A:CYS:HB2  | 1        | 1.18          |
| (2,90)  | 1:11:A:GLU:H    | 1:13:A:LYS:HD3  | 8        | 1.18          |
| (2,51)  | 1:24:A:PHE:HD1  | 1:13:A:LYS:HB3  | 2        | 1.18          |
| (3,383) | 1:22:A:SER:HB3  | 1:34:A:CYS:HB2  | 1        | 1.17          |
| (3,332) | 1:24:A:PHE:HD2  | 1:23:A:ILE:HD11 | 10       | 1.17          |
| (3,240) | 1:27:A:CYS:H    | 1:33:A:LYS:HB2  | 9        | 1.17          |
| (3,332) | 1:24:A:PHE:HD2  | 1:23:A:ILE:HD12 | 9        | 1.15          |
| (2,279) | 1:16:A:CYS:H    | 1:24:A:PHE:HA   | 7        | 1.15          |
| (2,89)  | 1:24:A:PHE:HE2  | 1:13:A:LYS:HD3  | 3        | 1.15          |
| (2,51)  | 1:24:A:PHE:HD1  | 1:13:A:LYS:HB3  | 7        | 1.15          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (3,460) | 1:5:A:ARG:HD2   | 1:4:A:MET:HE2   | 2        | 1.14          |
| (3,240) | 1:27:A:CYS:H    | 1:33:A:LYS:HB2  | 10       | 1.14          |
| (2,108) | 1:28:A:MET:H    | 1:33:A:LYS:HG2  | 10       | 1.14          |
| (2,89)  | 1:24:A:PHE:HE1  | 1:13:A:LYS:HD3  | 1        | 1.14          |
| (2,51)  | 1:24:A:PHE:HD2  | 1:13:A:LYS:HB3  | 1        | 1.13          |
| (2,51)  | 1:24:A:PHE:HD2  | 1:13:A:LYS:HB3  | 10       | 1.13          |
| (3,292) | 1:10:A:VAL:H    | 1:10:A:VAL:HG21 | 2        | 1.12          |
| (3,240) | 1:27:A:CYS:H    | 1:33:A:LYS:HB2  | 6        | 1.12          |
| (2,116) | 1:16:A:CYS:H    | 1:20:A:ILE:HD11 | 5        | 1.12          |
| (2,89)  | 1:24:A:PHE:HE2  | 1:13:A:LYS:HD3  | 7        | 1.12          |
| (3,460) | 1:5:A:ARG:HD2   | 1:4:A:MET:HE2   | 1        | 1.11          |
| (3,385) | 1:22:A:SER:HB2  | 1:34:A:CYS:HB2  | 3        | 1.11          |
| (3,385) | 1:22:A:SER:HB2  | 1:34:A:CYS:HB2  | 9        | 1.11          |
| (3,332) | 1:24:A:PHE:HD1  | 1:23:A:ILE:HD12 | 7        | 1.11          |
| (3,441) | 1:14:A:GLN:HA   | 1:17:A:LEU:HD12 | 8        | 1.1           |
| (3,292) | 1:10:A:VAL:H    | 1:10:A:VAL:HG23 | 1        | 1.1           |
| (2,218) | 1:12:A:CYS:HB3  | 1:13:A:LYS:HB2  | 10       | 1.1           |
| (2,90)  | 1:14:A:GLN:HE22 | 1:13:A:LYS:HD2  | 5        | 1.1           |
| (2,89)  | 1:24:A:PHE:HE1  | 1:13:A:LYS:HD3  | 9        | 1.1           |
| (2,51)  | 1:24:A:PHE:HD1  | 1:13:A:LYS:HB3  | 8        | 1.1           |
| (3,292) | 1:10:A:VAL:H    | 1:10:A:VAL:HG22 | 7        | 1.09          |
| (2,196) | 1:21:A:GLY:HA2  | 1:20:A:ILE:HD11 | 5        | 1.09          |
| (3,529) | 1:14:A:GLN:HG3  | 1:17:A:LEU:HD12 | 8        | 1.08          |
| (3,385) | 1:22:A:SER:HB2  | 1:34:A:CYS:HB2  | 6        | 1.08          |
| (3,332) | 1:24:A:PHE:HD2  | 1:23:A:ILE:HD12 | 1        | 1.08          |
| (2,51)  | 1:24:A:PHE:HD2  | 1:13:A:LYS:HB3  | 9        | 1.08          |
| (3,535) | 1:19:A:ALA:H    | 1:34:A:CYS:HB3  | 10       | 1.07          |
| (3,416) | 1:17:A:LEU:HA   | 1:16:A:CYS:HB3  | 4        | 1.07          |
| (3,281) | 1:25:A:GLY:H    | 1:13:A:LYS:HG3  | 2        | 1.07          |
| (3,257) | 1:19:A:ALA:H    | 1:15:A:LYS:HB2  | 10       | 1.07          |
| (3,292) | 1:10:A:VAL:H    | 1:10:A:VAL:HG22 | 6        | 1.06          |
| (3,257) | 1:19:A:ALA:H    | 1:15:A:LYS:HB2  | 1        | 1.06          |
| (3,257) | 1:19:A:ALA:H    | 1:15:A:LYS:HB2  | 6        | 1.06          |
| (2,51)  | 1:24:A:PHE:HD1  | 1:13:A:LYS:HB3  | 3        | 1.06          |
| (3,335) | 1:14:A:GLN:HE21 | 1:17:A:LEU:HD12 | 8        | 1.05          |
| (3,332) | 1:24:A:PHE:HD2  | 1:23:A:ILE:HD11 | 5        | 1.05          |
| (3,257) | 1:19:A:ALA:H    | 1:15:A:LYS:HB2  | 5        | 1.05          |
| (3,443) | 1:10:A:VAL:HA   | 1:10:A:VAL:HG12 | 2        | 1.04          |
| (3,292) | 1:10:A:VAL:H    | 1:10:A:VAL:HG22 | 10       | 1.04          |
| (3,257) | 1:19:A:ALA:H    | 1:15:A:LYS:HB2  | 8        | 1.04          |
| (2,221) | 1:13:A:LYS:HE3  | 1:10:A:VAL:HG13 | 5        | 1.04          |
| (3,257) | 1:19:A:ALA:H    | 1:15:A:LYS:HB2  | 9        | 1.03          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (3,218) | 1:29:A:ASN:HD22 | 1:28:A:MET:HB2  | 4        | 1.03          |
| (2,92)  | 1:24:A:PHE:HD1  | 1:17:A:LEU:HG   | 2        | 1.03          |
| (3,536) | 1:17:A:LEU:HD11 | 1:22:A:SER:HA   | 8        | 1.02          |
| (3,500) | 1:11:A:GLU:HB3  | 1:10:A:VAL:HG22 | 6        | 1.02          |
| (3,500) | 1:11:A:GLU:HB3  | 1:10:A:VAL:HG22 | 7        | 1.02          |
| (3,460) | 1:5:A:ARG:HD2   | 1:4:A:MET:HE3   | 6        | 1.02          |
| (3,443) | 1:10:A:VAL:HA   | 1:10:A:VAL:HG11 | 1        | 1.02          |
| (3,443) | 1:10:A:VAL:HA   | 1:10:A:VAL:HG13 | 10       | 1.02          |
| (3,332) | 1:24:A:PHE:HD1  | 1:23:A:ILE:HD12 | 3        | 1.02          |
| (2,258) | 1:19:A:ALA:HB3  | 1:20:A:ILE:HB   | 1        | 1.02          |
| (2,122) | 1:17:A:LEU:H    | 1:20:A:ILE:HD12 | 8        | 1.02          |
| (2,116) | 1:16:A:CYS:H    | 1:20:A:ILE:HG23 | 1        | 1.02          |
| (2,116) | 1:16:A:CYS:H    | 1:20:A:ILE:HD11 | 7        | 1.02          |
| (2,116) | 1:16:A:CYS:H    | 1:20:A:ILE:HG22 | 9        | 1.02          |
| (2,94)  | 1:24:A:PHE:HD1  | 1:26:A:LYS:HG2  | 10       | 1.02          |
| (3,240) | 1:27:A:CYS:H    | 1:33:A:LYS:HB2  | 4        | 1.01          |
| (2,258) | 1:19:A:ALA:HB2  | 1:20:A:ILE:HB   | 9        | 1.01          |
| (3,443) | 1:10:A:VAL:HA   | 1:10:A:VAL:HG13 | 6        | 1.0           |
| (3,388) | 1:22:A:SER:HB3  | 1:16:A:CYS:HB3  | 8        | 1.0           |
| (3,332) | 1:24:A:PHE:HD1  | 1:23:A:ILE:HD12 | 6        | 1.0           |
| (2,255) | 1:13:A:LYS:HG2  | 1:10:A:VAL:HG13 | 3        | 1.0           |
| (2,116) | 1:16:A:CYS:H    | 1:20:A:ILE:HG21 | 6        | 1.0           |
| (3,443) | 1:10:A:VAL:HA   | 1:10:A:VAL:HG11 | 7        | 0.99          |
| (2,116) | 1:16:A:CYS:H    | 1:20:A:ILE:HD12 | 8        | 0.99          |
| (3,528) | 1:14:A:GLN:HG2  | 1:17:A:LEU:HD12 | 8        | 0.98          |
| (3,425) | 1:19:A:ALA:HA   | 1:33:A:LYS:HB3  | 8        | 0.98          |
| (3,320) | 1:24:A:PHE:HE1  | 1:20:A:ILE:HD12 | 2        | 0.98          |
| (3,257) | 1:19:A:ALA:H    | 1:15:A:LYS:HB2  | 7        | 0.98          |
| (3,256) | 1:26:A:LYS:H    | 1:33:A:LYS:HB2  | 10       | 0.98          |
| (3,228) | 1:29:A:ASN:HD21 | 1:28:A:MET:HB2  | 7        | 0.98          |
| (3,146) | 1:14:A:GLN:H    | 1:16:A:CYS:HB2  | 4        | 0.98          |
| (2,279) | 1:16:A:CYS:H    | 1:24:A:PHE:HA   | 8        | 0.98          |
| (2,94)  | 1:24:A:PHE:HD1  | 1:26:A:LYS:HG2  | 7        | 0.98          |
| (3,281) | 1:25:A:GLY:H    | 1:13:A:LYS:HG3  | 3        | 0.97          |
| (3,257) | 1:19:A:ALA:H    | 1:15:A:LYS:HB2  | 2        | 0.97          |
| (2,258) | 1:19:A:ALA:HB3  | 1:20:A:ILE:HB   | 5        | 0.97          |
| (2,196) | 1:21:A:GLY:HA2  | 1:20:A:ILE:HD12 | 1        | 0.97          |
| (3,332) | 1:24:A:PHE:HD2  | 1:23:A:ILE:HD11 | 4        | 0.96          |
| (3,257) | 1:19:A:ALA:H    | 1:15:A:LYS:HB2  | 3        | 0.96          |
| (2,261) | 1:8:A:ALA:HB2   | 1:2:A:MET:HG2   | 3        | 0.96          |
| (2,258) | 1:19:A:ALA:HB3  | 1:20:A:ILE:HB   | 6        | 0.96          |
| (2,240) | 1:15:A:LYS:HB3  | 1:31:A:LYS:HB3  | 10       | 0.96          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (2,49)  | 1:12:A:CYS:H    | 1:14:A:GLN:HG3  | 4        | 0.96          |
| (2,258) | 1:19:A:ALA:HB3  | 1:20:A:ILE:HB   | 2        | 0.95          |
| (2,153) | 1:5:A:ARG:HG3   | 1:6:A:CYS:HA    | 5        | 0.95          |
| (2,121) | 1:18:A:LYS:H    | 1:17:A:LEU:HD12 | 1        | 0.95          |
| (2,121) | 1:23:A:ILE:H    | 1:17:A:LEU:HD13 | 5        | 0.95          |
| (2,51)  | 1:24:A:PHE:HD2  | 1:13:A:LYS:HB3  | 4        | 0.95          |
| (3,281) | 1:25:A:GLY:H    | 1:13:A:LYS:HG3  | 9        | 0.94          |
| (3,256) | 1:26:A:LYS:H    | 1:33:A:LYS:HB2  | 9        | 0.94          |
| (3,218) | 1:29:A:ASN:HD22 | 1:28:A:MET:HB2  | 7        | 0.94          |
| (3,183) | 1:4:A:MET:H     | 1:4:A:MET:HG3   | 8        | 0.94          |
| (2,279) | 1:16:A:CYS:H    | 1:34:A:CYS:HA   | 4        | 0.94          |
| (2,265) | 1:34:A:CYS:H    | 1:15:A:LYS:HA   | 5        | 0.94          |
| (2,198) | 1:21:A:GLY:HA3  | 1:20:A:ILE:HD11 | 8        | 0.94          |
| (2,191) | 1:7:A:SER:HB3   | 1:8:A:ALA:HB1   | 10       | 0.94          |
| (2,196) | 1:21:A:GLY:HA2  | 1:20:A:ILE:HD11 | 9        | 0.93          |
| (2,92)  | 1:24:A:PHE:HD2  | 1:17:A:LEU:HG   | 4        | 0.93          |
| (2,89)  | 1:24:A:PHE:HE2  | 1:13:A:LYS:HD2  | 5        | 0.93          |
| (3,302) | 1:21:A:GLY:H    | 1:17:A:LEU:HD12 | 9        | 0.92          |
| (3,218) | 1:29:A:ASN:HD22 | 1:28:A:MET:HB2  | 2        | 0.92          |
| (2,265) | 1:34:A:CYS:H    | 1:15:A:LYS:HA   | 3        | 0.92          |
| (2,258) | 1:19:A:ALA:HB3  | 1:20:A:ILE:HB   | 8        | 0.92          |
| (3,320) | 1:24:A:PHE:HE2  | 1:20:A:ILE:HD12 | 8        | 0.91          |
| (2,67)  | 1:28:A:MET:H    | 1:31:A:LYS:HD3  | 1        | 0.91          |
| (3,388) | 1:22:A:SER:HB3  | 1:16:A:CYS:HB3  | 5        | 0.9           |
| (3,320) | 1:24:A:PHE:HE2  | 1:20:A:ILE:HD13 | 4        | 0.9           |
| (2,231) | 1:28:A:MET:HG2  | 1:33:A:LYS:HD3  | 6        | 0.9           |
| (2,221) | 1:13:A:LYS:HE3  | 1:10:A:VAL:HG13 | 3        | 0.9           |
| (2,191) | 1:22:A:SER:HB2  | 1:19:A:ALA:HB3  | 1        | 0.9           |
| (2,122) | 1:17:A:LEU:H    | 1:20:A:ILE:HD11 | 9        | 0.9           |
| (2,90)  | 1:14:A:GLN:HE22 | 1:13:A:LYS:HD2  | 7        | 0.9           |
| (3,256) | 1:26:A:LYS:H    | 1:33:A:LYS:HB2  | 6        | 0.89          |
| (2,122) | 1:17:A:LEU:H    | 1:20:A:ILE:HD11 | 7        | 0.89          |
| (3,473) | 1:34:A:CYS:HB3  | 1:19:A:ALA:HB2  | 10       | 0.88          |
| (3,388) | 1:22:A:SER:HB3  | 1:16:A:CYS:HB3  | 7        | 0.88          |
| (3,281) | 1:25:A:GLY:H    | 1:13:A:LYS:HG3  | 5        | 0.88          |
| (2,265) | 1:34:A:CYS:H    | 1:17:A:LEU:HA   | 6        | 0.88          |
| (2,258) | 1:19:A:ALA:HB2  | 1:20:A:ILE:HB   | 10       | 0.88          |
| (2,252) | 1:31:A:LYS:HB3  | 1:15:A:LYS:HG2  | 6        | 0.88          |
| (2,122) | 1:17:A:LEU:H    | 1:20:A:ILE:HD11 | 5        | 0.88          |
| (3,320) | 1:24:A:PHE:HE2  | 1:20:A:ILE:HD11 | 10       | 0.87          |
| (3,293) | 1:16:A:CYS:H    | 1:17:A:LEU:HD12 | 10       | 0.87          |
| (3,281) | 1:25:A:GLY:H    | 1:13:A:LYS:HG3  | 1        | 0.87          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (2,240) | 1:15:A:LYS:HB3  | 1:31:A:LYS:HB3  | 9        | 0.87          |
| (2,153) | 1:5:A:ARG:HG3   | 1:6:A:CYS:HA    | 8        | 0.87          |
| (2,122) | 1:17:A:LEU:H    | 1:20:A:ILE:HG23 | 1        | 0.87          |
| (2,116) | 1:16:A:CYS:H    | 1:20:A:ILE:HD13 | 4        | 0.87          |
| (2,92)  | 1:24:A:PHE:HD1  | 1:13:A:LYS:HG2  | 6        | 0.87          |
| (3,380) | 1:11:A:GLU:HG2  | 1:11:A:GLU:HA   | 4        | 0.86          |
| (3,281) | 1:25:A:GLY:H    | 1:13:A:LYS:HG3  | 6        | 0.86          |
| (3,177) | 1:32:A:CYS:H    | 1:27:A:CYS:HB2  | 5        | 0.86          |
| (2,196) | 1:21:A:GLY:HA2  | 1:20:A:ILE:HD11 | 10       | 0.86          |
| (2,92)  | 1:24:A:PHE:HD1  | 1:13:A:LYS:HG2  | 8        | 0.86          |
| (2,89)  | 1:24:A:PHE:HE2  | 1:13:A:LYS:HD2  | 2        | 0.86          |
| (3,425) | 1:19:A:ALA:HA   | 1:33:A:LYS:HB3  | 4        | 0.85          |
| (3,329) | 1:24:A:PHE:HD2  | 1:23:A:ILE:HG23 | 8        | 0.85          |
| (3,281) | 1:25:A:GLY:H    | 1:13:A:LYS:HG3  | 7        | 0.85          |
| (2,258) | 1:15:A:LYS:HG3  | 1:14:A:GLN:HB3  | 3        | 0.85          |
| (2,258) | 1:19:A:ALA:HB3  | 1:20:A:ILE:HB   | 7        | 0.85          |
| (2,252) | 1:31:A:LYS:HB3  | 1:15:A:LYS:HG2  | 5        | 0.85          |
| (2,197) | 1:17:A:LEU:HA   | 1:20:A:ILE:HD12 | 8        | 0.85          |
| (2,116) | 1:16:A:CYS:H    | 1:20:A:ILE:HG21 | 3        | 0.85          |
| (2,94)  | 1:24:A:PHE:HD2  | 1:26:A:LYS:HG2  | 5        | 0.85          |
| (3,295) | 1:19:A:ALA:H    | 1:17:A:LEU:HD12 | 5        | 0.84          |
| (2,198) | 1:17:A:LEU:HA   | 1:20:A:ILE:HD13 | 4        | 0.84          |
| (2,93)  | 1:24:A:PHE:HE1  | 1:17:A:LEU:HG   | 2        | 0.84          |
| (2,92)  | 1:24:A:PHE:HD1  | 1:17:A:LEU:HG   | 5        | 0.84          |
| (3,499) | 1:11:A:GLU:HG2  | 1:10:A:VAL:HG21 | 2        | 0.83          |
| (3,299) | 1:25:A:GLY:H    | 1:23:A:ILE:HG21 | 2        | 0.83          |
| (3,177) | 1:32:A:CYS:H    | 1:27:A:CYS:HB2  | 4        | 0.83          |
| (3,177) | 1:32:A:CYS:H    | 1:27:A:CYS:HB2  | 9        | 0.83          |
| (2,265) | 1:34:A:CYS:H    | 1:15:A:LYS:HA   | 2        | 0.83          |
| (2,261) | 1:8:A:ALA:HB1   | 1:2:A:MET:HG2   | 4        | 0.83          |
| (2,216) | 1:24:A:PHE:HB2  | 1:26:A:LYS:HG2  | 3        | 0.83          |
| (2,108) | 1:28:A:MET:H    | 1:33:A:LYS:HG2  | 6        | 0.83          |
| (3,499) | 1:11:A:GLU:HG2  | 1:10:A:VAL:HG23 | 5        | 0.82          |
| (3,460) | 1:5:A:ARG:HD2   | 1:4:A:MET:HE3   | 3        | 0.82          |
| (2,198) | 1:21:A:GLY:HA3  | 1:20:A:ILE:HD13 | 7        | 0.82          |
| (2,98)  | 1:8:A:ALA:H     | 1:31:A:LYS:HD3  | 2        | 0.82          |
| (3,302) | 1:21:A:GLY:H    | 1:17:A:LEU:HD11 | 1        | 0.81          |
| (2,224) | 1:13:A:LYS:HE2  | 1:23:A:ILE:HG23 | 10       | 0.81          |
| (2,153) | 1:5:A:ARG:HG2   | 1:6:A:CYS:HA    | 4        | 0.81          |
| (3,536) | 1:17:A:LEU:HD12 | 1:22:A:SER:HA   | 10       | 0.8           |
| (3,298) | 1:25:A:GLY:H    | 1:20:A:ILE:HD11 | 3        | 0.8           |
| (2,121) | 1:18:A:LYS:H    | 1:17:A:LEU:HD13 | 7        | 0.8           |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (2,108) | 1:28:A:MET:H    | 1:33:A:LYS:HG2  | 4        | 0.8           |
| (2,94)  | 1:24:A:PHE:HD1  | 1:26:A:LYS:HG2  | 2        | 0.8           |
| (3,465) | 1:34:A:CYS:HB2  | 1:16:A:CYS:HB3  | 6        | 0.79          |
| (2,98)  | 1:8:A:ALA:H     | 1:31:A:LYS:HD3  | 6        | 0.79          |
| (2,279) | 1:16:A:CYS:H    | 1:34:A:CYS:HA   | 1        | 0.78          |
| (2,279) | 1:16:A:CYS:H    | 1:34:A:CYS:HA   | 6        | 0.78          |
| (2,258) | 1:15:A:LYS:HG3  | 1:14:A:GLN:HB2  | 4        | 0.78          |
| (2,93)  | 1:24:A:PHE:HE2  | 1:17:A:LEU:HG   | 6        | 0.78          |
| (2,90)  | 1:14:A:GLN:HE22 | 1:13:A:LYS:HD2  | 2        | 0.78          |
| (2,89)  | 1:24:A:PHE:HE1  | 1:13:A:LYS:HD2  | 6        | 0.78          |
| (2,86)  | 1:14:A:GLN:HE22 | 1:23:A:ILE:HB   | 6        | 0.78          |
| (2,49)  | 1:12:A:CYS:H    | 1:14:A:GLN:HG3  | 2        | 0.78          |
| (3,329) | 1:24:A:PHE:HD1  | 1:23:A:ILE:HG22 | 5        | 0.77          |
| (3,295) | 1:19:A:ALA:H    | 1:17:A:LEU:HD12 | 9        | 0.77          |
| (3,281) | 1:25:A:GLY:H    | 1:13:A:LYS:HG3  | 8        | 0.77          |
| (2,265) | 1:34:A:CYS:H    | 1:15:A:LYS:HA   | 10       | 0.77          |
| (2,93)  | 1:24:A:PHE:HE1  | 1:17:A:LEU:HG   | 5        | 0.77          |
| (2,49)  | 1:29:A:ASN:HD21 | 1:28:A:MET:HG2  | 7        | 0.77          |
| (3,409) | 1:23:A:ILE:HD11 | 1:23:A:ILE:HA   | 1        | 0.76          |
| (3,409) | 1:23:A:ILE:HD11 | 1:23:A:ILE:HA   | 3        | 0.76          |
| (3,409) | 1:23:A:ILE:HD12 | 1:23:A:ILE:HA   | 4        | 0.76          |
| (3,409) | 1:23:A:ILE:HD11 | 1:23:A:ILE:HA   | 7        | 0.76          |
| (3,409) | 1:23:A:ILE:HD13 | 1:23:A:ILE:HA   | 10       | 0.76          |
| (3,380) | 1:11:A:GLU:HG2  | 1:11:A:GLU:HA   | 3        | 0.76          |
| (3,299) | 1:25:A:GLY:H    | 1:23:A:ILE:HG21 | 8        | 0.76          |
| (3,281) | 1:25:A:GLY:H    | 1:13:A:LYS:HG3  | 10       | 0.76          |
| (3,256) | 1:26:A:LYS:H    | 1:33:A:LYS:HB2  | 4        | 0.76          |
| (2,255) | 1:8:A:ALA:HB1   | 1:10:A:VAL:HG12 | 5        | 0.76          |
| (2,153) | 1:5:A:ARG:HG2   | 1:6:A:CYS:HA    | 10       | 0.76          |
| (2,122) | 1:17:A:LEU:H    | 1:20:A:ILE:HD13 | 4        | 0.76          |
| (3,409) | 1:23:A:ILE:HD13 | 1:23:A:ILE:HA   | 5        | 0.75          |
| (3,409) | 1:23:A:ILE:HD13 | 1:23:A:ILE:HA   | 8        | 0.75          |
| (3,299) | 1:25:A:GLY:H    | 1:23:A:ILE:HG21 | 6        | 0.75          |
| (3,186) | 1:34:A:CYS:H    | 1:34:A:CYS:HB3  | 2        | 0.75          |
| (3,157) | 1:16:A:CYS:H    | 1:16:A:CYS:HB2  | 4        | 0.75          |
| (2,121) | 1:18:A:LYS:H    | 1:17:A:LEU:HD12 | 3        | 0.75          |
| (2,67)  | 1:28:A:MET:H    | 1:31:A:LYS:HD3  | 3        | 0.75          |
| (3,465) | 1:34:A:CYS:HB2  | 1:16:A:CYS:HB3  | 9        | 0.74          |
| (3,298) | 1:25:A:GLY:H    | 1:20:A:ILE:HD11 | 5        | 0.74          |
| (2,196) | 1:21:A:GLY:HA2  | 1:20:A:ILE:HD12 | 6        | 0.74          |
| (2,122) | 1:17:A:LEU:H    | 1:20:A:ILE:HD11 | 10       | 0.74          |
| (2,67)  | 1:28:A:MET:H    | 1:31:A:LYS:HD2  | 10       | 0.74          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (2,19)  | 1:1:A:GLN:HE21  | 1:9:A:SER:HB2   | 4        | 0.74          |
| (3,409) | 1:23:A:ILE:HD13 | 1:23:A:ILE:HA   | 2        | 0.73          |
| (3,409) | 1:23:A:ILE:HD11 | 1:23:A:ILE:HA   | 9        | 0.73          |
| (3,329) | 1:24:A:PHE:HD2  | 1:23:A:ILE:HG22 | 4        | 0.73          |
| (3,299) | 1:25:A:GLY:H    | 1:23:A:ILE:HG23 | 5        | 0.73          |
| (3,299) | 1:25:A:GLY:H    | 1:23:A:ILE:HG22 | 9        | 0.73          |
| (3,293) | 1:16:A:CYS:H    | 1:17:A:LEU:HD11 | 8        | 0.73          |
| (2,240) | 1:15:A:LYS:HB3  | 1:31:A:LYS:HB3  | 8        | 0.73          |
| (2,98)  | 1:8:A:ALA:H     | 1:31:A:LYS:HD3  | 7        | 0.73          |
| (2,93)  | 1:24:A:PHE:HE2  | 1:17:A:LEU:HG   | 4        | 0.73          |
| (3,320) | 1:24:A:PHE:HE1  | 1:20:A:ILE:HD11 | 7        | 0.72          |
| (3,299) | 1:25:A:GLY:H    | 1:23:A:ILE:HG23 | 10       | 0.72          |
| (3,298) | 1:25:A:GLY:H    | 1:20:A:ILE:HD11 | 9        | 0.72          |
| (3,297) | 1:8:A:ALA:H     | 1:10:A:VAL:HG12 | 3        | 0.72          |
| (2,261) | 1:8:A:ALA:HB2   | 1:2:A:MET:HG2   | 9        | 0.72          |
| (2,252) | 1:31:A:LYS:HB3  | 1:15:A:LYS:HG2  | 10       | 0.72          |
| (2,240) | 1:15:A:LYS:HB3  | 1:31:A:LYS:HB3  | 1        | 0.72          |
| (2,221) | 1:13:A:LYS:HE2  | 1:10:A:VAL:HG13 | 4        | 0.72          |
| (3,498) | 1:11:A:GLU:HG2  | 1:10:A:VAL:HG12 | 9        | 0.71          |
| (3,409) | 1:23:A:ILE:HD11 | 1:23:A:ILE:HA   | 6        | 0.71          |
| (3,329) | 1:24:A:PHE:HD2  | 1:23:A:ILE:HG22 | 10       | 0.71          |
| (3,299) | 1:25:A:GLY:H    | 1:23:A:ILE:HG23 | 1        | 0.71          |
| (3,299) | 1:25:A:GLY:H    | 1:23:A:ILE:HG21 | 7        | 0.71          |
| (3,298) | 1:25:A:GLY:H    | 1:20:A:ILE:HD11 | 7        | 0.71          |
| (3,295) | 1:19:A:ALA:H    | 1:17:A:LEU:HD12 | 2        | 0.71          |
| (3,257) | 1:19:A:ALA:H    | 1:15:A:LYS:HB2  | 4        | 0.71          |
| (3,183) | 1:4:A:MET:H     | 1:4:A:MET:HG3   | 1        | 0.71          |
| (2,196) | 1:21:A:GLY:HA2  | 1:20:A:ILE:HD11 | 2        | 0.71          |
| (2,122) | 1:17:A:LEU:H    | 1:20:A:ILE:HG21 | 6        | 0.71          |
| (2,94)  | 1:24:A:PHE:HD2  | 1:26:A:LYS:HG2  | 6        | 0.71          |
| (2,1)   | 1:14:A:GLN:H    | 1:32:A:CYS:H    | 7        | 0.71          |
| (3,536) | 1:17:A:LEU:HD13 | 1:22:A:SER:HA   | 3        | 0.7           |
| (3,476) | 1:12:A:CYS:HB3  | 1:15:A:LYS:HB3  | 4        | 0.7           |
| (3,465) | 1:34:A:CYS:HB2  | 1:16:A:CYS:HB3  | 5        | 0.7           |
| (3,442) | 1:17:A:LEU:HA   | 1:17:A:LEU:HD12 | 1        | 0.7           |
| (3,298) | 1:25:A:GLY:H    | 1:20:A:ILE:HD12 | 1        | 0.7           |
| (2,231) | 1:28:A:MET:HG2  | 1:33:A:LYS:HD3  | 9        | 0.7           |
| (2,121) | 1:18:A:LYS:H    | 1:17:A:LEU:HD13 | 4        | 0.7           |
| (3,536) | 1:17:A:LEU:HD13 | 1:22:A:SER:HA   | 9        | 0.69          |
| (3,500) | 1:11:A:GLU:HB3  | 1:10:A:VAL:HG21 | 2        | 0.69          |
| (3,333) | 1:14:A:GLN:HE21 | 1:10:A:VAL:HG11 | 9        | 0.69          |
| (3,298) | 1:25:A:GLY:H    | 1:20:A:ILE:HD12 | 6        | 0.69          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (3,296) | 1:8:A:ALA:H     | 1:10:A:VAL:HG22 | 8        | 0.69          |
| (3,231) | 1:8:A:ALA:H     | 1:11:A:GLU:HB3  | 5        | 0.69          |
| (2,64)  | 1:32:A:CYS:H    | 1:31:A:LYS:HD3  | 6        | 0.69          |
| (3,536) | 1:17:A:LEU:HD13 | 1:22:A:SER:HA   | 1        | 0.68          |
| (3,536) | 1:17:A:LEU:HD11 | 1:22:A:SER:HA   | 7        | 0.68          |
| (3,433) | 1:7:A:SER:HB2   | 1:8:A:ALA:HB2   | 6        | 0.68          |
| (3,383) | 1:22:A:SER:HB3  | 1:34:A:CYS:HB2  | 8        | 0.68          |
| (3,299) | 1:25:A:GLY:H    | 1:23:A:ILE:HG21 | 3        | 0.68          |
| (3,295) | 1:19:A:ALA:H    | 1:17:A:LEU:HD11 | 6        | 0.68          |
| (3,231) | 1:8:A:ALA:H     | 1:11:A:GLU:HB3  | 10       | 0.68          |
| (2,265) | 1:34:A:CYS:H    | 1:15:A:LYS:HA   | 1        | 0.68          |
| (2,261) | 1:8:A:ALA:HB3   | 1:2:A:MET:HG2   | 6        | 0.68          |
| (2,110) | 1:4:A:MET:H     | 1:31:A:LYS:HG2  | 1        | 0.68          |
| (2,82)  | 1:14:A:GLN:H    | 1:17:A:LEU:HB2  | 10       | 0.68          |
| (2,40)  | 1:5:A:ARG:H     | 1:6:A:CYS:HB3   | 4        | 0.68          |
| (3,554) | 1:5:A:ARG:H     | 1:5:A:ARG:HB3   | 8        | 0.67          |
| (3,385) | 1:22:A:SER:HB2  | 1:34:A:CYS:HB2  | 2        | 0.67          |
| (3,298) | 1:25:A:GLY:H    | 1:20:A:ILE:HD13 | 4        | 0.67          |
| (3,231) | 1:8:A:ALA:H     | 1:11:A:GLU:HB3  | 6        | 0.67          |
| (3,177) | 1:32:A:CYS:H    | 1:27:A:CYS:HB2  | 2        | 0.67          |
| (2,196) | 1:21:A:GLY:HA2  | 1:20:A:ILE:HD11 | 3        | 0.67          |
| (2,92)  | 1:24:A:PHE:HD1  | 1:17:A:LEU:HG   | 7        | 0.67          |
| (3,554) | 1:5:A:ARG:H     | 1:5:A:ARG:HB3   | 10       | 0.66          |
| (3,465) | 1:34:A:CYS:HB2  | 1:16:A:CYS:HB3  | 1        | 0.66          |
| (3,465) | 1:34:A:CYS:HB2  | 1:16:A:CYS:HB3  | 3        | 0.66          |
| (3,329) | 1:24:A:PHE:HD1  | 1:23:A:ILE:HG23 | 7        | 0.66          |
| (3,309) | 1:24:A:PHE:H    | 1:23:A:ILE:HD13 | 8        | 0.66          |
| (3,297) | 1:8:A:ALA:H     | 1:10:A:VAL:HG12 | 4        | 0.66          |
| (3,186) | 1:34:A:CYS:H    | 1:34:A:CYS:HB3  | 7        | 0.66          |
| (2,116) | 1:16:A:CYS:H    | 1:20:A:ILE:HD12 | 2        | 0.66          |
| (2,90)  | 1:14:A:GLN:HE22 | 1:13:A:LYS:HD2  | 4        | 0.66          |
| (2,67)  | 1:28:A:MET:H    | 1:31:A:LYS:HD3  | 8        | 0.66          |
| (3,329) | 1:24:A:PHE:HD2  | 1:23:A:ILE:HG23 | 6        | 0.65          |
| (3,231) | 1:8:A:ALA:H     | 1:11:A:GLU:HB3  | 1        | 0.65          |
| (2,42)  | 1:15:A:LYS:H    | 1:15:A:LYS:HE3  | 5        | 0.65          |
| (2,32)  | 1:4:A:MET:H     | 1:3:A:ASP:HB2   | 10       | 0.65          |
| (3,298) | 1:25:A:GLY:H    | 1:20:A:ILE:HD11 | 10       | 0.64          |
| (3,256) | 1:26:A:LYS:H    | 1:33:A:LYS:HB2  | 1        | 0.64          |
| (3,256) | 1:26:A:LYS:H    | 1:33:A:LYS:HB2  | 8        | 0.64          |
| (2,117) | 1:16:A:CYS:H    | 1:23:A:ILE:HG23 | 5        | 0.64          |
| (2,1)   | 1:14:A:GLN:H    | 1:32:A:CYS:H    | 3        | 0.64          |
| (3,329) | 1:24:A:PHE:HD2  | 1:23:A:ILE:HG22 | 1        | 0.63          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (3,297) | 1:8:A:ALA:H     | 1:10:A:VAL:HG11 | 8        | 0.63          |
| (2,224) | 1:13:A:LYS:HE2  | 1:23:A:ILE:HG21 | 5        | 0.63          |
| (2,122) | 1:17:A:LEU:H    | 1:20:A:ILE:HG21 | 3        | 0.63          |
| (3,442) | 1:17:A:LEU:HA   | 1:17:A:LEU:HD12 | 9        | 0.62          |
| (3,433) | 1:7:A:SER:HB2   | 1:8:A:ALA:HB1   | 3        | 0.62          |
| (3,368) | 1:4:A:MET:HG3   | 1:4:A:MET:HA    | 7        | 0.62          |
| (3,368) | 1:4:A:MET:HG3   | 1:4:A:MET:HA    | 9        | 0.62          |
| (3,309) | 1:24:A:PHE:H    | 1:23:A:ILE:HD13 | 4        | 0.62          |
| (3,298) | 1:25:A:GLY:H    | 1:20:A:ILE:HD12 | 2        | 0.62          |
| (3,295) | 1:19:A:ALA:H    | 1:17:A:LEU:HD12 | 1        | 0.62          |
| (3,231) | 1:8:A:ALA:H     | 1:11:A:GLU:HB3  | 8        | 0.62          |
| (2,265) | 1:34:A:CYS:H    | 1:15:A:LYS:HA   | 9        | 0.62          |
| (2,197) | 1:17:A:LEU:HA   | 1:20:A:ILE:HD11 | 10       | 0.62          |
| (2,94)  | 1:24:A:PHE:HD1  | 1:26:A:LYS:HG2  | 1        | 0.62          |
| (3,329) | 1:24:A:PHE:HD1  | 1:23:A:ILE:HG23 | 2        | 0.61          |
| (3,158) | 1:16:A:CYS:H    | 1:22:A:SER:HB3  | 4        | 0.61          |
| (2,265) | 1:34:A:CYS:H    | 1:15:A:LYS:HA   | 8        | 0.61          |
| (2,189) | 1:30:A:LYS:HA   | 1:30:A:LYS:HD2  | 9        | 0.61          |
| (2,78)  | 1:6:A:CYS:H     | 1:5:A:ARG:HB2   | 2        | 0.61          |
| (3,536) | 1:17:A:LEU:HD11 | 1:22:A:SER:HA   | 4        | 0.6           |
| (3,536) | 1:17:A:LEU:HD13 | 1:22:A:SER:HA   | 5        | 0.6           |
| (3,328) | 1:24:A:PHE:HZ   | 1:23:A:ILE:HG21 | 4        | 0.6           |
| (3,309) | 1:24:A:PHE:H    | 1:23:A:ILE:HD13 | 5        | 0.6           |
| (3,231) | 1:8:A:ALA:H     | 1:11:A:GLU:HB3  | 7        | 0.6           |
| (2,261) | 1:8:A:ALA:HB3   | 1:2:A:MET:HG2   | 2        | 0.6           |
| (2,121) | 1:23:A:ILE:H    | 1:17:A:LEU:HD12 | 6        | 0.6           |
| (2,49)  | 1:29:A:ASN:HD21 | 1:28:A:MET:HG2  | 3        | 0.6           |
| (2,11)  | 1:6:A:CYS:H     | 1:8:A:ALA:HA    | 1        | 0.6           |
| (3,554) | 1:5:A:ARG:H     | 1:5:A:ARG:HB3   | 5        | 0.59          |
| (3,329) | 1:24:A:PHE:HD2  | 1:23:A:ILE:HG21 | 9        | 0.59          |
| (3,299) | 1:25:A:GLY:H    | 1:23:A:ILE:HG23 | 4        | 0.59          |
| (3,295) | 1:19:A:ALA:H    | 1:17:A:LEU:HD13 | 7        | 0.59          |
| (3,177) | 1:32:A:CYS:H    | 1:27:A:CYS:HB2  | 8        | 0.59          |
| (2,218) | 1:16:A:CYS:HB3  | 1:13:A:LYS:HB3  | 6        | 0.59          |
| (2,175) | 1:9:A:SER:HB2   | 1:2:A:MET:HG3   | 5        | 0.59          |
| (2,110) | 1:4:A:MET:H     | 1:31:A:LYS:HG3  | 4        | 0.59          |
| (2,78)  | 1:6:A:CYS:H     | 1:5:A:ARG:HB2   | 4        | 0.59          |
| (2,66)  | 1:27:A:CYS:H    | 1:26:A:LYS:HD3  | 3        | 0.59          |
| (2,11)  | 1:6:A:CYS:H     | 1:8:A:ALA:HA    | 3        | 0.59          |
| (3,500) | 1:11:A:GLU:HB3  | 1:10:A:VAL:HG23 | 1        | 0.58          |
| (3,304) | 1:24:A:PHE:H    | 1:23:A:ILE:HG22 | 4        | 0.58          |
| (2,265) | 1:34:A:CYS:H    | 1:15:A:LYS:HA   | 7        | 0.58          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (2,221) | 1:13:A:LYS:HE3 | 1:10:A:VAL:HG12 | 8        | 0.58          |
| (2,189) | 1:30:A:LYS:HA  | 1:30:A:LYS:HD2  | 5        | 0.58          |
| (2,11)  | 1:6:A:CYS:H    | 1:27:A:CYS:HA   | 8        | 0.58          |
| (3,309) | 1:24:A:PHE:H   | 1:23:A:ILE:HD11 | 7        | 0.57          |
| (3,309) | 1:24:A:PHE:H   | 1:23:A:ILE:HD13 | 10       | 0.57          |
| (3,298) | 1:25:A:GLY:H   | 1:20:A:ILE:HD12 | 8        | 0.57          |
| (3,178) | 1:27:A:CYS:H   | 1:12:A:CYS:HB2  | 4        | 0.57          |
| (2,221) | 1:13:A:LYS:HE2 | 1:10:A:VAL:HG13 | 9        | 0.57          |
| (2,189) | 1:30:A:LYS:HA  | 1:30:A:LYS:HD2  | 4        | 0.57          |
| (2,116) | 1:16:A:CYS:H   | 1:20:A:ILE:HD11 | 10       | 0.57          |
| (2,82)  | 1:14:A:GLN:H   | 1:17:A:LEU:HB2  | 2        | 0.57          |
| (2,19)  | 1:1:A:GLN:HE21 | 1:9:A:SER:HB3   | 3        | 0.57          |
| (3,295) | 1:19:A:ALA:H   | 1:17:A:LEU:HD12 | 3        | 0.56          |
| (2,200) | 1:14:A:GLN:HA  | 1:23:A:ILE:HG22 | 9        | 0.56          |
| (2,189) | 1:30:A:LYS:HA  | 1:30:A:LYS:HD2  | 6        | 0.56          |
| (2,189) | 1:30:A:LYS:HA  | 1:30:A:LYS:HD2  | 7        | 0.56          |
| (2,109) | 1:28:A:MET:H   | 1:31:A:LYS:HG3  | 3        | 0.56          |
| (2,78)  | 1:6:A:CYS:H    | 1:5:A:ARG:HB2   | 8        | 0.56          |
| (3,500) | 1:11:A:GLU:HB3 | 1:10:A:VAL:HG22 | 10       | 0.55          |
| (3,316) | 1:11:A:GLU:H   | 1:10:A:VAL:HG22 | 7        | 0.55          |
| (3,302) | 1:21:A:GLY:H   | 1:17:A:LEU:HD13 | 3        | 0.55          |
| (3,295) | 1:19:A:ALA:H   | 1:17:A:LEU:HD13 | 4        | 0.55          |
| (2,252) | 1:31:A:LYS:HB3 | 1:15:A:LYS:HG2  | 1        | 0.55          |
| (2,207) | 1:18:A:LYS:HE2 | 1:18:A:LYS:HB2  | 3        | 0.55          |
| (2,198) | 1:21:A:GLY:HA3 | 1:20:A:ILE:HD13 | 5        | 0.55          |
| (2,78)  | 1:6:A:CYS:H    | 1:5:A:ARG:HB2   | 3        | 0.55          |
| (2,44)  | 1:24:A:PHE:HD1 | 1:13:A:LYS:HE3  | 6        | 0.55          |
| (3,329) | 1:24:A:PHE:HD1 | 1:23:A:ILE:HG23 | 3        | 0.54          |
| (3,281) | 1:25:A:GLY:H   | 1:13:A:LYS:HG3  | 4        | 0.54          |
| (2,255) | 1:13:A:LYS:HG2 | 1:10:A:VAL:HG12 | 8        | 0.54          |
| (2,246) | 1:26:A:LYS:HB2 | 1:33:A:LYS:HG3  | 2        | 0.54          |
| (2,224) | 1:13:A:LYS:HE2 | 1:23:A:ILE:HG22 | 7        | 0.54          |
| (2,207) | 1:18:A:LYS:HE2 | 1:18:A:LYS:HB2  | 6        | 0.54          |
| (2,175) | 1:9:A:SER:HB2  | 1:2:A:MET:HG3   | 2        | 0.54          |
| (2,111) | 1:27:A:CYS:H   | 1:26:A:LYS:HG2  | 3        | 0.54          |
| (2,93)  | 1:24:A:PHE:HE1 | 1:17:A:LEU:HG   | 7        | 0.54          |
| (2,78)  | 1:6:A:CYS:H    | 1:5:A:ARG:HB2   | 6        | 0.54          |
| (2,78)  | 1:6:A:CYS:H    | 1:5:A:ARG:HB2   | 7        | 0.54          |
| (2,67)  | 1:28:A:MET:H   | 1:31:A:LYS:HD3  | 2        | 0.54          |
| (2,64)  | 1:32:A:CYS:H   | 1:31:A:LYS:HD3  | 5        | 0.54          |
| (2,43)  | 1:24:A:PHE:HE1 | 1:13:A:LYS:HE3  | 8        | 0.54          |
| (2,11)  | 1:6:A:CYS:H    | 1:8:A:ALA:HA    | 7        | 0.54          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (2,11)  | 1:6:A:CYS:H     | 1:8:A:ALA:HA    | 10       | 0.54          |
| (3,309) | 1:24:A:PHE:H    | 1:23:A:ILE:HD11 | 1        | 0.53          |
| (3,247) | 1:4:A:MET:H     | 1:4:A:MET:HB3   | 5        | 0.53          |
| (3,186) | 1:34:A:CYS:H    | 1:34:A:CYS:HB3  | 1        | 0.53          |
| (2,191) | 1:7:A:SER:HB3   | 1:8:A:ALA:HB2   | 6        | 0.53          |
| (2,119) | 1:19:A:ALA:H    | 1:20:A:ILE:HG22 | 2        | 0.53          |
| (2,102) | 1:5:A:ARG:H     | 1:31:A:LYS:HG3  | 4        | 0.53          |
| (2,89)  | 1:24:A:PHE:HE1  | 1:13:A:LYS:HD2  | 10       | 0.53          |
| (2,88)  | 1:24:A:PHE:HD2  | 1:13:A:LYS:HD3  | 3        | 0.53          |
| (2,78)  | 1:6:A:CYS:H     | 1:5:A:ARG:HB2   | 1        | 0.53          |
| (2,11)  | 1:6:A:CYS:H     | 1:27:A:CYS:HA   | 9        | 0.53          |
| (3,442) | 1:17:A:LEU:HA   | 1:17:A:LEU:HD13 | 3        | 0.52          |
| (3,386) | 1:13:A:LYS:HA   | 1:16:A:CYS:HB2  | 4        | 0.52          |
| (3,247) | 1:4:A:MET:H     | 1:4:A:MET:HB3   | 3        | 0.52          |
| (3,186) | 1:34:A:CYS:H    | 1:34:A:CYS:HB3  | 10       | 0.52          |
| (2,229) | 1:28:A:MET:HG2  | 1:26:A:LYS:HG3  | 8        | 0.52          |
| (2,207) | 1:18:A:LYS:HE2  | 1:18:A:LYS:HB3  | 5        | 0.52          |
| (2,207) | 1:18:A:LYS:HE3  | 1:18:A:LYS:HB3  | 8        | 0.52          |
| (2,200) | 1:14:A:GLN:HA   | 1:23:A:ILE:HG23 | 1        | 0.52          |
| (2,193) | 1:15:A:LYS:HA   | 1:31:A:LYS:HG2  | 3        | 0.52          |
| (2,78)  | 1:6:A:CYS:H     | 1:5:A:ARG:HB2   | 9        | 0.52          |
| (3,320) | 1:24:A:PHE:HE2  | 1:20:A:ILE:HD12 | 1        | 0.51          |
| (2,207) | 1:18:A:LYS:HE3  | 1:18:A:LYS:HB2  | 10       | 0.51          |
| (2,153) | 1:5:A:ARG:HG2   | 1:6:A:CYS:HA    | 2        | 0.51          |
| (2,78)  | 1:6:A:CYS:H     | 1:5:A:ARG:HB2   | 10       | 0.51          |
| (2,67)  | 1:28:A:MET:H    | 1:31:A:LYS:HD3  | 5        | 0.51          |
| (2,40)  | 1:5:A:ARG:H     | 1:6:A:CYS:HB3   | 2        | 0.51          |
| (2,11)  | 1:6:A:CYS:H     | 1:8:A:ALA:HA    | 6        | 0.51          |
| (3,536) | 1:17:A:LEU:HD12 | 1:22:A:SER:HA   | 6        | 0.5           |
| (3,332) | 1:24:A:PHE:HD2  | 1:23:A:ILE:HD11 | 2        | 0.5           |
| (2,82)  | 1:14:A:GLN:H    | 1:17:A:LEU:HB2  | 8        | 0.5           |
| (2,78)  | 1:6:A:CYS:H     | 1:5:A:ARG:HB2   | 5        | 0.5           |
| (2,67)  | 1:28:A:MET:H    | 1:31:A:LYS:HD3  | 4        | 0.5           |
| (2,59)  | 1:3:A:ASP:H     | 1:2:A:MET:HB3   | 1        | 0.5           |
| (2,44)  | 1:24:A:PHE:HD1  | 1:13:A:LYS:HE3  | 8        | 0.5           |
| (3,535) | 1:19:A:ALA:H    | 1:34:A:CYS:HB3  | 6        | 0.49          |
| (3,320) | 1:24:A:PHE:HE1  | 1:20:A:ILE:HD11 | 3        | 0.49          |
| (3,320) | 1:24:A:PHE:HE2  | 1:20:A:ILE:HD12 | 6        | 0.49          |
| (3,309) | 1:24:A:PHE:H    | 1:23:A:ILE:HD11 | 3        | 0.49          |
| (3,309) | 1:24:A:PHE:H    | 1:23:A:ILE:HD11 | 9        | 0.49          |
| (3,247) | 1:4:A:MET:H     | 1:4:A:MET:HB3   | 2        | 0.49          |
| (3,202) | 1:14:A:GLN:H    | 1:14:A:GLN:HG3  | 3        | 0.49          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (2,207) | 1:18:A:LYS:HE3  | 1:18:A:LYS:HB2  | 7        | 0.49          |
| (2,195) | 1:9:A:SER:HB2   | 1:10:A:VAL:HG22 | 3        | 0.49          |
| (2,193) | 1:15:A:LYS:HA   | 1:31:A:LYS:HG2  | 5        | 0.49          |
| (2,175) | 1:9:A:SER:HB3   | 1:2:A:MET:HG2   | 7        | 0.49          |
| (2,94)  | 1:24:A:PHE:HD1  | 1:26:A:LYS:HG2  | 8        | 0.49          |
| (2,67)  | 1:28:A:MET:H    | 1:31:A:LYS:HD3  | 7        | 0.49          |
| (3,316) | 1:11:A:GLU:H    | 1:10:A:VAL:HG22 | 6        | 0.48          |
| (3,304) | 1:24:A:PHE:H    | 1:23:A:ILE:HG23 | 7        | 0.48          |
| (3,304) | 1:24:A:PHE:H    | 1:23:A:ILE:HG23 | 8        | 0.48          |
| (3,186) | 1:34:A:CYS:H    | 1:34:A:CYS:HB3  | 4        | 0.48          |
| (2,216) | 1:24:A:PHE:HB2  | 1:26:A:LYS:HG2  | 2        | 0.48          |
| (2,200) | 1:14:A:GLN:HA   | 1:23:A:ILE:HG23 | 5        | 0.48          |
| (2,191) | 1:7:A:SER:HB3   | 1:8:A:ALA:HB1   | 3        | 0.48          |
| (2,119) | 1:19:A:ALA:H    | 1:20:A:ILE:HG22 | 8        | 0.48          |
| (2,88)  | 1:24:A:PHE:HD1  | 1:13:A:LYS:HD3  | 4        | 0.48          |
| (2,88)  | 1:24:A:PHE:HD1  | 1:13:A:LYS:HD3  | 9        | 0.48          |
| (2,1)   | 1:6:A:CYS:H     | 1:32:A:CYS:H    | 6        | 0.48          |
| (3,309) | 1:24:A:PHE:H    | 1:23:A:ILE:HD11 | 6        | 0.47          |
| (2,240) | 1:15:A:LYS:HB3  | 1:31:A:LYS:HB3  | 7        | 0.47          |
| (2,216) | 1:24:A:PHE:HB2  | 1:26:A:LYS:HG2  | 10       | 0.47          |
| (2,122) | 1:17:A:LEU:H    | 1:20:A:ILE:HD12 | 2        | 0.47          |
| (2,64)  | 1:32:A:CYS:H    | 1:31:A:LYS:HD3  | 10       | 0.47          |
| (2,11)  | 1:6:A:CYS:H     | 1:27:A:CYS:HA   | 5        | 0.47          |
| (3,536) | 1:17:A:LEU:HD13 | 1:22:A:SER:HA   | 2        | 0.46          |
| (3,186) | 1:34:A:CYS:H    | 1:34:A:CYS:HB3  | 3        | 0.46          |
| (3,119) | 1:8:A:ALA:H     | 1:7:A:SER:HB3   | 7        | 0.46          |
| (2,216) | 1:24:A:PHE:HB2  | 1:26:A:LYS:HG2  | 7        | 0.46          |
| (2,207) | 1:18:A:LYS:HE2  | 1:18:A:LYS:HB2  | 1        | 0.46          |
| (2,67)  | 1:28:A:MET:H    | 1:31:A:LYS:HD3  | 6        | 0.46          |
| (2,64)  | 1:32:A:CYS:H    | 1:31:A:LYS:HD3  | 9        | 0.46          |
| (2,27)  | 1:14:A:GLN:HE21 | 1:17:A:LEU:HA   | 10       | 0.46          |
| (3,442) | 1:17:A:LEU:HA   | 1:17:A:LEU:HD11 | 7        | 0.45          |
| (3,380) | 1:11:A:GLU:HG2  | 1:11:A:GLU:HA   | 7        | 0.45          |
| (3,276) | 1:18:A:LYS:H    | 1:18:A:LYS:HG2  | 9        | 0.45          |
| (3,219) | 1:24:A:PHE:HD1  | 1:23:A:ILE:HB   | 2        | 0.45          |
| (3,186) | 1:34:A:CYS:H    | 1:34:A:CYS:HB3  | 5        | 0.45          |
| (3,164) | 1:32:A:CYS:H    | 1:32:A:CYS:HB3  | 9        | 0.45          |
| (2,240) | 1:15:A:LYS:HB3  | 1:31:A:LYS:HB3  | 5        | 0.45          |
| (2,198) | 1:21:A:GLY:HA3  | 1:20:A:ILE:HD13 | 9        | 0.45          |
| (2,164) | 1:23:A:ILE:HD11 | 1:24:A:PHE:HA   | 3        | 0.45          |
| (2,110) | 1:4:A:MET:H     | 1:31:A:LYS:HG3  | 5        | 0.45          |
| (2,88)  | 1:24:A:PHE:HD1  | 1:13:A:LYS:HD3  | 1        | 0.45          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (2,67)  | 1:28:A:MET:H    | 1:31:A:LYS:HD3  | 9        | 0.45          |
| (2,11)  | 1:6:A:CYS:H     | 1:8:A:ALA:HA    | 2        | 0.45          |
| (2,1)   | 1:6:A:CYS:H     | 1:32:A:CYS:H    | 1        | 0.45          |
| (3,442) | 1:17:A:LEU:HA   | 1:17:A:LEU:HD13 | 5        | 0.44          |
| (3,433) | 1:7:A:SER:HB2   | 1:8:A:ALA:HB3   | 8        | 0.44          |
| (3,380) | 1:11:A:GLU:HG2  | 1:11:A:GLU:HA   | 1        | 0.44          |
| (3,304) | 1:24:A:PHE:H    | 1:23:A:ILE:HG22 | 1        | 0.44          |
| (3,304) | 1:24:A:PHE:H    | 1:23:A:ILE:HG21 | 9        | 0.44          |
| (3,296) | 1:8:A:ALA:H     | 1:10:A:VAL:HG22 | 3        | 0.44          |
| (3,119) | 1:8:A:ALA:H     | 1:7:A:SER:HB3   | 1        | 0.44          |
| (2,207) | 1:18:A:LYS:HE3  | 1:18:A:LYS:HB3  | 4        | 0.44          |
| (2,169) | 1:14:A:GLN:HA   | 1:18:A:LYS:HE3  | 4        | 0.44          |
| (2,119) | 1:19:A:ALA:H    | 1:20:A:ILE:HG22 | 9        | 0.44          |
| (2,87)  | 1:11:A:GLU:H    | 1:13:A:LYS:HB3  | 3        | 0.44          |
| (2,82)  | 1:14:A:GLN:H    | 1:17:A:LEU:HB2  | 5        | 0.44          |
| (2,58)  | 1:3:A:ASP:H     | 1:1:A:GLN:HB3   | 2        | 0.44          |
| (2,58)  | 1:3:A:ASP:H     | 1:1:A:GLN:HB3   | 3        | 0.44          |
| (2,35)  | 1:26:A:LYS:H    | 1:12:A:CYS:HB3  | 3        | 0.44          |
| (3,218) | 1:29:A:ASN:HD22 | 1:28:A:MET:HB2  | 8        | 0.43          |
| (3,164) | 1:32:A:CYS:H    | 1:32:A:CYS:HB3  | 2        | 0.43          |
| (3,145) | 1:6:A:CYS:H     | 1:5:A:ARG:HD3   | 2        | 0.43          |
| (2,246) | 1:26:A:LYS:HB2  | 1:33:A:LYS:HG3  | 5        | 0.43          |
| (2,218) | 1:16:A:CYS:HB3  | 1:15:A:LYS:HB2  | 3        | 0.43          |
| (2,215) | 1:32:A:CYS:HB3  | 1:26:A:LYS:HG3  | 10       | 0.43          |
| (2,162) | 1:20:A:ILE:HD12 | 1:16:A:CYS:HA   | 8        | 0.43          |
| (2,98)  | 1:8:A:ALA:H     | 1:31:A:LYS:HD2  | 8        | 0.43          |
| (2,64)  | 1:32:A:CYS:H    | 1:31:A:LYS:HD3  | 2        | 0.43          |
| (3,554) | 1:5:A:ARG:H     | 1:5:A:ARG:HB3   | 4        | 0.42          |
| (3,442) | 1:17:A:LEU:HA   | 1:17:A:LEU:HD12 | 6        | 0.42          |
| (3,385) | 1:22:A:SER:HB2  | 1:34:A:CYS:HB2  | 5        | 0.42          |
| (3,335) | 1:14:A:GLN:HE21 | 1:17:A:LEU:HD12 | 3        | 0.42          |
| (3,320) | 1:24:A:PHE:HE1  | 1:20:A:ILE:HD11 | 5        | 0.42          |
| (3,302) | 1:21:A:GLY:H    | 1:17:A:LEU:HD11 | 7        | 0.42          |
| (3,164) | 1:32:A:CYS:H    | 1:32:A:CYS:HB3  | 8        | 0.42          |
| (3,164) | 1:32:A:CYS:H    | 1:32:A:CYS:HB3  | 10       | 0.42          |
| (2,224) | 1:13:A:LYS:HE3  | 1:23:A:ILE:HG22 | 8        | 0.42          |
| (2,215) | 1:32:A:CYS:HB3  | 1:31:A:LYS:HG2  | 4        | 0.42          |
| (2,164) | 1:23:A:ILE:HD13 | 1:22:A:SER:HA   | 1        | 0.42          |
| (2,164) | 1:23:A:ILE:HD11 | 1:24:A:PHE:HA   | 6        | 0.42          |
| (2,58)  | 1:3:A:ASP:H     | 1:1:A:GLN:HB2   | 4        | 0.42          |
| (2,27)  | 1:14:A:GLN:HE21 | 1:17:A:LEU:HA   | 1        | 0.42          |
| (3,442) | 1:17:A:LEU:HA   | 1:17:A:LEU:HD11 | 4        | 0.41          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (3,304) | 1:24:A:PHE:H    | 1:23:A:ILE:HG22 | 10       | 0.41          |
| (3,186) | 1:34:A:CYS:H    | 1:34:A:CYS:HB3  | 9        | 0.41          |
| (2,279) | 1:16:A:CYS:H    | 1:34:A:CYS:HA   | 3        | 0.41          |
| (2,168) | 1:11:A:GLU:HA   | 1:15:A:LYS:HE3  | 7        | 0.41          |
| (2,107) | 1:16:A:CYS:H    | 1:19:A:ALA:HB3  | 6        | 0.41          |
| (2,60)  | 1:10:A:VAL:H    | 1:2:A:MET:HB3   | 8        | 0.41          |
| (2,43)  | 1:24:A:PHE:HE1  | 1:13:A:LYS:HE3  | 4        | 0.41          |
| (3,460) | 1:5:A:ARG:HD2   | 1:4:A:MET:HE2   | 5        | 0.4           |
| (3,442) | 1:17:A:LEU:HA   | 1:17:A:LEU:HD13 | 2        | 0.4           |
| (3,415) | 1:22:A:SER:HB2  | 1:16:A:CYS:HB3  | 4        | 0.4           |
| (3,328) | 1:24:A:PHE:HZ   | 1:23:A:ILE:HG23 | 7        | 0.4           |
| (3,304) | 1:24:A:PHE:H    | 1:23:A:ILE:HG22 | 5        | 0.4           |
| (3,297) | 1:8:A:ALA:H     | 1:10:A:VAL:HG12 | 9        | 0.4           |
| (3,164) | 1:32:A:CYS:H    | 1:32:A:CYS:HB3  | 4        | 0.4           |
| (2,252) | 1:31:A:LYS:HB3  | 1:15:A:LYS:HG2  | 8        | 0.4           |
| (2,246) | 1:26:A:LYS:HB2  | 1:33:A:LYS:HG3  | 7        | 0.4           |
| (2,198) | 1:21:A:GLY:HA3  | 1:20:A:ILE:HD11 | 1        | 0.4           |
| (2,162) | 1:20:A:ILE:HG21 | 1:16:A:CYS:HA   | 5        | 0.4           |
| (2,119) | 1:19:A:ALA:H    | 1:20:A:ILE:HG23 | 7        | 0.4           |
| (2,111) | 1:27:A:CYS:H    | 1:26:A:LYS:HG2  | 7        | 0.4           |
| (2,109) | 1:28:A:MET:H    | 1:31:A:LYS:HG3  | 5        | 0.4           |
| (2,109) | 1:28:A:MET:H    | 1:31:A:LYS:HG3  | 7        | 0.4           |
| (2,58)  | 1:3:A:ASP:H     | 1:1:A:GLN:HB3   | 7        | 0.4           |
| (2,35)  | 1:26:A:LYS:H    | 1:12:A:CYS:HB3  | 6        | 0.4           |
| (2,11)  | 1:6:A:CYS:H     | 1:27:A:CYS:HA   | 4        | 0.4           |
| (3,505) | 1:4:A:MET:HB3   | 1:8:A:ALA:HB1   | 1        | 0.39          |
| (3,433) | 1:7:A:SER:HB2   | 1:8:A:ALA:HB1   | 9        | 0.39          |
| (3,304) | 1:24:A:PHE:H    | 1:23:A:ILE:HG23 | 3        | 0.39          |
| (3,252) | 1:16:A:CYS:H    | 1:15:A:LYS:HB3  | 3        | 0.39          |
| (3,199) | 1:26:A:LYS:H    | 1:28:A:MET:HG3  | 2        | 0.39          |
| (3,164) | 1:32:A:CYS:H    | 1:32:A:CYS:HB3  | 1        | 0.39          |
| (2,279) | 1:16:A:CYS:H    | 1:34:A:CYS:HA   | 9        | 0.39          |
| (2,266) | 1:6:A:CYS:HB2   | 1:27:A:CYS:HA   | 6        | 0.39          |
| (2,164) | 1:23:A:ILE:HD12 | 1:22:A:SER:HA   | 5        | 0.39          |
| (2,132) | 1:22:A:SER:HB3  | 1:16:A:CYS:HA   | 8        | 0.39          |
| (2,111) | 1:27:A:CYS:H    | 1:26:A:LYS:HG2  | 5        | 0.39          |
| (2,111) | 1:27:A:CYS:H    | 1:26:A:LYS:HG2  | 8        | 0.39          |
| (2,98)  | 1:8:A:ALA:H     | 1:31:A:LYS:HD2  | 10       | 0.39          |
| (2,43)  | 1:24:A:PHE:HE1  | 1:13:A:LYS:HE2  | 1        | 0.39          |
| (2,37)  | 1:8:A:ALA:H     | 1:2:A:MET:HG2   | 10       | 0.39          |
| (2,27)  | 1:14:A:GLN:HE21 | 1:17:A:LEU:HA   | 4        | 0.39          |
| (2,27)  | 1:14:A:GLN:HE21 | 1:17:A:LEU:HA   | 5        | 0.39          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (2,1)   | 1:6:A:CYS:H     | 1:32:A:CYS:H    | 9        | 0.39          |
| (3,514) | 1:17:A:LEU:HB2  | 1:17:A:LEU:HD12 | 8        | 0.38          |
| (3,514) | 1:17:A:LEU:HB2  | 1:17:A:LEU:HD12 | 10       | 0.38          |
| (3,380) | 1:11:A:GLU:HG2  | 1:11:A:GLU:HA   | 10       | 0.38          |
| (3,231) | 1:8:A:ALA:H     | 1:11:A:GLU:HB3  | 9        | 0.38          |
| (3,186) | 1:34:A:CYS:H    | 1:34:A:CYS:HB3  | 6        | 0.38          |
| (3,164) | 1:32:A:CYS:H    | 1:32:A:CYS:HB3  | 7        | 0.38          |
| (2,224) | 1:13:A:LYS:HE2  | 1:23:A:ILE:HG22 | 2        | 0.38          |
| (2,193) | 1:15:A:LYS:HA   | 1:31:A:LYS:HG2  | 2        | 0.38          |
| (2,193) | 1:15:A:LYS:HA   | 1:31:A:LYS:HG2  | 7        | 0.38          |
| (2,175) | 1:9:A:SER:HB2   | 1:2:A:MET:HG2   | 10       | 0.38          |
| (2,119) | 1:19:A:ALA:H    | 1:20:A:ILE:HG23 | 10       | 0.38          |
| (2,117) | 1:16:A:CYS:H    | 1:23:A:ILE:HG21 | 6        | 0.38          |
| (2,111) | 1:27:A:CYS:H    | 1:26:A:LYS:HG2  | 4        | 0.38          |
| (2,106) | 1:34:A:CYS:H    | 1:33:A:LYS:HG2  | 5        | 0.38          |
| (2,82)  | 1:14:A:GLN:H    | 1:17:A:LEU:HB2  | 4        | 0.38          |
| (2,43)  | 1:24:A:PHE:HE2  | 1:13:A:LYS:HE2  | 5        | 0.38          |
| (2,43)  | 1:24:A:PHE:HE2  | 1:13:A:LYS:HE2  | 7        | 0.38          |
| (2,37)  | 1:8:A:ALA:H     | 1:2:A:MET:HG3   | 7        | 0.38          |
| (2,37)  | 1:8:A:ALA:H     | 1:2:A:MET:HG3   | 9        | 0.38          |
| (2,19)  | 1:1:A:GLN:HE21  | 1:9:A:SER:HB3   | 6        | 0.38          |
| (3,252) | 1:16:A:CYS:H    | 1:15:A:LYS:HB3  | 4        | 0.37          |
| (3,246) | 1:28:A:MET:H    | 1:28:A:MET:HB3  | 1        | 0.37          |
| (3,164) | 1:32:A:CYS:H    | 1:32:A:CYS:HB3  | 5        | 0.37          |
| (3,164) | 1:32:A:CYS:H    | 1:32:A:CYS:HB3  | 6        | 0.37          |
| (2,246) | 1:26:A:LYS:HB2  | 1:33:A:LYS:HG2  | 4        | 0.37          |
| (2,246) | 1:26:A:LYS:HB2  | 1:33:A:LYS:HG2  | 6        | 0.37          |
| (2,193) | 1:15:A:LYS:HA   | 1:31:A:LYS:HG2  | 9        | 0.37          |
| (2,111) | 1:27:A:CYS:H    | 1:26:A:LYS:HG2  | 9        | 0.37          |
| (2,110) | 1:4:A:MET:H     | 1:31:A:LYS:HG3  | 9        | 0.37          |
| (2,109) | 1:28:A:MET:H    | 1:31:A:LYS:HG3  | 8        | 0.37          |
| (2,88)  | 1:24:A:PHE:HD2  | 1:13:A:LYS:HD3  | 7        | 0.37          |
| (2,58)  | 1:3:A:ASP:H     | 1:1:A:GLN:HB3   | 6        | 0.37          |
| (2,35)  | 1:26:A:LYS:H    | 1:12:A:CYS:HB3  | 5        | 0.37          |
| (3,31)  | 1:24:A:PHE:HD2  | 1:25:A:GLY:H    | 2        | 0.36          |
| (2,193) | 1:15:A:LYS:HA   | 1:31:A:LYS:HG2  | 8        | 0.36          |
| (2,162) | 1:20:A:ILE:HD11 | 1:16:A:CYS:HA   | 7        | 0.36          |
| (2,126) | 1:14:A:GLN:HE21 | 1:17:A:LEU:HD23 | 3        | 0.36          |
| (2,119) | 1:19:A:ALA:H    | 1:20:A:ILE:HG21 | 5        | 0.36          |
| (2,111) | 1:27:A:CYS:H    | 1:26:A:LYS:HG2  | 2        | 0.36          |
| (2,111) | 1:27:A:CYS:H    | 1:26:A:LYS:HG2  | 6        | 0.36          |
| (2,71)  | 1:30:A:LYS:H    | 1:30:A:LYS:HD2  | 9        | 0.36          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (2,58)  | 1:3:A:ASP:H     | 1:1:A:GLN:HB3   | 5        | 0.36          |
| (2,43)  | 1:24:A:PHE:HE2  | 1:13:A:LYS:HE2  | 3        | 0.36          |
| (3,445) | 1:21:A:GLY:HA3  | 1:17:A:LEU:HD23 | 10       | 0.35          |
| (3,322) | 1:22:A:SER:H    | 1:20:A:ILE:HD12 | 8        | 0.35          |
| (3,302) | 1:21:A:GLY:H    | 1:17:A:LEU:HD11 | 4        | 0.35          |
| (3,219) | 1:24:A:PHE:HD2  | 1:23:A:ILE:HB   | 6        | 0.35          |
| (3,164) | 1:32:A:CYS:H    | 1:32:A:CYS:HB3  | 3        | 0.35          |
| (2,279) | 1:16:A:CYS:H    | 1:34:A:CYS:HA   | 5        | 0.35          |
| (2,198) | 1:21:A:GLY:HA3  | 1:20:A:ILE:HD13 | 10       | 0.35          |
| (2,197) | 1:17:A:LEU:HA   | 1:20:A:ILE:HD12 | 1        | 0.35          |
| (2,197) | 1:17:A:LEU:HA   | 1:20:A:ILE:HD11 | 7        | 0.35          |
| (2,164) | 1:23:A:ILE:HD12 | 1:22:A:SER:HA   | 8        | 0.35          |
| (2,110) | 1:4:A:MET:H     | 1:31:A:LYS:HG3  | 2        | 0.35          |
| (2,109) | 1:28:A:MET:H    | 1:31:A:LYS:HG3  | 2        | 0.35          |
| (2,98)  | 1:8:A:ALA:H     | 1:31:A:LYS:HD2  | 3        | 0.35          |
| (2,94)  | 1:24:A:PHE:HD1  | 1:26:A:LYS:HG2  | 9        | 0.35          |
| (3,533) | 1:24:A:PHE:HD1  | 1:13:A:LYS:HA   | 2        | 0.34          |
| (3,246) | 1:28:A:MET:H    | 1:28:A:MET:HB3  | 6        | 0.34          |
| (3,184) | 1:16:A:CYS:H    | 1:12:A:CYS:HB2  | 2        | 0.34          |
| (2,252) | 1:31:A:LYS:HB3  | 1:15:A:LYS:HG2  | 9        | 0.34          |
| (2,246) | 1:26:A:LYS:HB2  | 1:33:A:LYS:HG3  | 3        | 0.34          |
| (2,200) | 1:14:A:GLN:HA   | 1:23:A:ILE:HG21 | 3        | 0.34          |
| (2,107) | 1:16:A:CYS:H    | 1:19:A:ALA:HB3  | 8        | 0.34          |
| (2,59)  | 1:3:A:ASP:H     | 1:2:A:MET:HB3   | 10       | 0.34          |
| (2,50)  | 1:14:A:GLN:HE21 | 1:18:A:LYS:HB3  | 3        | 0.34          |
| (2,49)  | 1:29:A:ASN:HD21 | 1:28:A:MET:HG2  | 8        | 0.34          |
| (2,43)  | 1:24:A:PHE:HE1  | 1:13:A:LYS:HE3  | 9        | 0.34          |
| (3,328) | 1:24:A:PHE:HZ   | 1:23:A:ILE:HG23 | 3        | 0.33          |
| (3,158) | 1:16:A:CYS:H    | 1:22:A:SER:HB3  | 8        | 0.33          |
| (2,246) | 1:26:A:LYS:HB2  | 1:33:A:LYS:HG2  | 10       | 0.33          |
| (2,197) | 1:17:A:LEU:HA   | 1:20:A:ILE:HD11 | 9        | 0.33          |
| (2,193) | 1:15:A:LYS:HA   | 1:31:A:LYS:HG2  | 6        | 0.33          |
| (2,111) | 1:27:A:CYS:H    | 1:26:A:LYS:HG2  | 10       | 0.33          |
| (2,106) | 1:34:A:CYS:H    | 1:33:A:LYS:HG2  | 2        | 0.33          |
| (2,106) | 1:34:A:CYS:H    | 1:33:A:LYS:HG2  | 3        | 0.33          |
| (2,24)  | 1:10:A:VAL:H    | 1:9:A:SER:HB2   | 3        | 0.33          |
| (3,304) | 1:24:A:PHE:H    | 1:23:A:ILE:HG23 | 6        | 0.32          |
| (3,246) | 1:28:A:MET:H    | 1:28:A:MET:HB3  | 5        | 0.32          |
| (3,246) | 1:28:A:MET:H    | 1:28:A:MET:HB3  | 7        | 0.32          |
| (3,246) | 1:28:A:MET:H    | 1:28:A:MET:HB3  | 9        | 0.32          |
| (3,246) | 1:28:A:MET:H    | 1:28:A:MET:HB3  | 10       | 0.32          |
| (3,158) | 1:16:A:CYS:H    | 1:22:A:SER:HB3  | 5        | 0.32          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (2,274) | 1:23:A:ILE:HA   | 1:13:A:LYS:HG2  | 8        | 0.32          |
| (2,261) | 1:8:A:ALA:HB3   | 1:2:A:MET:HG2   | 7        | 0.32          |
| (2,224) | 1:13:A:LYS:HE3  | 1:23:A:ILE:HG23 | 4        | 0.32          |
| (2,216) | 1:24:A:PHE:HB2  | 1:26:A:LYS:HG2  | 5        | 0.32          |
| (2,191) | 1:7:A:SER:HB3   | 1:8:A:ALA:HB2   | 2        | 0.32          |
| (2,175) | 1:9:A:SER:HB2   | 1:2:A:MET:HG3   | 9        | 0.32          |
| (2,164) | 1:23:A:ILE:HD11 | 1:24:A:PHE:HA   | 9        | 0.32          |
| (2,119) | 1:19:A:ALA:H    | 1:20:A:ILE:HG23 | 1        | 0.32          |
| (2,119) | 1:19:A:ALA:H    | 1:20:A:ILE:HG21 | 6        | 0.32          |
| (2,110) | 1:4:A:MET:H     | 1:31:A:LYS:HG3  | 8        | 0.32          |
| (2,27)  | 1:14:A:GLN:HE21 | 1:17:A:LEU:HA   | 7        | 0.32          |
| (2,24)  | 1:10:A:VAL:H    | 1:9:A:SER:HB2   | 1        | 0.32          |
| (3,433) | 1:7:A:SER:HB2   | 1:8:A:ALA:HB2   | 2        | 0.31          |
| (3,380) | 1:11:A:GLU:HG2  | 1:11:A:GLU:HA   | 5        | 0.31          |
| (2,162) | 1:20:A:ILE:HG22 | 1:16:A:CYS:HA   | 2        | 0.31          |
| (2,110) | 1:4:A:MET:H     | 1:31:A:LYS:HG3  | 6        | 0.31          |
| (2,109) | 1:28:A:MET:H    | 1:31:A:LYS:HG3  | 6        | 0.31          |
| (2,109) | 1:28:A:MET:H    | 1:31:A:LYS:HG3  | 10       | 0.31          |
| (2,107) | 1:16:A:CYS:H    | 1:15:A:LYS:HG3  | 5        | 0.31          |
| (2,98)  | 1:8:A:ALA:H     | 1:31:A:LYS:HD2  | 9        | 0.31          |
| (3,433) | 1:7:A:SER:HB2   | 1:8:A:ALA:HB3   | 5        | 0.3           |
| (3,380) | 1:11:A:GLU:HG2  | 1:11:A:GLU:HA   | 6        | 0.3           |
| (3,328) | 1:24:A:PHE:HZ   | 1:23:A:ILE:HG21 | 9        | 0.3           |
| (3,302) | 1:21:A:GLY:H    | 1:17:A:LEU:HD13 | 5        | 0.3           |
| (3,302) | 1:21:A:GLY:H    | 1:17:A:LEU:HD12 | 6        | 0.3           |
| (3,219) | 1:24:A:PHE:HD2  | 1:23:A:ILE:HB   | 5        | 0.3           |
| (3,31)  | 1:24:A:PHE:HD2  | 1:25:A:GLY:H    | 6        | 0.3           |
| (2,172) | 1:30:A:LYS:HA   | 1:6:A:CYS:HB2   | 4        | 0.3           |
| (2,120) | 1:21:A:GLY:H    | 1:20:A:ILE:HG22 | 8        | 0.3           |
| (2,119) | 1:19:A:ALA:H    | 1:20:A:ILE:HG21 | 3        | 0.3           |
| (2,119) | 1:19:A:ALA:H    | 1:20:A:ILE:HG21 | 4        | 0.3           |
| (2,107) | 1:16:A:CYS:H    | 1:19:A:ALA:HB3  | 1        | 0.3           |
| (2,102) | 1:5:A:ARG:H     | 1:31:A:LYS:HG3  | 3        | 0.3           |
| (2,102) | 1:5:A:ARG:H     | 1:31:A:LYS:HG3  | 5        | 0.3           |
| (2,64)  | 1:32:A:CYS:H    | 1:31:A:LYS:HD3  | 4        | 0.3           |
| (2,57)  | 1:16:A:CYS:H    | 1:14:A:GLN:HB2  | 10       | 0.3           |
| (2,49)  | 1:29:A:ASN:HD21 | 1:28:A:MET:HG2  | 9        | 0.3           |
| (2,44)  | 1:24:A:PHE:HD1  | 1:13:A:LYS:HE3  | 9        | 0.3           |
| (2,1)   | 1:6:A:CYS:H     | 1:32:A:CYS:H    | 5        | 0.3           |
| (3,246) | 1:28:A:MET:H    | 1:28:A:MET:HB3  | 2        | 0.29          |
| (3,246) | 1:28:A:MET:H    | 1:28:A:MET:HB3  | 3        | 0.29          |
| (3,246) | 1:28:A:MET:H    | 1:28:A:MET:HB3  | 8        | 0.29          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (2,239) | 1:5:A:ARG:HB2   | 1:5:A:ARG:HG3   | 8        | 0.29          |
| (2,228) | 1:28:A:MET:HG3  | 1:26:A:LYS:HG3  | 9        | 0.29          |
| (2,164) | 1:23:A:ILE:HD13 | 1:22:A:SER:HA   | 7        | 0.29          |
| (2,64)  | 1:32:A:CYS:H    | 1:31:A:LYS:HD3  | 8        | 0.29          |
| (2,59)  | 1:3:A:ASP:H     | 1:2:A:MET:HB3   | 8        | 0.29          |
| (2,37)  | 1:8:A:ALA:H     | 1:2:A:MET:HG3   | 1        | 0.29          |
| (3,554) | 1:5:A:ARG:H     | 1:5:A:ARG:HB3   | 2        | 0.28          |
| (3,445) | 1:21:A:GLY:HA3  | 1:17:A:LEU:HD21 | 2        | 0.28          |
| (3,328) | 1:24:A:PHE:HZ   | 1:23:A:ILE:HG22 | 1        | 0.28          |
| (3,31)  | 1:24:A:PHE:HD1  | 1:25:A:GLY:H    | 7        | 0.28          |
| (2,224) | 1:13:A:LYS:HE2  | 1:23:A:ILE:HG22 | 3        | 0.28          |
| (2,121) | 1:23:A:ILE:H    | 1:17:A:LEU:HD13 | 2        | 0.28          |
| (2,117) | 1:16:A:CYS:H    | 1:23:A:ILE:HG21 | 3        | 0.28          |
| (2,111) | 1:27:A:CYS:H    | 1:26:A:LYS:HG2  | 1        | 0.28          |
| (2,110) | 1:4:A:MET:H     | 1:31:A:LYS:HG3  | 10       | 0.28          |
| (2,82)  | 1:6:A:CYS:H     | 1:5:A:ARG:HG3   | 9        | 0.28          |
| (2,43)  | 1:24:A:PHE:HE2  | 1:13:A:LYS:HE2  | 2        | 0.28          |
| (2,43)  | 1:24:A:PHE:HE1  | 1:13:A:LYS:HE2  | 10       | 0.28          |
| (2,35)  | 1:26:A:LYS:H    | 1:12:A:CYS:HB3  | 7        | 0.28          |
| (2,35)  | 1:26:A:LYS:H    | 1:12:A:CYS:HB3  | 9        | 0.28          |
| (2,19)  | 1:1:A:GLN:HE21  | 1:9:A:SER:HB3   | 7        | 0.28          |
| (3,473) | 1:34:A:CYS:HB3  | 1:19:A:ALA:HB3  | 6        | 0.27          |
| (3,246) | 1:28:A:MET:H    | 1:28:A:MET:HB3  | 4        | 0.27          |
| (3,183) | 1:4:A:MET:H     | 1:4:A:MET:HG3   | 7        | 0.27          |
| (3,31)  | 1:24:A:PHE:HD1  | 1:25:A:GLY:H    | 10       | 0.27          |
| (2,250) | 1:18:A:LYS:HD3  | 1:18:A:LYS:HG2  | 3        | 0.27          |
| (2,216) | 1:24:A:PHE:HB2  | 1:26:A:LYS:HG2  | 1        | 0.27          |
| (2,175) | 1:9:A:SER:HB2   | 1:2:A:MET:HG3   | 6        | 0.27          |
| (2,109) | 1:28:A:MET:H    | 1:31:A:LYS:HG3  | 9        | 0.27          |
| (2,49)  | 1:29:A:ASN:HD21 | 1:28:A:MET:HG2  | 1        | 0.27          |
| (2,49)  | 1:29:A:ASN:HD21 | 1:28:A:MET:HG2  | 10       | 0.27          |
| (2,35)  | 1:26:A:LYS:H    | 1:12:A:CYS:HB3  | 8        | 0.27          |
| (3,47)  | 1:2:A:MET:H     | 1:8:A:ALA:HA    | 4        | 0.26          |
| (2,240) | 1:15:A:LYS:HB3  | 1:31:A:LYS:HB3  | 2        | 0.26          |
| (2,102) | 1:5:A:ARG:H     | 1:31:A:LYS:HG2  | 1        | 0.26          |
| (2,93)  | 1:24:A:PHE:HE1  | 1:17:A:LEU:HG   | 3        | 0.26          |
| (2,17)  | 1:11:A:GLU:H    | 1:9:A:SER:HB2   | 10       | 0.26          |
| (3,497) | 1:34:A:CYS:HB3  | 1:20:A:ILE:HG12 | 4        | 0.25          |
| (3,333) | 1:14:A:GLN:HE21 | 1:10:A:VAL:HG11 | 1        | 0.25          |
| (3,252) | 1:16:A:CYS:H    | 1:15:A:LYS:HB3  | 8        | 0.25          |
| (3,218) | 1:29:A:ASN:HD22 | 1:28:A:MET:HB2  | 9        | 0.25          |
| (3,202) | 1:14:A:GLN:H    | 1:14:A:GLN:HG3  | 7        | 0.25          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (3,119) | 1:8:A:ALA:H     | 1:7:A:SER:HB3   | 10       | 0.25          |
| (2,250) | 1:18:A:LYS:HD3  | 1:18:A:LYS:HG2  | 5        | 0.25          |
| (2,246) | 1:26:A:LYS:HB2  | 1:33:A:LYS:HG2  | 9        | 0.25          |
| (2,193) | 1:15:A:LYS:HA   | 1:31:A:LYS:HG3  | 1        | 0.25          |
| (2,175) | 1:9:A:SER:HB3   | 1:2:A:MET:HG3   | 3        | 0.25          |
| (2,92)  | 1:24:A:PHE:HD1  | 1:17:A:LEU:HG   | 3        | 0.25          |
| (2,40)  | 1:5:A:ARG:H     | 1:6:A:CYS:HB3   | 9        | 0.25          |
| (2,35)  | 1:26:A:LYS:H    | 1:12:A:CYS:HB3  | 1        | 0.25          |
| (3,296) | 1:8:A:ALA:H     | 1:10:A:VAL:HG23 | 4        | 0.24          |
| (3,218) | 1:29:A:ASN:HD22 | 1:28:A:MET:HB2  | 10       | 0.24          |
| (3,183) | 1:4:A:MET:H     | 1:4:A:MET:HG3   | 9        | 0.24          |
| (3,158) | 1:16:A:CYS:H    | 1:22:A:SER:HB3  | 7        | 0.24          |
| (3,151) | 1:25:A:GLY:H    | 1:16:A:CYS:HB2  | 4        | 0.24          |
| (3,31)  | 1:24:A:PHE:HD2  | 1:25:A:GLY:H    | 1        | 0.24          |
| (3,31)  | 1:24:A:PHE:HD2  | 1:25:A:GLY:H    | 9        | 0.24          |
| (3,13)  | 1:5:A:ARG:H     | 1:4:A:MET:H     | 5        | 0.24          |
| (2,241) | 1:13:A:LYS:HB2  | 1:13:A:LYS:HG2  | 9        | 0.24          |
| (2,235) | 1:2:A:MET:HG2   | 1:2:A:MET:HB3   | 10       | 0.24          |
| (2,216) | 1:24:A:PHE:HB2  | 1:26:A:LYS:HG2  | 8        | 0.24          |
| (2,107) | 1:16:A:CYS:H    | 1:19:A:ALA:HB2  | 3        | 0.24          |
| (2,88)  | 1:24:A:PHE:HD2  | 1:13:A:LYS:HD3  | 2        | 0.24          |
| (2,40)  | 1:5:A:ARG:H     | 1:6:A:CYS:HB3   | 7        | 0.24          |
| (2,17)  | 1:11:A:GLU:H    | 1:9:A:SER:HB2   | 1        | 0.24          |
| (3,478) | 1:34:A:CYS:HB3  | 1:20:A:ILE:HD12 | 8        | 0.23          |
| (3,387) | 1:13:A:LYS:HA   | 1:25:A:GLY:HA3  | 7        | 0.23          |
| (2,261) | 1:8:A:ALA:HB1   | 1:2:A:MET:HG2   | 5        | 0.23          |
| (2,250) | 1:18:A:LYS:HD3  | 1:18:A:LYS:HG2  | 7        | 0.23          |
| (2,250) | 1:13:A:LYS:HD3  | 1:13:A:LYS:HG2  | 8        | 0.23          |
| (2,239) | 1:5:A:ARG:HB2   | 1:5:A:ARG:HG3   | 2        | 0.23          |
| (2,197) | 1:17:A:LEU:HA   | 1:20:A:ILE:HD11 | 5        | 0.23          |
| (2,183) | 1:1:A:GLN:HA    | 1:2:A:MET:HB2   | 4        | 0.23          |
| (2,164) | 1:23:A:ILE:HD12 | 1:22:A:SER:HA   | 10       | 0.23          |
| (2,89)  | 1:24:A:PHE:HE1  | 1:13:A:LYS:HD2  | 8        | 0.23          |
| (2,82)  | 1:6:A:CYS:H     | 1:5:A:ARG:HG2   | 3        | 0.23          |
| (2,66)  | 1:27:A:CYS:H    | 1:26:A:LYS:HD3  | 8        | 0.23          |
| (2,43)  | 1:24:A:PHE:HE1  | 1:13:A:LYS:HE3  | 6        | 0.23          |
| (2,40)  | 1:5:A:ARG:H     | 1:6:A:CYS:HB3   | 6        | 0.23          |
| (2,40)  | 1:5:A:ARG:H     | 1:6:A:CYS:HB3   | 8        | 0.23          |
| (2,37)  | 1:8:A:ALA:H     | 1:2:A:MET:HG3   | 2        | 0.23          |
| (3,276) | 1:18:A:LYS:H    | 1:18:A:LYS:HG2  | 3        | 0.22          |
| (3,31)  | 1:24:A:PHE:HD2  | 1:25:A:GLY:H    | 5        | 0.22          |
| (2,250) | 1:18:A:LYS:HD3  | 1:18:A:LYS:HG2  | 1        | 0.22          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (2,250) | 1:13:A:LYS:HD3  | 1:13:A:LYS:HG2  | 4        | 0.22          |
| (2,250) | 1:13:A:LYS:HD3  | 1:13:A:LYS:HG2  | 10       | 0.22          |
| (2,241) | 1:13:A:LYS:HB2  | 1:13:A:LYS:HG2  | 1        | 0.22          |
| (2,241) | 1:13:A:LYS:HB2  | 1:13:A:LYS:HG2  | 6        | 0.22          |
| (2,239) | 1:5:A:ARG:HB2   | 1:5:A:ARG:HG3   | 4        | 0.22          |
| (2,229) | 1:28:A:MET:HG2  | 1:26:A:LYS:HG3  | 2        | 0.22          |
| (2,193) | 1:15:A:LYS:HA   | 1:31:A:LYS:HG2  | 10       | 0.22          |
| (2,191) | 1:7:A:SER:HB3   | 1:8:A:ALA:HB1   | 9        | 0.22          |
| (2,132) | 1:22:A:SER:HB3  | 1:25:A:GLY:HA2  | 4        | 0.22          |
| (2,86)  | 1:14:A:GLN:HE22 | 1:18:A:LYS:HB2  | 9        | 0.22          |
| (2,41)  | 1:31:A:LYS:H    | 1:6:A:CYS:HB2   | 5        | 0.22          |
| (2,24)  | 1:10:A:VAL:H    | 1:9:A:SER:HB2   | 2        | 0.22          |
| (2,17)  | 1:11:A:GLU:H    | 1:9:A:SER:HB3   | 7        | 0.22          |
| (3,535) | 1:19:A:ALA:H    | 1:34:A:CYS:HB3  | 9        | 0.21          |
| (3,476) | 1:12:A:CYS:HB3  | 1:15:A:LYS:HB3  | 3        | 0.21          |
| (3,387) | 1:13:A:LYS:HA   | 1:25:A:GLY:HA3  | 3        | 0.21          |
| (3,380) | 1:11:A:GLU:HG2  | 1:11:A:GLU:HA   | 8        | 0.21          |
| (3,276) | 1:18:A:LYS:H    | 1:18:A:LYS:HG2  | 4        | 0.21          |
| (2,250) | 1:13:A:LYS:HD3  | 1:13:A:LYS:HG2  | 2        | 0.21          |
| (2,250) | 1:18:A:LYS:HD3  | 1:18:A:LYS:HG2  | 9        | 0.21          |
| (2,235) | 1:2:A:MET:HG3   | 1:2:A:MET:HB2   | 3        | 0.21          |
| (2,218) | 1:16:A:CYS:HB3  | 1:13:A:LYS:HB3  | 5        | 0.21          |
| (2,215) | 1:32:A:CYS:HB3  | 1:26:A:LYS:HG3  | 3        | 0.21          |
| (2,198) | 1:21:A:GLY:HA3  | 1:20:A:ILE:HD11 | 6        | 0.21          |
| (2,132) | 1:22:A:SER:HB3  | 1:25:A:GLY:HA2  | 5        | 0.21          |
| (2,117) | 1:16:A:CYS:H    | 1:23:A:ILE:HG23 | 1        | 0.21          |
| (2,94)  | 1:24:A:PHE:HD2  | 1:26:A:LYS:HG2  | 4        | 0.21          |
| (2,88)  | 1:24:A:PHE:HD2  | 1:13:A:LYS:HD3  | 5        | 0.21          |
| (2,88)  | 1:24:A:PHE:HD1  | 1:13:A:LYS:HD2  | 10       | 0.21          |
| (2,50)  | 1:14:A:GLN:HE21 | 1:18:A:LYS:HB3  | 6        | 0.21          |
| (2,35)  | 1:26:A:LYS:H    | 1:12:A:CYS:HB3  | 10       | 0.21          |
| (3,318) | 1:14:A:GLN:HE22 | 1:17:A:LEU:HD13 | 10       | 0.2           |
| (3,252) | 1:16:A:CYS:H    | 1:15:A:LYS:HB3  | 2        | 0.2           |
| (3,219) | 1:24:A:PHE:HD2  | 1:23:A:ILE:HB   | 10       | 0.2           |
| (3,202) | 1:14:A:GLN:H    | 1:14:A:GLN:HG3  | 6        | 0.2           |
| (3,56)  | 1:3:A:ASP:H     | 1:2:A:MET:HA    | 7        | 0.2           |
| (2,241) | 1:13:A:LYS:HB2  | 1:13:A:LYS:HG2  | 3        | 0.2           |
| (2,239) | 1:5:A:ARG:HB2   | 1:5:A:ARG:HG3   | 1        | 0.2           |
| (2,235) | 1:2:A:MET:HG3   | 1:2:A:MET:HB2   | 7        | 0.2           |
| (2,235) | 1:2:A:MET:HG3   | 1:2:A:MET:HB2   | 9        | 0.2           |
| (2,121) | 1:18:A:LYS:H    | 1:17:A:LEU:HD12 | 10       | 0.2           |
| (2,120) | 1:21:A:GLY:H    | 1:20:A:ILE:HG23 | 7        | 0.2           |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (2,106) | 1:34:A:CYS:H    | 1:33:A:LYS:HG2  | 7        | 0.2           |
| (2,64)  | 1:32:A:CYS:H    | 1:15:A:LYS:HD3  | 3        | 0.2           |
| (2,58)  | 1:3:A:ASP:H     | 1:1:A:GLN:HB3   | 9        | 0.2           |
| (2,57)  | 1:16:A:CYS:H    | 1:14:A:GLN:HB2  | 2        | 0.2           |
| (2,54)  | 1:6:A:CYS:H     | 1:30:A:LYS:HB3  | 10       | 0.2           |
| (2,41)  | 1:31:A:LYS:H    | 1:6:A:CYS:HB2   | 8        | 0.2           |
| (2,40)  | 1:5:A:ARG:H     | 1:6:A:CYS:HB2   | 1        | 0.2           |
| (2,40)  | 1:5:A:ARG:H     | 1:6:A:CYS:HB3   | 3        | 0.2           |
| (2,35)  | 1:26:A:LYS:H    | 1:16:A:CYS:HB3  | 2        | 0.2           |
| (2,17)  | 1:11:A:GLU:H    | 1:9:A:SER:HB2   | 3        | 0.2           |
| (3,387) | 1:13:A:LYS:HA   | 1:25:A:GLY:HA3  | 6        | 0.19          |
| (3,294) | 1:19:A:ALA:H    | 1:17:A:LEU:HD23 | 10       | 0.19          |
| (2,277) | 1:16:A:CYS:HA   | 1:15:A:LYS:HA   | 10       | 0.19          |
| (2,235) | 1:2:A:MET:HG3   | 1:2:A:MET:HB2   | 2        | 0.19          |
| (2,227) | 1:4:A:MET:HG3   | 1:31:A:LYS:HG3  | 10       | 0.19          |
| (2,215) | 1:32:A:CYS:HB3  | 1:26:A:LYS:HG3  | 6        | 0.19          |
| (2,198) | 1:21:A:GLY:HA3  | 1:20:A:ILE:HD13 | 3        | 0.19          |
| (2,175) | 1:9:A:SER:HB2   | 1:2:A:MET:HG3   | 1        | 0.19          |
| (2,117) | 1:16:A:CYS:H    | 1:23:A:ILE:HG23 | 4        | 0.19          |
| (2,72)  | 1:30:A:LYS:H    | 1:30:A:LYS:HD3  | 4        | 0.19          |
| (2,41)  | 1:31:A:LYS:H    | 1:6:A:CYS:HB2   | 4        | 0.19          |
| (2,41)  | 1:31:A:LYS:H    | 1:6:A:CYS:HB2   | 9        | 0.19          |
| (2,32)  | 1:4:A:MET:H     | 1:4:A:MET:HG2   | 3        | 0.19          |
| (2,23)  | 1:8:A:ALA:H     | 1:9:A:SER:HB2   | 10       | 0.19          |
| (2,17)  | 1:11:A:GLU:H    | 1:9:A:SER:HB3   | 6        | 0.19          |
| (2,5)   | 1:1:A:GLN:HE22  | 1:1:A:GLN:HE21  | 1        | 0.19          |
| (2,5)   | 1:1:A:GLN:HE22  | 1:1:A:GLN:HE21  | 2        | 0.19          |
| (2,5)   | 1:29:A:ASN:HD22 | 1:29:A:ASN:HD21 | 3        | 0.19          |
| (2,5)   | 1:29:A:ASN:HD22 | 1:29:A:ASN:HD21 | 4        | 0.19          |
| (2,5)   | 1:29:A:ASN:HD22 | 1:29:A:ASN:HD21 | 5        | 0.19          |
| (2,5)   | 1:1:A:GLN:HE22  | 1:1:A:GLN:HE21  | 6        | 0.19          |
| (2,5)   | 1:29:A:ASN:HD22 | 1:29:A:ASN:HD21 | 7        | 0.19          |
| (2,5)   | 1:1:A:GLN:HE22  | 1:1:A:GLN:HE21  | 8        | 0.19          |
| (2,5)   | 1:29:A:ASN:HD22 | 1:29:A:ASN:HD21 | 9        | 0.19          |
| (2,5)   | 1:29:A:ASN:HD22 | 1:29:A:ASN:HD21 | 10       | 0.19          |
| (3,533) | 1:24:A:PHE:HD1  | 1:13:A:LYS:HA   | 5        | 0.18          |
| (3,533) | 1:24:A:PHE:HD1  | 1:13:A:LYS:HA   | 8        | 0.18          |
| (3,387) | 1:13:A:LYS:HA   | 1:25:A:GLY:HA3  | 1        | 0.18          |
| (3,166) | 1:27:A:CYS:H    | 1:27:A:CYS:HB3  | 2        | 0.18          |
| (3,166) | 1:27:A:CYS:H    | 1:27:A:CYS:HB3  | 4        | 0.18          |
| (3,166) | 1:27:A:CYS:H    | 1:27:A:CYS:HB3  | 5        | 0.18          |
| (3,31)  | 1:24:A:PHE:HD1  | 1:25:A:GLY:H    | 3        | 0.18          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (3,24)  | 1:11:A:GLU:H    | 1:10:A:VAL:H    | 1        | 0.18          |
| (3,24)  | 1:11:A:GLU:H    | 1:10:A:VAL:H    | 7        | 0.18          |
| (2,250) | 1:13:A:LYS:HD3  | 1:13:A:LYS:HG2  | 6        | 0.18          |
| (2,241) | 1:13:A:LYS:HB2  | 1:13:A:LYS:HG2  | 2        | 0.18          |
| (2,241) | 1:13:A:LYS:HB2  | 1:13:A:LYS:HG2  | 7        | 0.18          |
| (2,235) | 1:2:A:MET:HG2   | 1:2:A:MET:HB3   | 4        | 0.18          |
| (2,126) | 1:14:A:GLN:HE21 | 1:17:A:LEU:HD22 | 9        | 0.18          |
| (2,72)  | 1:30:A:LYS:H    | 1:30:A:LYS:HD3  | 8        | 0.18          |
| (2,71)  | 1:30:A:LYS:H    | 1:31:A:LYS:HD2  | 8        | 0.18          |
| (2,66)  | 1:27:A:CYS:H    | 1:26:A:LYS:HD3  | 9        | 0.18          |
| (2,37)  | 1:8:A:ALA:H     | 1:2:A:MET:HG3   | 6        | 0.18          |
| (3,387) | 1:13:A:LYS:HA   | 1:25:A:GLY:HA3  | 8        | 0.17          |
| (3,322) | 1:22:A:SER:H    | 1:20:A:ILE:HD11 | 7        | 0.17          |
| (3,316) | 1:11:A:GLU:H    | 1:10:A:VAL:HG23 | 1        | 0.17          |
| (3,166) | 1:27:A:CYS:H    | 1:27:A:CYS:HB3  | 9        | 0.17          |
| (2,277) | 1:16:A:CYS:HA   | 1:15:A:LYS:HA   | 1        | 0.17          |
| (2,274) | 1:23:A:ILE:HA   | 1:13:A:LYS:HG2  | 10       | 0.17          |
| (2,241) | 1:13:A:LYS:HB2  | 1:13:A:LYS:HG2  | 4        | 0.17          |
| (2,239) | 1:5:A:ARG:HB2   | 1:5:A:ARG:HG3   | 5        | 0.17          |
| (2,239) | 1:5:A:ARG:HB2   | 1:5:A:ARG:HG3   | 10       | 0.17          |
| (2,231) | 1:28:A:MET:HG2  | 1:33:A:LYS:HD3  | 4        | 0.17          |
| (2,228) | 1:28:A:MET:HG3  | 1:26:A:LYS:HG3  | 8        | 0.17          |
| (2,216) | 1:24:A:PHE:HB2  | 1:26:A:LYS:HG2  | 6        | 0.17          |
| (2,200) | 1:14:A:GLN:HA   | 1:23:A:ILE:HG23 | 4        | 0.17          |
| (2,175) | 1:9:A:SER:HB2   | 1:2:A:MET:HG2   | 4        | 0.17          |
| (2,175) | 1:9:A:SER:HB2   | 1:2:A:MET:HG3   | 8        | 0.17          |
| (2,117) | 1:16:A:CYS:H    | 1:23:A:ILE:HG22 | 9        | 0.17          |
| (2,107) | 1:16:A:CYS:H    | 1:19:A:ALA:HB2  | 4        | 0.17          |
| (2,107) | 1:16:A:CYS:H    | 1:19:A:ALA:HB2  | 9        | 0.17          |
| (2,102) | 1:5:A:ARG:H     | 1:31:A:LYS:HG3  | 9        | 0.17          |
| (2,84)  | 1:31:A:LYS:H    | 1:31:A:LYS:HD3  | 1        | 0.17          |
| (2,76)  | 1:5:A:ARG:H     | 1:5:A:ARG:HG3   | 8        | 0.17          |
| (3,530) | 1:22:A:SER:HB3  | 1:19:A:ALA:HB2  | 4        | 0.16          |
| (3,445) | 1:21:A:GLY:HA3  | 1:17:A:LEU:HD23 | 8        | 0.16          |
| (3,387) | 1:13:A:LYS:HA   | 1:25:A:GLY:HA3  | 10       | 0.16          |
| (3,293) | 1:16:A:CYS:H    | 1:17:A:LEU:HD12 | 6        | 0.16          |
| (3,228) | 1:29:A:ASN:HD21 | 1:28:A:MET:HB2  | 2        | 0.16          |
| (3,166) | 1:27:A:CYS:H    | 1:27:A:CYS:HB3  | 8        | 0.16          |
| (3,56)  | 1:3:A:ASP:H     | 1:2:A:MET:HA    | 5        | 0.16          |
| (3,47)  | 1:2:A:MET:H     | 1:8:A:ALA:HA    | 6        | 0.16          |
| (2,277) | 1:16:A:CYS:HA   | 1:17:A:LEU:HA   | 5        | 0.16          |
| (2,277) | 1:16:A:CYS:HA   | 1:17:A:LEU:HA   | 7        | 0.16          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (2,277) | 1:16:A:CYS:HA   | 1:17:A:LEU:HA   | 9        | 0.16          |
| (2,235) | 1:2:A:MET:HG3   | 1:2:A:MET:HB2   | 5        | 0.16          |
| (2,224) | 1:13:A:LYS:HE2  | 1:23:A:ILE:HG21 | 1        | 0.16          |
| (2,189) | 1:30:A:LYS:HA   | 1:31:A:LYS:HD2  | 8        | 0.16          |
| (2,168) | 1:11:A:GLU:HA   | 1:31:A:LYS:HE2  | 10       | 0.16          |
| (2,82)  | 1:6:A:CYS:H     | 1:5:A:ARG:HG3   | 7        | 0.16          |
| (2,63)  | 1:33:A:LYS:H    | 1:33:A:LYS:HD3  | 9        | 0.16          |
| (3,436) | 1:13:A:LYS:HA   | 1:13:A:LYS:HG3  | 1        | 0.15          |
| (3,436) | 1:13:A:LYS:HA   | 1:13:A:LYS:HG3  | 4        | 0.15          |
| (3,320) | 1:24:A:PHE:HE2  | 1:20:A:ILE:HD11 | 9        | 0.15          |
| (3,219) | 1:24:A:PHE:HD1  | 1:23:A:ILE:HB   | 8        | 0.15          |
| (3,205) | 1:31:A:LYS:H    | 1:32:A:CYS:HB3  | 5        | 0.15          |
| (3,78)  | 1:6:A:CYS:H     | 1:5:A:ARG:HA    | 6        | 0.15          |
| (3,31)  | 1:24:A:PHE:HD2  | 1:25:A:GLY:H    | 4        | 0.15          |
| (3,13)  | 1:5:A:ARG:H     | 1:4:A:MET:H     | 7        | 0.15          |
| (2,277) | 1:16:A:CYS:HA   | 1:15:A:LYS:HA   | 6        | 0.15          |
| (2,254) | 1:17:A:LEU:HB2  | 1:17:A:LEU:HD22 | 9        | 0.15          |
| (2,241) | 1:13:A:LYS:HB2  | 1:13:A:LYS:HG2  | 5        | 0.15          |
| (2,239) | 1:5:A:ARG:HB2   | 1:5:A:ARG:HG3   | 6        | 0.15          |
| (2,239) | 1:5:A:ARG:HB2   | 1:5:A:ARG:HG3   | 9        | 0.15          |
| (2,235) | 1:2:A:MET:HG3   | 1:2:A:MET:HB2   | 6        | 0.15          |
| (2,228) | 1:28:A:MET:HG3  | 1:26:A:LYS:HG3  | 2        | 0.15          |
| (2,215) | 1:32:A:CYS:HB3  | 1:26:A:LYS:HG3  | 8        | 0.15          |
| (2,76)  | 1:5:A:ARG:H     | 1:5:A:ARG:HG3   | 10       | 0.15          |
| (2,57)  | 1:16:A:CYS:H    | 1:14:A:GLN:HB2  | 4        | 0.15          |
| (2,38)  | 1:14:A:GLN:H    | 1:14:A:GLN:HG2  | 1        | 0.15          |
| (2,27)  | 1:14:A:GLN:HE21 | 1:17:A:LEU:HA   | 2        | 0.15          |
| (2,1)   | 1:6:A:CYS:H     | 1:32:A:CYS:H    | 10       | 0.15          |
| (3,476) | 1:12:A:CYS:HB3  | 1:15:A:LYS:HB3  | 2        | 0.14          |
| (3,415) | 1:22:A:SER:HB2  | 1:16:A:CYS:HB3  | 3        | 0.14          |
| (3,387) | 1:13:A:LYS:HA   | 1:25:A:GLY:HA3  | 5        | 0.14          |
| (3,293) | 1:16:A:CYS:H    | 1:17:A:LEU:HD13 | 5        | 0.14          |
| (3,276) | 1:18:A:LYS:H    | 1:18:A:LYS:HG2  | 1        | 0.14          |
| (3,49)  | 1:32:A:CYS:H    | 1:12:A:CYS:HA   | 4        | 0.14          |
| (3,38)  | 1:7:A:SER:H     | 1:6:A:CYS:HA    | 2        | 0.14          |
| (3,24)  | 1:11:A:GLU:H    | 1:10:A:VAL:H    | 6        | 0.14          |
| (3,24)  | 1:11:A:GLU:H    | 1:10:A:VAL:H    | 10       | 0.14          |
| (3,13)  | 1:5:A:ARG:H     | 1:4:A:MET:H     | 9        | 0.14          |
| (2,240) | 1:15:A:LYS:HB3  | 1:31:A:LYS:HB2  | 4        | 0.14          |
| (2,239) | 1:5:A:ARG:HB2   | 1:5:A:ARG:HG3   | 3        | 0.14          |
| (2,239) | 1:5:A:ARG:HB2   | 1:5:A:ARG:HG3   | 7        | 0.14          |
| (2,215) | 1:32:A:CYS:HB3  | 1:26:A:LYS:HG3  | 1        | 0.14          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (2,197) | 1:17:A:LEU:HA   | 1:20:A:ILE:HD13 | 4        | 0.14          |
| (2,68)  | 1:28:A:MET:H    | 1:26:A:LYS:HB2  | 9        | 0.14          |
| (2,66)  | 1:27:A:CYS:H    | 1:26:A:LYS:HD3  | 5        | 0.14          |
| (2,44)  | 1:24:A:PHE:HD1  | 1:13:A:LYS:HE2  | 1        | 0.14          |
| (2,40)  | 1:5:A:ARG:H     | 1:6:A:CYS:HB3   | 10       | 0.14          |
| (2,30)  | 1:7:A:SER:H     | 1:6:A:CYS:HB3   | 5        | 0.14          |
| (2,23)  | 1:8:A:ALA:H     | 1:9:A:SER:HB2   | 8        | 0.14          |
| (2,22)  | 1:18:A:LYS:H    | 1:18:A:LYS:HA   | 9        | 0.14          |
| (3,533) | 1:24:A:PHE:HD2  | 1:13:A:LYS:HA   | 10       | 0.13          |
| (3,436) | 1:13:A:LYS:HA   | 1:13:A:LYS:HG3  | 5        | 0.13          |
| (3,415) | 1:22:A:SER:HB2  | 1:16:A:CYS:HB3  | 6        | 0.13          |
| (3,415) | 1:22:A:SER:HB2  | 1:16:A:CYS:HB3  | 9        | 0.13          |
| (3,413) | 1:10:A:VAL:HG22 | 1:11:A:GLU:HA   | 7        | 0.13          |
| (3,387) | 1:13:A:LYS:HA   | 1:25:A:GLY:HA3  | 9        | 0.13          |
| (3,328) | 1:24:A:PHE:HZ   | 1:23:A:ILE:HG22 | 10       | 0.13          |
| (3,327) | 1:24:A:PHE:HE2  | 1:23:A:ILE:HG22 | 4        | 0.13          |
| (3,316) | 1:11:A:GLU:H    | 1:10:A:VAL:HG22 | 10       | 0.13          |
| (3,256) | 1:26:A:LYS:H    | 1:33:A:LYS:HB2  | 2        | 0.13          |
| (3,249) | 1:3:A:ASP:H     | 1:5:A:ARG:HB2   | 9        | 0.13          |
| (3,205) | 1:31:A:LYS:H    | 1:32:A:CYS:HB3  | 3        | 0.13          |
| (3,186) | 1:34:A:CYS:H    | 1:34:A:CYS:HB3  | 8        | 0.13          |
| (3,85)  | 1:24:A:PHE:HE2  | 1:22:A:SER:HA   | 8        | 0.13          |
| (3,47)  | 1:2:A:MET:H     | 1:8:A:ALA:HA    | 2        | 0.13          |
| (3,13)  | 1:5:A:ARG:H     | 1:4:A:MET:H     | 3        | 0.13          |
| (2,277) | 1:16:A:CYS:HA   | 1:15:A:LYS:HA   | 8        | 0.13          |
| (2,254) | 1:17:A:LEU:HB2  | 1:17:A:LEU:HD22 | 1        | 0.13          |
| (2,223) | 1:18:A:LYS:HE3  | 1:17:A:LEU:HD12 | 2        | 0.13          |
| (2,200) | 1:14:A:GLN:HA   | 1:23:A:ILE:HG21 | 7        | 0.13          |
| (2,189) | 1:30:A:LYS:HA   | 1:31:A:LYS:HD2  | 3        | 0.13          |
| (2,120) | 1:21:A:GLY:H    | 1:20:A:ILE:HG21 | 4        | 0.13          |
| (2,72)  | 1:30:A:LYS:H    | 1:31:A:LYS:HB2  | 5        | 0.13          |
| (2,40)  | 1:5:A:ARG:H     | 1:6:A:CYS:HB3   | 5        | 0.13          |
| (2,17)  | 1:11:A:GLU:H    | 1:9:A:SER:HB3   | 5        | 0.13          |
| (3,452) | 1:22:A:SER:HB3  | 1:20:A:ILE:HG12 | 8        | 0.12          |
| (3,445) | 1:21:A:GLY:HA3  | 1:17:A:LEU:HD22 | 4        | 0.12          |
| (3,436) | 1:13:A:LYS:HA   | 1:13:A:LYS:HG3  | 6        | 0.12          |
| (3,436) | 1:13:A:LYS:HA   | 1:13:A:LYS:HG3  | 7        | 0.12          |
| (3,436) | 1:13:A:LYS:HA   | 1:13:A:LYS:HG3  | 9        | 0.12          |
| (3,264) | 1:17:A:LEU:H    | 1:17:A:LEU:HB3  | 1        | 0.12          |
| (3,85)  | 1:24:A:PHE:HE2  | 1:22:A:SER:HA   | 4        | 0.12          |
| (3,56)  | 1:3:A:ASP:H     | 1:2:A:MET:HA    | 3        | 0.12          |
| (3,31)  | 1:24:A:PHE:HD1  | 1:25:A:GLY:H    | 8        | 0.12          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (3,13)  | 1:5:A:ARG:H     | 1:4:A:MET:H     | 6        | 0.12          |
| (2,254) | 1:17:A:LEU:HB2  | 1:17:A:LEU:HD23 | 5        | 0.12          |
| (2,235) | 1:2:A:MET:HG2   | 1:2:A:MET:HB3   | 1        | 0.12          |
| (2,235) | 1:2:A:MET:HG2   | 1:2:A:MET:HB3   | 8        | 0.12          |
| (2,179) | 1:15:A:LYS:HA   | 1:14:A:GLN:HB3  | 10       | 0.12          |
| (2,170) | 1:15:A:LYS:HA   | 1:15:A:LYS:HE2  | 7        | 0.12          |
| (2,162) | 1:20:A:ILE:HG21 | 1:16:A:CYS:HA   | 4        | 0.12          |
| (2,117) | 1:16:A:CYS:H    | 1:23:A:ILE:HG21 | 7        | 0.12          |
| (2,68)  | 1:28:A:MET:H    | 1:26:A:LYS:HB2  | 10       | 0.12          |
| (2,60)  | 1:10:A:VAL:H    | 1:2:A:MET:HB3   | 10       | 0.12          |
| (2,22)  | 1:18:A:LYS:H    | 1:18:A:LYS:HA   | 10       | 0.12          |
| (3,473) | 1:34:A:CYS:HB3  | 1:19:A:ALA:HB3  | 8        | 0.11          |
| (3,465) | 1:34:A:CYS:HB2  | 1:16:A:CYS:HB3  | 8        | 0.11          |
| (3,445) | 1:21:A:GLY:HA3  | 1:17:A:LEU:HD21 | 6        | 0.11          |
| (3,436) | 1:13:A:LYS:HA   | 1:13:A:LYS:HG3  | 2        | 0.11          |
| (3,436) | 1:13:A:LYS:HA   | 1:13:A:LYS:HG3  | 3        | 0.11          |
| (3,357) | 1:5:A:ARG:HD3   | 1:5:A:ARG:HA    | 7        | 0.11          |
| (3,357) | 1:5:A:ARG:HD3   | 1:5:A:ARG:HA    | 9        | 0.11          |
| (3,293) | 1:16:A:CYS:H    | 1:17:A:LEU:HD11 | 7        | 0.11          |
| (3,254) | 1:34:A:CYS:H    | 1:33:A:LYS:HD3  | 2        | 0.11          |
| (3,193) | 1:8:A:ALA:H     | 1:3:A:ASP:HB3   | 1        | 0.11          |
| (3,85)  | 1:24:A:PHE:HE2  | 1:22:A:SER:HA   | 1        | 0.11          |
| (3,78)  | 1:6:A:CYS:H     | 1:5:A:ARG:HA    | 7        | 0.11          |
| (2,254) | 1:17:A:LEU:HB2  | 1:23:A:ILE:HG21 | 3        | 0.11          |
| (2,240) | 1:15:A:LYS:HB3  | 1:31:A:LYS:HB3  | 6        | 0.11          |
| (2,107) | 1:16:A:CYS:H    | 1:19:A:ALA:HB3  | 2        | 0.11          |
| (2,107) | 1:16:A:CYS:H    | 1:19:A:ALA:HB2  | 10       | 0.11          |
| (2,76)  | 1:5:A:ARG:H     | 1:5:A:ARG:HG3   | 2        | 0.11          |
| (2,57)  | 1:16:A:CYS:H    | 1:14:A:GLN:HB2  | 5        | 0.11          |
| (2,23)  | 1:8:A:ALA:H     | 1:9:A:SER:HB2   | 1        | 0.11          |
| (2,22)  | 1:18:A:LYS:H    | 1:18:A:LYS:HA   | 1        | 0.11          |
| (2,22)  | 1:18:A:LYS:H    | 1:18:A:LYS:HA   | 8        | 0.11          |
| (3,368) | 1:4:A:MET:HG3   | 1:4:A:MET:HA    | 8        | 0.1           |
| (3,205) | 1:31:A:LYS:H    | 1:32:A:CYS:HB3  | 8        | 0.1           |
| (3,56)  | 1:3:A:ASP:H     | 1:2:A:MET:HA    | 6        | 0.1           |
| (3,47)  | 1:2:A:MET:H     | 1:8:A:ALA:HA    | 3        | 0.1           |
| (2,88)  | 1:24:A:PHE:HD1  | 1:13:A:LYS:HD2  | 6        | 0.1           |
| (2,68)  | 1:28:A:MET:H    | 1:26:A:LYS:HB2  | 8        | 0.1           |
| (2,66)  | 1:27:A:CYS:H    | 1:26:A:LYS:HD2  | 4        | 0.1           |
| (2,44)  | 1:24:A:PHE:HD2  | 1:13:A:LYS:HE2  | 3        | 0.1           |

## 10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found