



# Full wwPDB NMR Structure Validation Report ⓘ

Mar 6, 2026 – 04:31 AM UTC

PDB ID : 8CJR / pdb\_00008cjr  
BMRB ID : 34793  
Title : JzTx-34 toxin peptide W25A mutant  
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Deposited on : 2023-02-13

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

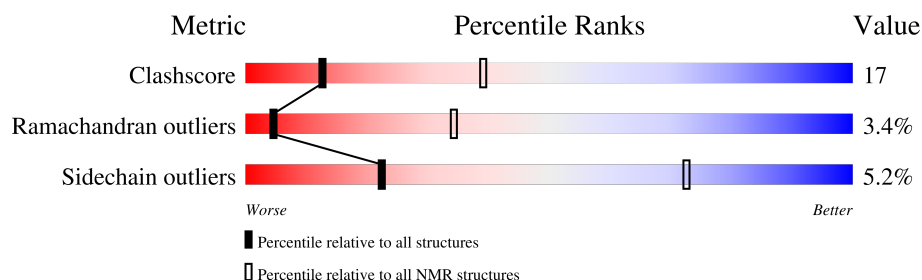
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 57%.

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   | C     | 35     |                  |

## 2 Ensemble composition and analysis

This entry contains 10 models. Model 4 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                                    | C:2-C:33 (32)         | 0.35              | 4            |

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 2 clusters and 2 single-model clusters were found.

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

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 535 atoms, of which 255 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Mu-theraphotoxin-Cg1a.

| Mol | Chain | Residues | Atoms |     |     |    |    |   | Trace |
|-----|-------|----------|-------|-----|-----|----|----|---|-------|
| 1   | C     | 35       | Total | C   | H   | N  | O  | S | 0     |
|     |       |          | 535   | 174 | 255 | 51 | 49 | 6 |       |

There is a discrepancy between the modelled and reference sequences:

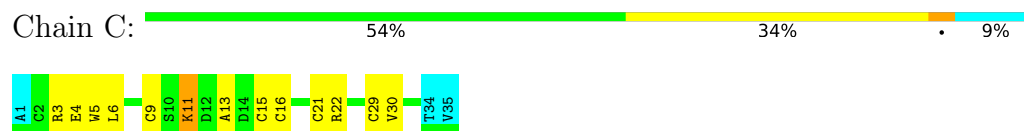
| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| C     | 25      | ALA      | TRP    | engineered mutation | UNP B1P1F7 |

## 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: Mu-theraphotoxin-Cg1a

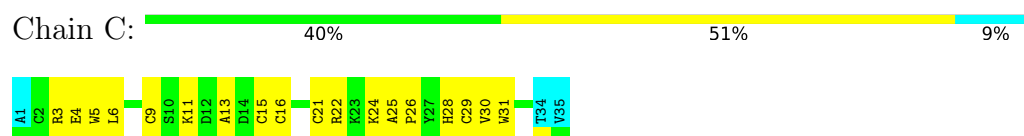


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

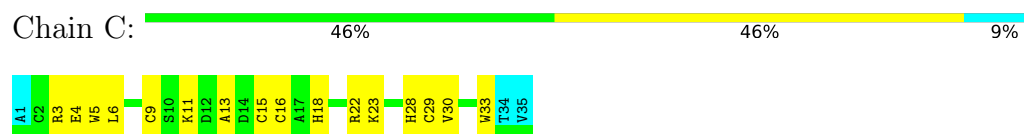
#### 4.2.1 Score per residue for model 1

- Molecule 1: Mu-theraphotoxin-Cg1a



#### 4.2.2 Score per residue for model 2

- Molecule 1: Mu-theraphotoxin-Cg1a



### 4.2.3 Score per residue for model 3

- Molecule 1: Mu-theraphotoxin-Cg1a



### 4.2.4 Score per residue for model 4 (medoid)

- Molecule 1: Mu-theraphotoxin-Cg1a



### 4.2.5 Score per residue for model 5

- Molecule 1: Mu-theraphotoxin-Cg1a



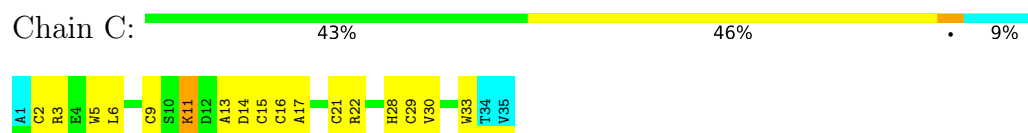
### 4.2.6 Score per residue for model 6

- Molecule 1: Mu-theraphotoxin-Cg1a



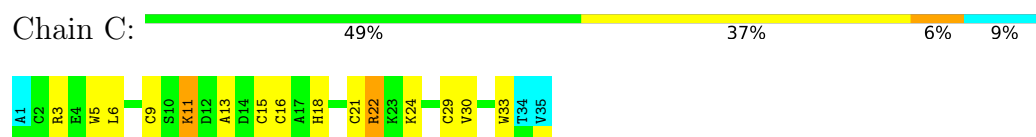
### 4.2.7 Score per residue for model 7

- Molecule 1: Mu-theraphotoxin-Cg1a



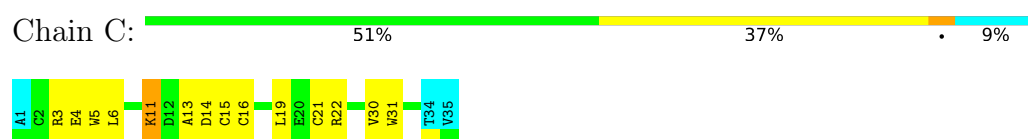
#### 4.2.8 Score per residue for model 8

- Molecule 1: Mu-theraphotoxin-Cg1a



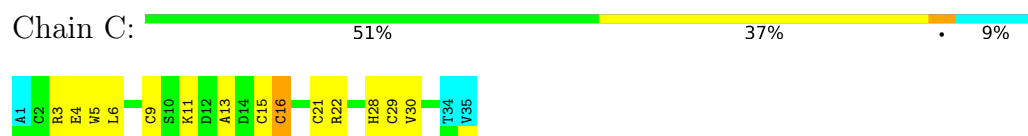
#### 4.2.9 Score per residue for model 9

- Molecule 1: Mu-theraphotoxin-Cg1a



#### 4.2.10 Score per residue for model 10

- Molecule 1: Mu-theraphotoxin-Cg1a



## 5 Refinement protocol and experimental data overview

The models were refined using the following method: *molecular dynamics*.

Of the 250 calculated structures, 10 were deposited, based on the following criterion: *structures with the lowest energy*.

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

| Software name | Classification        | Version |
|---------------|-----------------------|---------|
| ARIA          | refinement            | 2.3     |
| ARIA          | structure calculation | 2.3     |

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                       | 260            |
| Number of shifts mapped to atoms             | 260            |
| Number of unparsed shifts                    | 0              |
| Number of shifts with mapping errors         | 0              |
| Number of shifts with mapping warnings       | 0              |
| Assignment completeness (well-defined parts) | 57%            |



## 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   | C     | 260   | 232      | 230      | 8±2     |
| All | All   | 2600  | 2320     | 2300     | 82      |

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 17.

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

| Atom-1         | Atom-2         | Clash(Å) | Distance(Å) | Models |       |
|----------------|----------------|----------|-------------|--------|-------|
|                |                |          |             | Worst  | Total |
| 1:C:11:LYS:HD3 | 1:C:13:ALA:HB3 | 0.62     | 1.72        | 3      | 9     |
| 1:C:3:ARG:O    | 1:C:16:CYS:HB2 | 0.57     | 2.00        | 5      | 9     |
| 1:C:5:TRP:CE2  | 1:C:6:LEU:HD13 | 0.52     | 2.39        | 2      | 8     |
| 1:C:9:CYS:HB3  | 1:C:29:CYS:SG  | 0.50     | 2.46        | 5      | 6     |
| 1:C:14:ASP:OD2 | 1:C:17:ALA:HA  | 0.49     | 2.07        | 7      | 1     |
| 1:C:22:ARG:HB2 | 1:C:28:HIS:O   | 0.49     | 2.08        | 2      | 5     |
| 1:C:5:TRP:CD1  | 1:C:30:VAL:HA  | 0.48     | 2.43        | 5      | 10    |
| 1:C:22:ARG:C   | 1:C:24:LYS:H   | 0.47     | 2.17        | 8      | 1     |
| 1:C:4:GLU:HG2  | 1:C:5:TRP:H    | 0.47     | 1.69        | 3      | 5     |
| 1:C:11:LYS:O   | 1:C:21:CYS:HB2 | 0.47     | 2.10        | 9      | 6     |
| 1:C:14:ASP:HB3 | 1:C:19:LEU:C   | 0.46     | 2.34        | 9      | 1     |
| 1:C:23:LYS:HD3 | 1:C:23:LYS:N   | 0.46     | 2.26        | 3      | 1     |
| 1:C:11:LYS:CD  | 1:C:13:ALA:HB3 | 0.45     | 2.42        | 9      | 6     |
| 1:C:25:ALA:HA  | 1:C:26:PRO:C   | 0.44     | 2.36        | 1      | 1     |

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| Atom-1         | Atom-2         | Clash(Å) | Distance(Å) | Models |       |
|----------------|----------------|----------|-------------|--------|-------|
|                |                |          |             | Worst  | Total |
| 1:C:4:GLU:HG3  | 1:C:5:TRP:H    | 0.43     | 1.72        | 1      | 2     |
| 1:C:14:ASP:O   | 1:C:16:CYS:N   | 0.42     | 2.52        | 6      | 2     |
| 1:C:4:GLU:HG2  | 1:C:5:TRP:N    | 0.42     | 2.30        | 3      | 2     |
| 1:C:18:HIS:HB3 | 1:C:33:TRP:CZ3 | 0.41     | 2.50        | 8      | 1     |
| 1:C:18:HIS:HB3 | 1:C:33:TRP:CH2 | 0.41     | 2.51        | 2      | 3     |
| 1:C:14:ASP:O   | 1:C:15:CYS:SG  | 0.41     | 2.79        | 6      | 1     |
| 1:C:5:TRP:NE1  | 1:C:30:VAL:HA  | 0.41     | 2.31        | 4      | 1     |
| 1:C:11:LYS:HD2 | 1:C:11:LYS:H   | 0.40     | 1.76        | 5      | 1     |

## 6.3 Torsion angles [i](#)

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

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

| Mol | Chain | Analysed      | Favoured     | Allowed     | Outliers   | Percentiles |    |
|-----|-------|---------------|--------------|-------------|------------|-------------|----|
| 1   | C     | 32/35 (91%)   | 24±1 (75±4%) | 7±1 (22±5%) | 1±0 (3±1%) | 4           | 34 |
| All | All   | 320/350 (91%) | 239 (75%)    | 70 (22%)    | 11 (3%)    | 4           | 34 |

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

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | C     | 15  | CYS  | 10             |
| 1   | C     | 22  | ARG  | 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   | C     | 27/29 (93%)   | 26±1 (95±4%) | 1±1 (5±4%) | 22          | 72 |
| All | All   | 270/290 (93%) | 256 (95%)    | 14 (5%)    | 22          | 72 |

All 6 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   | C     | 11  | LYS  | 5              |
| 1   | C     | 23  | LYS  | 3              |
| 1   | C     | 16  | CYS  | 2              |
| 1   | C     | 22  | ARG  | 2              |
| 1   | C     | 24  | LYS  | 1              |
| 1   | C     | 2   | CYS  | 1              |

### 6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 6.7 Other polymers [i](#)

There are no such molecules in this entry.

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

There are no chain breaks in this entry.

## 7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 57% for the well-defined parts and 57% 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

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                  | 260 |
| Number of shifts mapped to atoms        | 260 |
| 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

The following table shows the suggested chemical shift referencing corrections.

| Nucleus                | # values | Correction $\pm$ precision, ppm | Suggested action         |
|------------------------|----------|---------------------------------|--------------------------|
| $^{13}\text{C}_\alpha$ | 0        | —                               | None (insufficient data) |
| $^{13}\text{C}_\beta$  | 0        | —                               | None (insufficient data) |
| $^{13}\text{C}'$       | 0        | —                               | None (insufficient data) |
| $^{15}\text{N}$        | 32       | $1.13 \pm 0.46$                 | Should be applied        |

#### 7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 57%, i.e. 239 atoms were assigned a chemical shift out of a possible 418. 0 out of 3 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total         | $^1\text{H}$  | $^{13}\text{C}$ | $^{15}\text{N}$ |
|-----------|---------------|---------------|-----------------|-----------------|
| Backbone  | 95/160 (59%)  | 65/65 (100%)  | 0/64 (0%)       | 30/31 (97%)     |
| Sidechain | 118/197 (60%) | 118/126 (94%) | 0/62 (0%)       | 0/9 (0%)        |

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|          | Total         | <sup>1</sup> H | <sup>13</sup> C | <sup>15</sup> N |
|----------|---------------|----------------|-----------------|-----------------|
| Aromatic | 26/61 (43%)   | 26/30 (87%)    | 0/24 (0%)       | 0/7 (0%)        |
| Overall  | 239/418 (57%) | 209/221 (95%)  | 0/150 (0%)      | 30/47 (64%)     |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 57%, i.e. 260 atoms were assigned a chemical shift out of a possible 453. 0 out of 4 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total         | <sup>1</sup> H | <sup>13</sup> C | <sup>15</sup> N |
|-----------|---------------|----------------|-----------------|-----------------|
| Backbone  | 102/175 (58%) | 70/71 (99%)    | 0/70 (0%)       | 32/34 (94%)     |
| Sidechain | 132/217 (61%) | 132/140 (94%)  | 0/68 (0%)       | 0/9 (0%)        |
| Aromatic  | 26/61 (43%)   | 26/30 (87%)    | 0/24 (0%)       | 0/7 (0%)        |
| Overall   | 260/453 (57%) | 228/241 (95%)  | 0/162 (0%)      | 32/50 (64%)     |

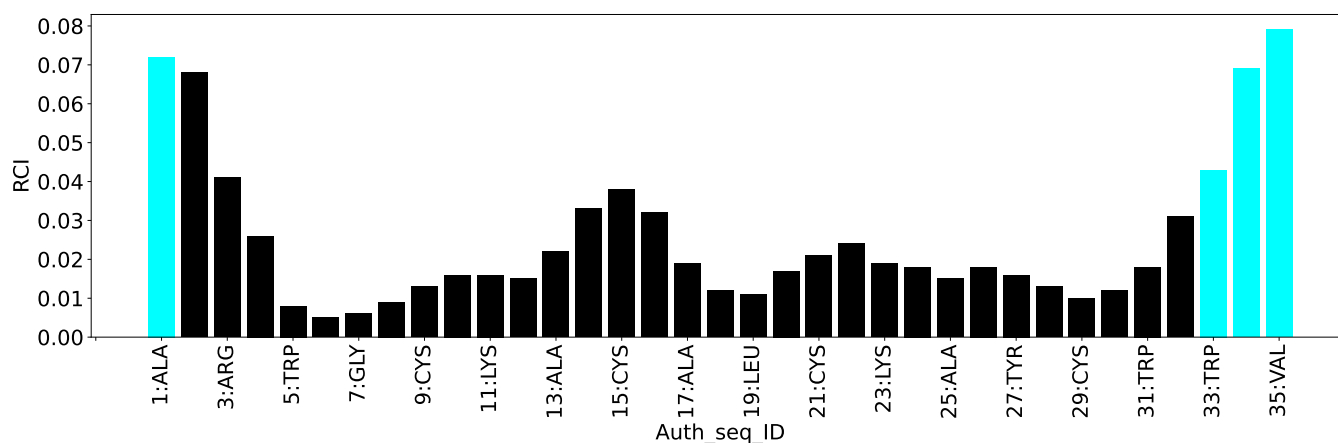
#### 7.1.4 Statistically unusual chemical shifts [i](#)

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 C:



## 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                                | 815   |
| Intra-residue ( $ i-j =0$ )                              | 362   |
| Sequential ( $ i-j =1$ )                                 | 145   |
| Medium range ( $ i-j >1$ and $ i-j <5$ )                 | 92    |
| Long range ( $ i-j \geq 5$ )                             | 216   |
| Inter-chain                                              | 0     |
| Hydrogen bond restraints                                 | 0     |
| Disulfide bond restraints                                | 0     |
| Total dihedral-angle restraints                          | 0     |
| Number of unmapped restraints                            | 0     |
| Number of restraints per residue                         | 23.3  |
| Number of long range restraints per residue <sup>1</sup> | 6.2   |

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

### 8.2 Residual restraint violations

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

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

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

| Bins (Å)         | Average number of violations per model | Max (Å) |
|------------------|----------------------------------------|---------|
| 0.1-0.2 (Small)  | 24.6                                   | 0.2     |
| 0.2-0.5 (Medium) | 50.0                                   | 0.5     |
| >0.5 (Large)     | 53.2                                   | 4.02    |

### 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 ⓘ

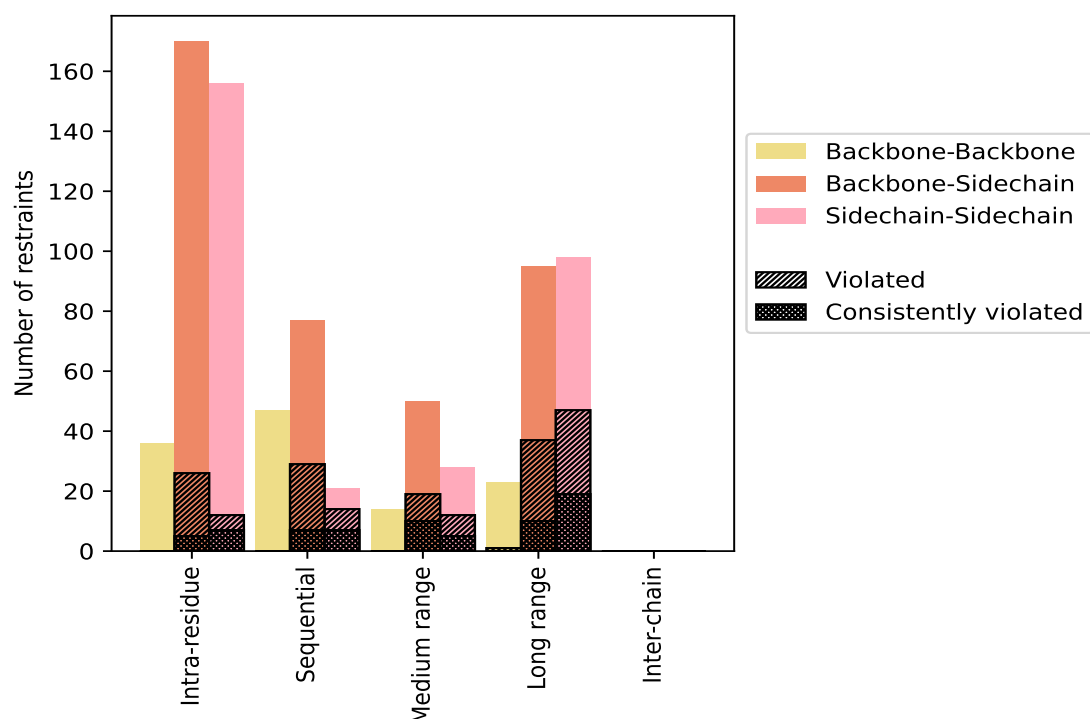
The following table shows the summary of distance violations in different restraint categories based on the sequence separation of the atoms involved. Each category is further sub-divided into three sub-categories based on the atoms involved. Violations less than 0.1 Å are not included in the statistics.

| 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="#">362</a> | <a href="#">44.4</a>  | <a href="#">38</a>    | <a href="#">10.5</a> | <a href="#">4.7</a>  | <a href="#">12</a>                 | <a href="#">3.3</a>  | <a href="#">1.5</a> |
| Backbone-Backbone                                          | 36                  | 4.4                   | 0                     | 0.0                  | 0.0                  | 0                                  | 0.0                  | 0.0                 |
| Backbone-Sidechain                                         | 170                 | 20.9                  | 26                    | 15.3                 | 3.2                  | 5                                  | 2.9                  | 0.6                 |
| Sidechain-Sidechain                                        | 156                 | 19.1                  | 12                    | 7.7                  | 1.5                  | 7                                  | 4.5                  | 0.9                 |
| <a href="#">Sequential ( i-j =1)</a>                       | <a href="#">145</a> | <a href="#">17.8</a>  | <a href="#">43</a>    | <a href="#">29.7</a> | <a href="#">5.3</a>  | <a href="#">14</a>                 | <a href="#">9.7</a>  | <a href="#">1.7</a> |
| Backbone-Backbone                                          | 47                  | 5.8                   | 0                     | 0.0                  | 0.0                  | 0                                  | 0.0                  | 0.0                 |
| Backbone-Sidechain                                         | 77                  | 9.4                   | 29                    | 37.7                 | 3.6                  | 7                                  | 9.1                  | 0.9                 |
| Sidechain-Sidechain                                        | 21                  | 2.6                   | 14                    | 66.7                 | 1.7                  | 7                                  | 33.3                 | 0.9                 |
| <a href="#">Medium range ( i-j &gt;1 &amp;  i-j &lt;5)</a> | <a href="#">92</a>  | <a href="#">11.3</a>  | <a href="#">31</a>    | <a href="#">33.7</a> | <a href="#">3.8</a>  | <a href="#">15</a>                 | <a href="#">16.3</a> | <a href="#">1.8</a> |
| Backbone-Backbone                                          | 14                  | 1.7                   | 0                     | 0.0                  | 0.0                  | 0                                  | 0.0                  | 0.0                 |
| Backbone-Sidechain                                         | 50                  | 6.1                   | 19                    | 38.0                 | 2.3                  | 10                                 | 20.0                 | 1.2                 |
| Sidechain-Sidechain                                        | 28                  | 3.4                   | 12                    | 42.9                 | 1.5                  | 5                                  | 17.9                 | 0.6                 |
| <a href="#">Long range ( i-j ≥5)</a>                       | <a href="#">216</a> | <a href="#">26.5</a>  | <a href="#">85</a>    | <a href="#">39.4</a> | <a href="#">10.4</a> | <a href="#">29</a>                 | <a href="#">13.4</a> | <a href="#">3.6</a> |
| Backbone-Backbone                                          | 23                  | 2.8                   | 1                     | 4.3                  | 0.1                  | 0                                  | 0.0                  | 0.0                 |
| Backbone-Sidechain                                         | 95                  | 11.7                  | 37                    | 38.9                 | 4.5                  | 10                                 | 10.5                 | 1.2                 |
| Sidechain-Sidechain                                        | 98                  | 12.0                  | 47                    | 48.0                 | 5.8                  | 19                                 | 19.4                 | 2.3                 |
| <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="#">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="#">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="#">815</a> | <a href="#">100.0</a> | <a href="#">197</a>   | <a href="#">24.2</a> | <a href="#">24.2</a> | <a href="#">70</a>                 | <a href="#">8.6</a>  | <a href="#">8.6</a> |
| Backbone-Backbone                                          | 120                 | 14.7                  | 1                     | 0.8                  | 0.1                  | 0                                  | 0.0                  | 0.0                 |
| Backbone-Sidechain                                         | 392                 | 48.1                  | 111                   | 28.3                 | 13.6                 | 32                                 | 8.2                  | 3.9                 |
| Sidechain-Sidechain                                        | 303                 | 37.2                  | 85                    | 28.1                 | 10.4                 | 38                                 | 12.5                 | 4.7                 |

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

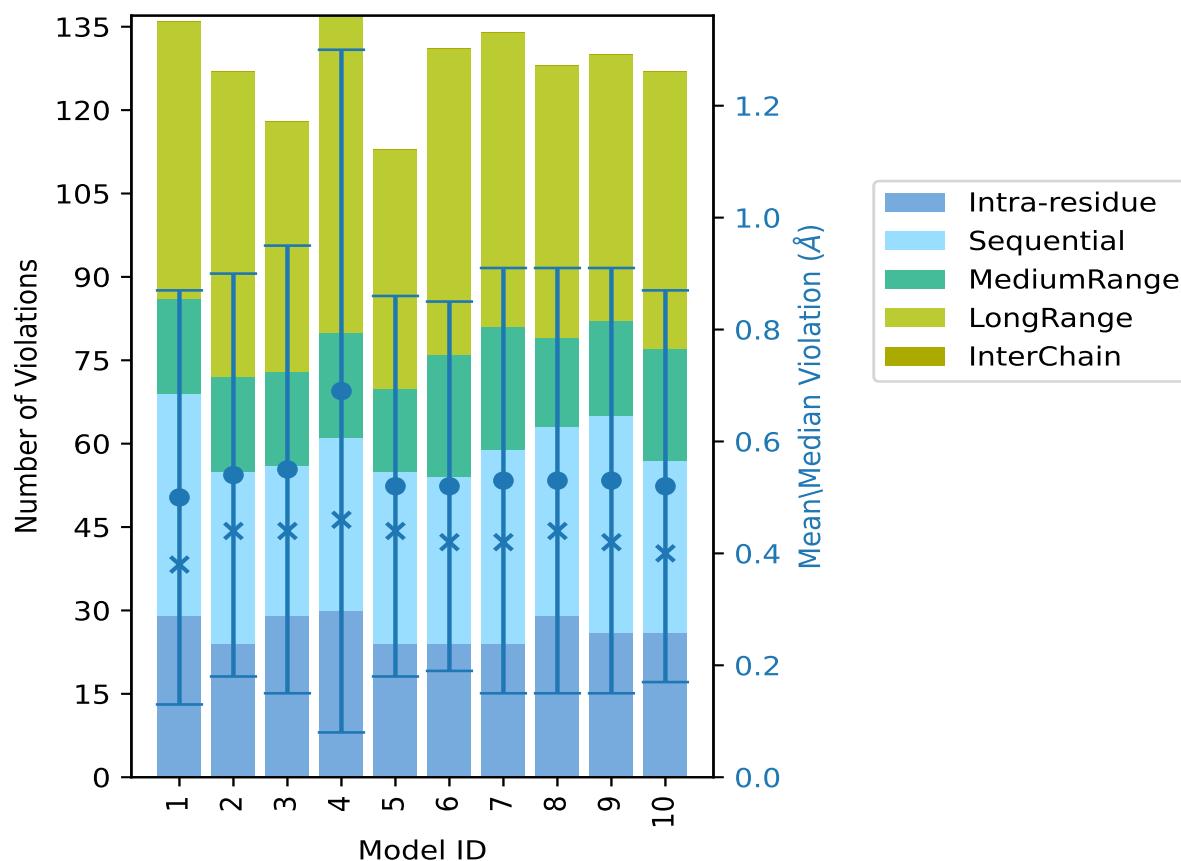
## 9.2 Distance violation statistics for each model [i](#)

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

| Model ID | Number of violations |                 |                 |                 |                 |       | Mean (Å) | Max (Å) | SD <sup>6</sup> (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
|          | IR <sup>1</sup>      | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total |          |         |                     |            |
| 1        | 29                   | 40              | 17              | 50              | 0               | 136   | 0.5      | 1.9     | 0.37                | 0.38       |
| 2        | 24                   | 31              | 17              | 55              | 0               | 127   | 0.54     | 1.89    | 0.36                | 0.44       |
| 3        | 29                   | 27              | 17              | 45              | 0               | 118   | 0.55     | 2.26    | 0.4                 | 0.44       |
| 4        | 30                   | 31              | 19              | 57              | 0               | 137   | 0.69     | 4.02    | 0.61                | 0.46       |
| 5        | 24                   | 31              | 15              | 43              | 0               | 113   | 0.52     | 2.03    | 0.34                | 0.44       |
| 6        | 24                   | 30              | 22              | 55              | 0               | 131   | 0.52     | 1.54    | 0.33                | 0.42       |
| 7        | 24                   | 35              | 22              | 53              | 0               | 134   | 0.53     | 2.4     | 0.38                | 0.42       |
| 8        | 29                   | 34              | 16              | 49              | 0               | 128   | 0.53     | 1.96    | 0.38                | 0.44       |
| 9        | 26                   | 39              | 17              | 48              | 0               | 130   | 0.53     | 1.63    | 0.38                | 0.42       |
| 10       | 26                   | 31              | 20              | 50              | 0               | 127   | 0.52     | 1.91    | 0.35                | 0.4        |

<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, 618(IR:324, SQ:102, MR:61, LR:131, IC:0) restraints are not violated in the ensemble.

| Number of violated restraints |                 |                 |                 |                 |       | Fraction of the ensemble |      |
|-------------------------------|-----------------|-----------------|-----------------|-----------------|-------|--------------------------|------|
| IR <sup>1</sup>               | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total | Count <sup>6</sup>       | %    |
| 9                             | 3               | 5               | 19              | 0               | 36    | 1                        | 10.0 |
| 2                             | 2               | 2               | 5               | 0               | 11    | 2                        | 20.0 |
| 3                             | 3               | 0               | 2               | 0               | 8     | 3                        | 30.0 |

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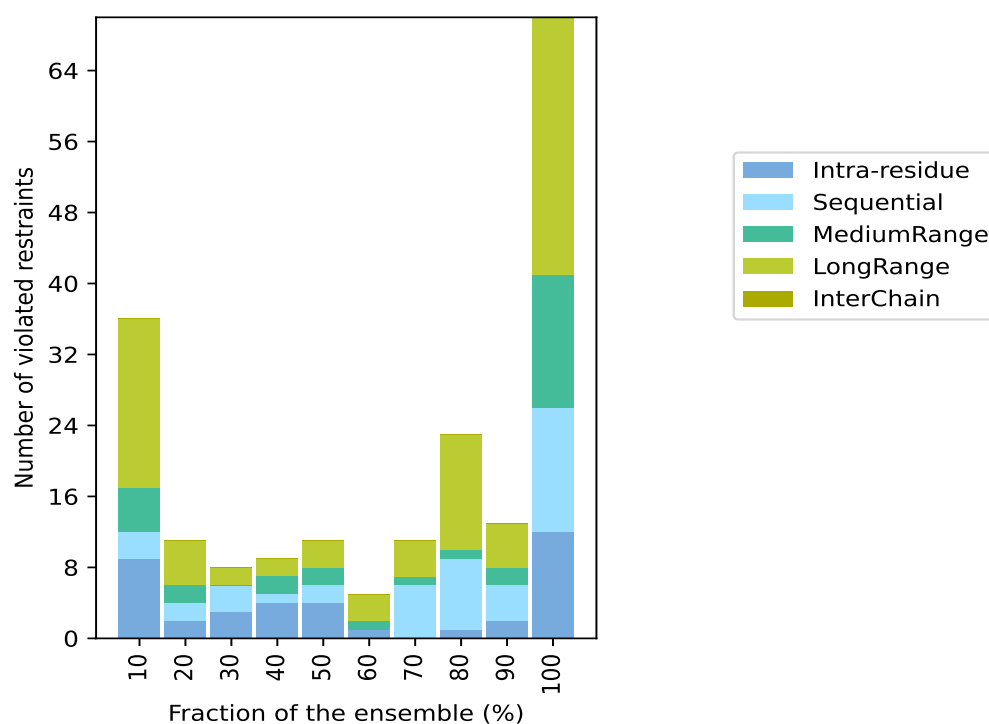
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| Number of violated restraints |                 |                 |                 |                 |       | Fraction of the ensemble |       |
|-------------------------------|-----------------|-----------------|-----------------|-----------------|-------|--------------------------|-------|
| 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>       | %     |
| 4                             | 1               | 2               | 2               | 0               | 9     | 4                        | 40.0  |
| 4                             | 2               | 2               | 3               | 0               | 11    | 5                        | 50.0  |
| 1                             | 0               | 1               | 3               | 0               | 5     | 6                        | 60.0  |
| 0                             | 6               | 1               | 4               | 0               | 11    | 7                        | 70.0  |
| 1                             | 8               | 1               | 13              | 0               | 23    | 8                        | 80.0  |
| 2                             | 4               | 2               | 5               | 0               | 13    | 9                        | 90.0  |
| 12                            | 14              | 15              | 29              | 0               | 70    | 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](#)

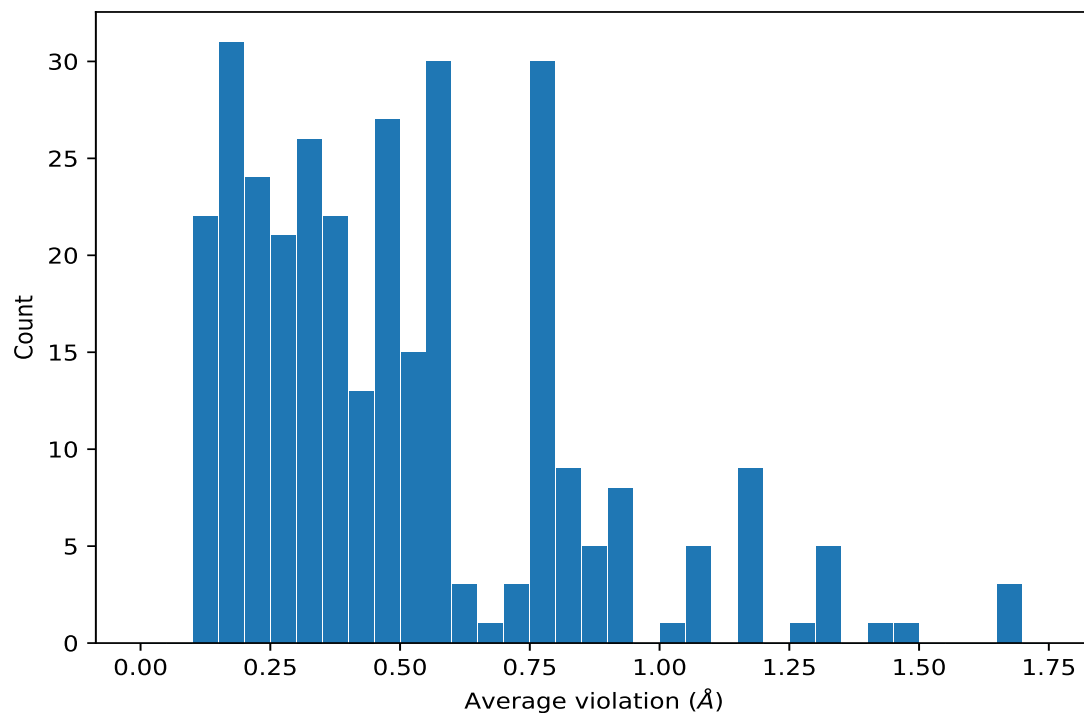


## 9.4 Most violated distance restraints in the ensemble [i](#)

### 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) |
|---------|-----------------|----------------|---------------------|----------|---------------------|------------|
| (1,506) | 1:19:C:LEU:HD23 | 1:14:C:ASP:HB3 | 10                  | 1.7      | 0.47                | 1.92       |
| (1,506) | 1:19:C:LEU:HD21 | 1:14:C:ASP:HB3 | 10                  | 1.7      | 0.47                | 1.92       |
| (1,506) | 1:19:C:LEU:HD22 | 1:14:C:ASP:HB3 | 10                  | 1.7      | 0.47                | 1.92       |
| (1,454) | 1:3:C:ARG:HG3   | 1:1:C:ALA:HA   | 10                  | 1.34     | 0.24                | 1.48       |
| (1,503) | 1:17:C:ALA:HB1  | 1:16:C:CYS:HB2 | 10                  | 1.3      | 0.21                | 1.39       |
| (1,503) | 1:17:C:ALA:HB2  | 1:16:C:CYS:HB2 | 10                  | 1.3      | 0.21                | 1.39       |
| (1,503) | 1:17:C:ALA:HB3  | 1:16:C:CYS:HB2 | 10                  | 1.3      | 0.21                | 1.39       |
| (1,382) | 1:11:C:LYS:HD3  | 1:14:C:ASP:HA  | 10                  | 1.25     | 0.37                | 1.37       |
| (1,301) | 1:3:C:ARG:H     | 1:15:C:CYS:HB3 | 10                  | 1.18     | 0.17                | 1.19       |
| (1,155) | 1:31:C:TRP:HH2  | 1:18:C:HIS:HB3 | 10                  | 1.18     | 0.1                 | 1.16       |
| (3,91)  | 1:30:C:VAL:HG21 | 1:31:C:TRP:HB3 | 10                  | 1.18     | 0.1                 | 1.16       |
| (3,91)  | 1:30:C:VAL:HG22 | 1:31:C:TRP:HB3 | 10                  | 1.18     | 0.1                 | 1.16       |
| (3,91)  | 1:30:C:VAL:HG23 | 1:31:C:TRP:HB3 | 10                  | 1.18     | 0.1                 | 1.16       |
| (4,93)  | 1:30:C:VAL:HG21 | 1:31:C:TRP:HB3 | 10                  | 1.17     | 0.1                 | 1.15       |
| (4,93)  | 1:30:C:VAL:HG22 | 1:31:C:TRP:HB3 | 10                  | 1.17     | 0.1                 | 1.15       |

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| Key     | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (4,93)  | 1:30:C:VAL:HG23 | 1:31:C:TRP:HB3  | 10                  | 1.17     | 0.1                 | 1.15       |
| (1,524) | 1:19:C:LEU:HD22 | 1:5:C:TRP:HB3   | 10                  | 1.09     | 0.07                | 1.1        |
| (1,524) | 1:19:C:LEU:HD23 | 1:5:C:TRP:HB3   | 10                  | 1.09     | 0.07                | 1.1        |
| (1,524) | 1:19:C:LEU:HD21 | 1:5:C:TRP:HB3   | 10                  | 1.09     | 0.07                | 1.1        |
| (1,200) | 1:15:C:CYS:H    | 1:15:C:CYS:HB2  | 10                  | 1.07     | 0.01                | 1.07       |
| (3,49)  | 1:31:C:TRP:HD1  | 1:19:C:LEU:HD23 | 10                  | 0.92     | 0.08                | 0.96       |
| (3,49)  | 1:31:C:TRP:HD1  | 1:19:C:LEU:HD21 | 10                  | 0.92     | 0.08                | 0.96       |
| (3,49)  | 1:31:C:TRP:HD1  | 1:19:C:LEU:HD22 | 10                  | 0.92     | 0.08                | 0.96       |
| (4,51)  | 1:31:C:TRP:HD1  | 1:19:C:LEU:HD23 | 10                  | 0.92     | 0.08                | 0.94       |
| (4,51)  | 1:31:C:TRP:HD1  | 1:19:C:LEU:HD21 | 10                  | 0.92     | 0.08                | 0.94       |
| (4,51)  | 1:31:C:TRP:HD1  | 1:19:C:LEU:HD22 | 10                  | 0.92     | 0.08                | 0.94       |
| (1,521) | 1:6:C:LEU:HD11  | 1:29:C:CYS:HB3  | 10                  | 0.9      | 1.04                | 0.55       |
| (1,521) | 1:6:C:LEU:HD13  | 1:29:C:CYS:HB3  | 10                  | 0.9      | 1.04                | 0.55       |
| (1,296) | 1:28:C:HIS:HE1  | 1:30:C:VAL:HG13 | 10                  | 0.87     | 0.12                | 0.9        |
| (1,296) | 1:28:C:HIS:HE1  | 1:30:C:VAL:HG12 | 10                  | 0.87     | 0.12                | 0.9        |
| (1,296) | 1:28:C:HIS:HE1  | 1:30:C:VAL:HG11 | 10                  | 0.87     | 0.12                | 0.9        |
| (1,224) | 1:31:C:TRP:HD1  | 1:31:C:TRP:HB3  | 10                  | 0.87     | 0.02                | 0.86       |
| (1,329) | 1:12:C:ASP:H    | 1:11:C:LYS:HB3  | 10                  | 0.86     | 0.06                | 0.84       |
| (3,51)  | 1:21:C:CYS:HB3  | 1:14:C:ASP:HA   | 10                  | 0.84     | 0.18                | 0.86       |
| (3,51)  | 1:21:C:CYS:HB3  | 1:29:C:CYS:HA   | 10                  | 0.84     | 0.18                | 0.86       |
| (4,53)  | 1:21:C:CYS:HB3  | 1:14:C:ASP:HA   | 10                  | 0.84     | 0.19                | 0.86       |
| (4,53)  | 1:21:C:CYS:HB3  | 1:29:C:CYS:HA   | 10                  | 0.84     | 0.19                | 0.86       |
| (1,311) | 1:10:C:SER:H    | 1:15:C:CYS:HB2  | 10                  | 0.84     | 0.32                | 0.84       |
| (1,197) | 1:5:C:TRP:HE3   | 1:5:C:TRP:HB2   | 10                  | 0.82     | 0.01                | 0.82       |
| (1,323) | 1:21:C:CYS:H    | 1:20:C:GLU:HB3  | 10                  | 0.8      | 0.06                | 0.8        |
| (1,593) | 1:19:C:LEU:HD23 | 1:30:C:VAL:HG21 | 10                  | 0.78     | 0.08                | 0.79       |
| (1,593) | 1:19:C:LEU:HD21 | 1:30:C:VAL:HG21 | 10                  | 0.78     | 0.08                | 0.79       |
| (1,593) | 1:19:C:LEU:HD23 | 1:30:C:VAL:HG22 | 10                  | 0.78     | 0.08                | 0.79       |
| (1,593) | 1:19:C:LEU:HD22 | 1:30:C:VAL:HG21 | 10                  | 0.78     | 0.08                | 0.79       |
| (1,593) | 1:19:C:LEU:HD22 | 1:30:C:VAL:HG23 | 10                  | 0.78     | 0.08                | 0.79       |
| (1,593) | 1:19:C:LEU:HD22 | 1:30:C:VAL:HG22 | 10                  | 0.78     | 0.08                | 0.79       |
| (1,593) | 1:19:C:LEU:HD21 | 1:30:C:VAL:HG23 | 10                  | 0.78     | 0.08                | 0.79       |
| (3,28)  | 1:27:C:TYR:HE1  | 1:23:C:LYS:HD3  | 10                  | 0.77     | 0.25                | 0.78       |
| (3,28)  | 1:27:C:TYR:HE1  | 1:23:C:LYS:HD2  | 10                  | 0.77     | 0.25                | 0.78       |
| (3,28)  | 1:27:C:TYR:HE2  | 1:23:C:LYS:HD3  | 10                  | 0.77     | 0.25                | 0.78       |
| (3,28)  | 1:27:C:TYR:HE2  | 1:24:C:LYS:HB2  | 10                  | 0.77     | 0.25                | 0.78       |
| (3,28)  | 1:27:C:TYR:HE1  | 1:24:C:LYS:HB2  | 10                  | 0.77     | 0.25                | 0.78       |
| (3,28)  | 1:27:C:TYR:HE2  | 1:23:C:LYS:HD2  | 10                  | 0.77     | 0.25                | 0.78       |
| (1,195) | 1:28:C:HIS:H    | 1:22:C:ARG:HD2  | 10                  | 0.76     | 0.03                | 0.76       |
| (4,30)  | 1:27:C:TYR:HE1  | 1:23:C:LYS:HD3  | 10                  | 0.76     | 0.25                | 0.78       |
| (4,30)  | 1:27:C:TYR:HE1  | 1:23:C:LYS:HD2  | 10                  | 0.76     | 0.25                | 0.78       |
| (4,30)  | 1:27:C:TYR:HE2  | 1:23:C:LYS:HD3  | 10                  | 0.76     | 0.25                | 0.78       |

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| Key     | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (4,30)  | 1:27:C:TYR:HE2  | 1:24:C:LYS:HB2  | 10                  | 0.76     | 0.25                | 0.78       |
| (4,30)  | 1:27:C:TYR:HE1  | 1:24:C:LYS:HB2  | 10                  | 0.76     | 0.25                | 0.78       |
| (4,30)  | 1:27:C:TYR:HE2  | 1:23:C:LYS:HD2  | 10                  | 0.76     | 0.25                | 0.78       |
| (1,234) | 1:31:C:TRP:HE3  | 1:31:C:TRP:HB2  | 10                  | 0.75     | 0.01                | 0.75       |
| (3,86)  | 1:20:C:GLU:HB2  | 1:32:C:ASP:HB2  | 10                  | 0.72     | 0.26                | 0.67       |
| (4,88)  | 1:20:C:GLU:HB2  | 1:32:C:ASP:HB2  | 10                  | 0.72     | 0.26                | 0.67       |
| (1,153) | 1:18:C:HIS:HD2  | 1:18:C:HIS:HB3  | 10                  | 0.7      | 0.02                | 0.69       |
| (1,201) | 1:22:C:ARG:H    | 1:22:C:ARG:HD2  | 10                  | 0.64     | 0.11                | 0.64       |
| (1,227) | 1:31:C:TRP:H    | 1:31:C:TRP:HB3  | 10                  | 0.61     | 0.01                | 0.61       |
| (1,199) | 1:33:C:TRP:H    | 1:32:C:ASP:HB2  | 10                  | 0.6      | 0.15                | 0.62       |
| (1,241) | 1:13:C:ALA:H    | 1:11:C:LYS:HB3  | 10                  | 0.6      | 0.07                | 0.6        |
| (1,115) | 1:32:C:ASP:H    | 1:18:C:HIS:HB2  | 10                  | 0.59     | 0.08                | 0.59       |
| (3,46)  | 1:29:C:CYS:H    | 1:19:C:LEU:HD21 | 10                  | 0.57     | 0.1                 | 0.62       |
| (3,46)  | 1:29:C:CYS:H    | 1:19:C:LEU:HD22 | 10                  | 0.57     | 0.1                 | 0.62       |
| (3,46)  | 1:16:C:CYS:H    | 1:19:C:LEU:HD23 | 10                  | 0.57     | 0.1                 | 0.62       |
| (3,46)  | 1:29:C:CYS:H    | 1:19:C:LEU:HD23 | 10                  | 0.57     | 0.1                 | 0.62       |
| (3,46)  | 1:16:C:CYS:H    | 1:19:C:LEU:HD22 | 10                  | 0.57     | 0.1                 | 0.62       |
| (4,48)  | 1:29:C:CYS:H    | 1:19:C:LEU:HD21 | 10                  | 0.57     | 0.1                 | 0.62       |
| (4,48)  | 1:29:C:CYS:H    | 1:19:C:LEU:HD22 | 10                  | 0.57     | 0.1                 | 0.62       |
| (4,48)  | 1:16:C:CYS:H    | 1:19:C:LEU:HD23 | 10                  | 0.57     | 0.1                 | 0.62       |
| (4,48)  | 1:29:C:CYS:H    | 1:19:C:LEU:HD23 | 10                  | 0.57     | 0.1                 | 0.62       |
| (4,48)  | 1:16:C:CYS:H    | 1:19:C:LEU:HD22 | 10                  | 0.57     | 0.1                 | 0.62       |
| (1,308) | 1:32:C:ASP:H    | 1:31:C:TRP:HB2  | 10                  | 0.57     | 0.06                | 0.54       |
| (3,80)  | 1:19:C:LEU:HD12 | 1:4:C:GLU:HB2   | 10                  | 0.56     | 0.21                | 0.48       |
| (3,80)  | 1:19:C:LEU:HD11 | 1:4:C:GLU:HG2   | 10                  | 0.56     | 0.21                | 0.48       |
| (3,80)  | 1:19:C:LEU:HD12 | 1:4:C:GLU:HG2   | 10                  | 0.56     | 0.21                | 0.48       |
| (3,80)  | 1:19:C:LEU:HD13 | 1:4:C:GLU:HG2   | 10                  | 0.56     | 0.21                | 0.48       |
| (4,82)  | 1:19:C:LEU:HD12 | 1:4:C:GLU:HB2   | 10                  | 0.56     | 0.21                | 0.48       |
| (4,82)  | 1:19:C:LEU:HD11 | 1:4:C:GLU:HG2   | 10                  | 0.56     | 0.21                | 0.48       |
| (4,82)  | 1:19:C:LEU:HD12 | 1:4:C:GLU:HG2   | 10                  | 0.56     | 0.21                | 0.48       |
| (4,82)  | 1:19:C:LEU:HD13 | 1:4:C:GLU:HG2   | 10                  | 0.56     | 0.21                | 0.48       |
| (1,291) | 1:2:C:CYS:H     | 1:1:C:ALA:HB3   | 10                  | 0.55     | 0.1                 | 0.55       |
| (1,291) | 1:2:C:CYS:H     | 1:1:C:ALA:HB2   | 10                  | 0.55     | 0.1                 | 0.55       |
| (1,291) | 1:2:C:CYS:H     | 1:1:C:ALA:HB1   | 10                  | 0.55     | 0.1                 | 0.55       |
| (1,567) | 1:25:C:ALA:HB1  | 1:26:C:PRO:HB2  | 10                  | 0.55     | 0.13                | 0.6        |
| (1,567) | 1:25:C:ALA:HB3  | 1:26:C:PRO:HB2  | 10                  | 0.55     | 0.13                | 0.6        |
| (1,567) | 1:25:C:ALA:HB2  | 1:26:C:PRO:HB2  | 10                  | 0.55     | 0.13                | 0.6        |
| (3,39)  | 1:7:C:GLY:H     | 1:4:C:GLU:HB2   | 10                  | 0.52     | 0.13                | 0.47       |
| (3,39)  | 1:7:C:GLY:H     | 1:4:C:GLU:HG2   | 10                  | 0.52     | 0.13                | 0.47       |
| (4,41)  | 1:7:C:GLY:H     | 1:4:C:GLU:HB2   | 10                  | 0.51     | 0.13                | 0.46       |
| (4,41)  | 1:7:C:GLY:H     | 1:4:C:GLU:HG2   | 10                  | 0.51     | 0.13                | 0.46       |
| (1,354) | 1:31:C:TRP:HE1  | 1:6:C:LEU:HD13  | 10                  | 0.5      | 0.3                 | 0.4        |

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| Key     | Atom-1         | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,354) | 1:31:C:TRP:HE1 | 1:6:C:LEU:HD12  | 10                  | 0.5      | 0.3                 | 0.4        |
| (1,353) | 1:31:C:TRP:HE1 | 1:19:C:LEU:HD22 | 10                  | 0.49     | 0.06                | 0.53       |
| (1,353) | 1:31:C:TRP:HE1 | 1:19:C:LEU:HD23 | 10                  | 0.49     | 0.06                | 0.53       |
| (1,353) | 1:31:C:TRP:HE1 | 1:19:C:LEU:HD21 | 10                  | 0.49     | 0.06                | 0.53       |
| (1,300) | 1:16:C:CYS:H   | 1:15:C:CYS:HB3  | 10                  | 0.48     | 0.03                | 0.49       |
| (1,218) | 1:31:C:TRP:HH2 | 1:5:C:TRP:HB3   | 10                  | 0.47     | 0.17                | 0.51       |
| (1,366) | 1:5:C:TRP:HD1  | 1:6:C:LEU:HD11  | 10                  | 0.46     | 0.73                | 0.22       |
| (1,366) | 1:5:C:TRP:HD1  | 1:6:C:LEU:HD12  | 10                  | 0.46     | 0.73                | 0.22       |
| (1,366) | 1:5:C:TRP:HD1  | 1:6:C:LEU:HD13  | 10                  | 0.46     | 0.73                | 0.22       |
| (1,191) | 1:27:C:TYR:HE2 | 1:27:C:TYR:HB2  | 10                  | 0.45     | 0.05                | 0.44       |
| (1,191) | 1:27:C:TYR:HE1 | 1:27:C:TYR:HB2  | 10                  | 0.45     | 0.05                | 0.44       |
| (4,8)   | 1:2:C:CYS:H    | 1:3:C:ARG:HD3   | 10                  | 0.45     | 0.06                | 0.42       |
| (4,8)   | 1:2:C:CYS:H    | 1:3:C:ARG:HD2   | 10                  | 0.45     | 0.06                | 0.42       |
| (1,222) | 1:5:C:TRP:HD1  | 1:5:C:TRP:HB3   | 10                  | 0.42     | 0.01                | 0.42       |
| (1,297) | 1:18:C:HIS:HE1 | 1:17:C:ALA:HB3  | 10                  | 0.42     | 0.06                | 0.42       |
| (1,297) | 1:18:C:HIS:HE1 | 1:17:C:ALA:HB1  | 10                  | 0.42     | 0.06                | 0.42       |
| (1,297) | 1:18:C:HIS:HE1 | 1:17:C:ALA:HB2  | 10                  | 0.42     | 0.06                | 0.42       |
| (1,262) | 1:5:C:TRP:HD1  | 1:30:C:VAL:HG11 | 10                  | 0.41     | 0.04                | 0.41       |
| (1,262) | 1:5:C:TRP:HD1  | 1:30:C:VAL:HG13 | 10                  | 0.41     | 0.04                | 0.41       |
| (1,262) | 1:5:C:TRP:HD1  | 1:30:C:VAL:HG12 | 10                  | 0.41     | 0.04                | 0.41       |
| (1,264) | 1:28:C:HIS:HD2 | 1:30:C:VAL:HG22 | 10                  | 0.39     | 0.06                | 0.42       |
| (1,264) | 1:28:C:HIS:HD2 | 1:30:C:VAL:HG23 | 10                  | 0.39     | 0.06                | 0.42       |
| (1,264) | 1:28:C:HIS:HD2 | 1:30:C:VAL:HG21 | 10                  | 0.39     | 0.06                | 0.42       |
| (1,343) | 1:32:C:ASP:H   | 1:30:C:VAL:HG21 | 10                  | 0.39     | 0.03                | 0.4        |
| (1,343) | 1:32:C:ASP:H   | 1:30:C:VAL:HG22 | 10                  | 0.39     | 0.03                | 0.4        |
| (1,343) | 1:32:C:ASP:H   | 1:30:C:VAL:HG23 | 10                  | 0.39     | 0.03                | 0.4        |
| (1,193) | 1:28:C:HIS:HD2 | 1:22:C:ARG:HD2  | 10                  | 0.38     | 0.04                | 0.4        |
| (1,156) | 1:31:C:TRP:HZ3 | 1:18:C:HIS:HB3  | 10                  | 0.38     | 0.11                | 0.37       |
| (3,93)  | 1:19:C:LEU:HB3 | 1:20:C:GLU:HG3  | 10                  | 0.37     | 0.19                | 0.29       |
| (4,95)  | 1:19:C:LEU:HB3 | 1:20:C:GLU:HG3  | 10                  | 0.36     | 0.19                | 0.29       |
| (1,62)  | 1:27:C:TYR:HD1 | 1:27:C:TYR:HE1  | 10                  | 0.35     | 0.0                 | 0.35       |
| (1,62)  | 1:27:C:TYR:HD2 | 1:27:C:TYR:HE2  | 10                  | 0.35     | 0.0                 | 0.35       |
| (1,464) | 1:25:C:ALA:HB3 | 1:24:C:LYS:HA   | 10                  | 0.33     | 0.04                | 0.32       |
| (1,464) | 1:25:C:ALA:HB2 | 1:24:C:LYS:HA   | 10                  | 0.33     | 0.04                | 0.32       |
| (1,464) | 1:25:C:ALA:HB1 | 1:24:C:LYS:HA   | 10                  | 0.33     | 0.04                | 0.32       |
| (3,10)  | 1:31:C:TRP:HD1 | 1:31:C:TRP:HA   | 10                  | 0.31     | 0.02                | 0.31       |
| (4,11)  | 1:31:C:TRP:HD1 | 1:31:C:TRP:HA   | 10                  | 0.3      | 0.02                | 0.31       |
| (1,352) | 1:6:C:LEU:H    | 1:19:C:LEU:HD21 | 10                  | 0.28     | 0.05                | 0.29       |
| (1,352) | 1:6:C:LEU:H    | 1:19:C:LEU:HD22 | 10                  | 0.28     | 0.05                | 0.29       |
| (1,352) | 1:6:C:LEU:H    | 1:19:C:LEU:HD23 | 10                  | 0.28     | 0.05                | 0.29       |
| (1,273) | 1:15:C:CYS:H   | 1:13:C:ALA:HB2  | 10                  | 0.24     | 0.04                | 0.24       |
| (1,273) | 1:15:C:CYS:H   | 1:13:C:ALA:HB3  | 10                  | 0.24     | 0.04                | 0.24       |

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| Key     | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,273) | 1:15:C:CYS:H    | 1:13:C:ALA:HB1  | 10                  | 0.24     | 0.04                | 0.24       |
| (3,25)  | 1:28:C:HIS:HD2  | 1:22:C:ARG:HG3  | 10                  | 0.23     | 0.03                | 0.22       |
| (4,27)  | 1:28:C:HIS:HD2  | 1:22:C:ARG:HG3  | 10                  | 0.23     | 0.04                | 0.22       |
| (1,2)   | 1:5:C:TRP:H     | 1:5:C:TRP:HB3   | 10                  | 0.16     | 0.02                | 0.16       |
| (3,38)  | 1:29:C:CYS:H    | 1:29:C:CYS:HB3  | 10                  | 0.15     | 0.01                | 0.16       |
| (4,40)  | 1:29:C:CYS:H    | 1:29:C:CYS:HB3  | 10                  | 0.15     | 0.01                | 0.15       |
| (1,534) | 1:11:C:LYS:HD3  | 1:15:C:CYS:HB2  | 9                   | 1.49     | 0.11                | 1.49       |
| (1,540) | 1:3:C:ARG:HG3   | 1:11:C:LYS:HE3  | 9                   | 1.34     | 0.76                | 1.56       |
| (1,175) | 1:17:C:ALA:H    | 1:16:C:CYS:HB2  | 9                   | 1.01     | 0.1                 | 1.05       |
| (1,293) | 1:13:C:ALA:H    | 1:11:C:LYS:HG2  | 9                   | 0.82     | 0.09                | 0.83       |
| (1,345) | 1:5:C:TRP:HE1   | 1:6:C:LEU:HD13  | 9                   | 0.47     | 0.61                | 0.24       |
| (1,345) | 1:5:C:TRP:HE1   | 1:6:C:LEU:HD12  | 9                   | 0.47     | 0.61                | 0.24       |
| (3,41)  | 1:20:C:GLU:H    | 1:30:C:VAL:HB   | 9                   | 0.39     | 0.1                 | 0.36       |
| (4,43)  | 1:20:C:GLU:H    | 1:30:C:VAL:HB   | 9                   | 0.38     | 0.1                 | 0.35       |
| (1,280) | 1:31:C:TRP:HE3  | 1:19:C:LEU:HD12 | 9                   | 0.37     | 0.08                | 0.4        |
| (1,280) | 1:31:C:TRP:HE3  | 1:19:C:LEU:HD11 | 9                   | 0.37     | 0.08                | 0.4        |
| (1,280) | 1:31:C:TRP:HE3  | 1:19:C:LEU:HD13 | 9                   | 0.37     | 0.08                | 0.4        |
| (1,600) | 1:5:C:TRP:HH2   | 1:6:C:LEU:HD13  | 9                   | 0.32     | 0.02                | 0.32       |
| (1,600) | 1:5:C:TRP:HH2   | 1:6:C:LEU:HD12  | 9                   | 0.32     | 0.02                | 0.32       |
| (1,341) | 1:12:C:ASP:H    | 1:11:C:LYS:HG2  | 9                   | 0.3      | 0.09                | 0.33       |
| (1,162) | 1:18:C:HIS:HD2  | 1:18:C:HIS:HA   | 9                   | 0.19     | 0.03                | 0.2        |
| (1,289) | 1:13:C:ALA:H    | 1:13:C:ALA:HB3  | 9                   | 0.18     | 0.04                | 0.19       |
| (1,289) | 1:13:C:ALA:H    | 1:13:C:ALA:HB1  | 9                   | 0.18     | 0.04                | 0.19       |
| (1,289) | 1:13:C:ALA:H    | 1:13:C:ALA:HB2  | 9                   | 0.18     | 0.04                | 0.19       |
| (4,10)  | 1:18:C:HIS:HD2  | 1:18:C:HIS:HA   | 9                   | 0.18     | 0.02                | 0.19       |
| (1,513) | 1:19:C:LEU:HB3  | 1:14:C:ASP:HB3  | 8                   | 1.18     | 0.02                | 1.19       |
| (1,491) | 1:19:C:LEU:HB2  | 1:14:C:ASP:HB3  | 8                   | 0.83     | 0.02                | 0.83       |
| (3,57)  | 1:34:C:THR:HG23 | 1:33:C:TRP:HA   | 8                   | 0.52     | 0.21                | 0.52       |
| (3,57)  | 1:34:C:THR:HG22 | 1:33:C:TRP:HA   | 8                   | 0.52     | 0.21                | 0.52       |
| (3,57)  | 1:34:C:THR:HG21 | 1:33:C:TRP:HA   | 8                   | 0.52     | 0.21                | 0.52       |
| (3,57)  | 1:34:C:THR:HG21 | 1:31:C:TRP:HA   | 8                   | 0.52     | 0.21                | 0.52       |
| (4,59)  | 1:34:C:THR:HG23 | 1:33:C:TRP:HA   | 8                   | 0.52     | 0.21                | 0.51       |
| (4,59)  | 1:34:C:THR:HG22 | 1:33:C:TRP:HA   | 8                   | 0.52     | 0.21                | 0.51       |
| (4,59)  | 1:34:C:THR:HG21 | 1:33:C:TRP:HA   | 8                   | 0.52     | 0.21                | 0.51       |
| (4,59)  | 1:34:C:THR:HG21 | 1:31:C:TRP:HA   | 8                   | 0.52     | 0.21                | 0.51       |
| (3,29)  | 1:31:C:TRP:H    | 1:30:C:VAL:HG11 | 8                   | 0.48     | 0.09                | 0.49       |
| (3,29)  | 1:31:C:TRP:H    | 1:30:C:VAL:HG13 | 8                   | 0.48     | 0.09                | 0.49       |
| (3,29)  | 1:31:C:TRP:H    | 1:34:C:THR:HG22 | 8                   | 0.48     | 0.09                | 0.49       |
| (3,29)  | 1:31:C:TRP:H    | 1:30:C:VAL:HG12 | 8                   | 0.48     | 0.09                | 0.49       |
| (3,29)  | 1:31:C:TRP:H    | 1:34:C:THR:HG23 | 8                   | 0.48     | 0.09                | 0.49       |
| (4,31)  | 1:31:C:TRP:H    | 1:30:C:VAL:HG11 | 8                   | 0.48     | 0.1                 | 0.49       |
| (4,31)  | 1:31:C:TRP:H    | 1:30:C:VAL:HG13 | 8                   | 0.48     | 0.1                 | 0.49       |

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| Key     | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (4,31)  | 1:31:C:TRP:H    | 1:34:C:THR:HG22 | 8                   | 0.48     | 0.1                 | 0.49       |
| (4,31)  | 1:31:C:TRP:H    | 1:30:C:VAL:HG12 | 8                   | 0.48     | 0.1                 | 0.49       |
| (4,31)  | 1:31:C:TRP:H    | 1:34:C:THR:HG23 | 8                   | 0.48     | 0.1                 | 0.49       |
| (3,84)  | 1:24:C:LYS:HD3  | 1:23:C:LYS:HE2  | 8                   | 0.42     | 0.16                | 0.36       |
| (3,84)  | 1:24:C:LYS:HD2  | 1:23:C:LYS:HE2  | 8                   | 0.42     | 0.16                | 0.36       |
| (3,84)  | 1:24:C:LYS:HD2  | 1:23:C:LYS:HE3  | 8                   | 0.42     | 0.16                | 0.36       |
| (4,86)  | 1:24:C:LYS:HD3  | 1:23:C:LYS:HE2  | 8                   | 0.42     | 0.15                | 0.36       |
| (4,86)  | 1:24:C:LYS:HD2  | 1:23:C:LYS:HE2  | 8                   | 0.42     | 0.15                | 0.36       |
| (4,86)  | 1:24:C:LYS:HD2  | 1:23:C:LYS:HE3  | 8                   | 0.42     | 0.15                | 0.36       |
| (1,267) | 1:31:C:TRP:HZ3  | 1:19:C:LEU:HD11 | 8                   | 0.36     | 0.04                | 0.36       |
| (1,267) | 1:31:C:TRP:HZ3  | 1:19:C:LEU:HD12 | 8                   | 0.36     | 0.04                | 0.36       |
| (1,267) | 1:31:C:TRP:HZ3  | 1:19:C:LEU:HD13 | 8                   | 0.36     | 0.04                | 0.36       |
| (1,598) | 1:11:C:LYS:H    | 1:10:C:SER:HB3  | 8                   | 0.35     | 0.08                | 0.36       |
| (1,570) | 1:30:C:VAL:HG13 | 1:22:C:ARG:HB3  | 8                   | 0.34     | 0.1                 | 0.32       |
| (1,570) | 1:30:C:VAL:HG12 | 1:22:C:ARG:HB3  | 8                   | 0.34     | 0.1                 | 0.32       |
| (1,570) | 1:30:C:VAL:HG11 | 1:22:C:ARG:HB3  | 8                   | 0.34     | 0.1                 | 0.32       |
| (1,360) | 1:31:C:TRP:H    | 1:19:C:LEU:HD23 | 8                   | 0.24     | 0.09                | 0.25       |
| (1,360) | 1:31:C:TRP:H    | 1:19:C:LEU:HD21 | 8                   | 0.24     | 0.09                | 0.25       |
| (1,360) | 1:31:C:TRP:H    | 1:19:C:LEU:HD22 | 8                   | 0.24     | 0.09                | 0.25       |
| (1,322) | 1:21:C:CYS:H    | 1:20:C:GLU:HG2  | 8                   | 0.23     | 0.07                | 0.22       |
| (1,346) | 1:5:C:TRP:HE1   | 1:19:C:LEU:HD21 | 8                   | 0.22     | 0.09                | 0.18       |
| (1,346) | 1:5:C:TRP:HE1   | 1:19:C:LEU:HD22 | 8                   | 0.22     | 0.09                | 0.18       |
| (1,346) | 1:5:C:TRP:HE1   | 1:19:C:LEU:HD23 | 8                   | 0.22     | 0.09                | 0.18       |
| (1,573) | 1:30:C:VAL:HG22 | 1:22:C:ARG:HB2  | 8                   | 0.21     | 0.04                | 0.2        |
| (1,573) | 1:30:C:VAL:HG21 | 1:22:C:ARG:HB2  | 8                   | 0.21     | 0.04                | 0.2        |
| (1,573) | 1:30:C:VAL:HG23 | 1:22:C:ARG:HB2  | 8                   | 0.21     | 0.04                | 0.2        |
| (1,355) | 1:5:C:TRP:H     | 1:19:C:LEU:HD23 | 8                   | 0.21     | 0.04                | 0.21       |
| (1,355) | 1:5:C:TRP:H     | 1:19:C:LEU:HD21 | 8                   | 0.21     | 0.04                | 0.21       |
| (1,355) | 1:5:C:TRP:H     | 1:19:C:LEU:HD22 | 8                   | 0.21     | 0.04                | 0.21       |
| (3,11)  | 1:33:C:TRP:HZ3  | 1:33:C:TRP:HB3  | 8                   | 0.18     | 0.03                | 0.17       |
| (3,11)  | 1:22:C:ARG:HE   | 1:26:C:PRO:HD3  | 8                   | 0.18     | 0.03                | 0.17       |
| (4,12)  | 1:33:C:TRP:HZ3  | 1:33:C:TRP:HB3  | 8                   | 0.18     | 0.03                | 0.17       |
| (4,12)  | 1:22:C:ARG:HE   | 1:26:C:PRO:HD3  | 8                   | 0.18     | 0.03                | 0.17       |
| (1,266) | 1:31:C:TRP:HH2  | 1:19:C:LEU:HD11 | 8                   | 0.18     | 0.04                | 0.18       |
| (1,266) | 1:31:C:TRP:HH2  | 1:19:C:LEU:HD12 | 8                   | 0.18     | 0.04                | 0.18       |
| (1,266) | 1:31:C:TRP:HH2  | 1:19:C:LEU:HD13 | 8                   | 0.18     | 0.04                | 0.18       |
| (1,283) | 1:5:C:TRP:H     | 1:19:C:LEU:HD11 | 8                   | 0.18     | 0.02                | 0.18       |
| (1,283) | 1:5:C:TRP:H     | 1:19:C:LEU:HD12 | 8                   | 0.18     | 0.02                | 0.18       |
| (1,283) | 1:5:C:TRP:H     | 1:19:C:LEU:HD13 | 8                   | 0.18     | 0.02                | 0.18       |
| (3,68)  | 1:15:C:CYS:HB2  | 1:9:C:CYS:HB3   | 8                   | 0.16     | 0.04                | 0.15       |
| (4,70)  | 1:15:C:CYS:HB2  | 1:9:C:CYS:HB3   | 8                   | 0.16     | 0.04                | 0.15       |
| (1,605) | 1:5:C:TRP:HZ2   | 1:30:C:VAL:HA   | 8                   | 0.13     | 0.02                | 0.13       |

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| Key     | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (3,65)  | 1:35:C:VAL:HG11 | 1:34:C:THR:HB   | 7                   | 0.78     | 0.19                | 0.67       |
| (3,65)  | 1:35:C:VAL:HG13 | 1:34:C:THR:HB   | 7                   | 0.78     | 0.19                | 0.67       |
| (3,65)  | 1:35:C:VAL:HG12 | 1:34:C:THR:HB   | 7                   | 0.78     | 0.19                | 0.67       |
| (4,67)  | 1:35:C:VAL:HG11 | 1:34:C:THR:HB   | 7                   | 0.77     | 0.19                | 0.67       |
| (4,67)  | 1:35:C:VAL:HG13 | 1:34:C:THR:HB   | 7                   | 0.77     | 0.19                | 0.67       |
| (4,67)  | 1:35:C:VAL:HG12 | 1:34:C:THR:HB   | 7                   | 0.77     | 0.19                | 0.67       |
| (3,8)   | 1:2:C:CYS:H     | 1:3:C:ARG:HD3   | 7                   | 0.47     | 0.07                | 0.44       |
| (3,8)   | 1:2:C:CYS:H     | 1:3:C:ARG:HD2   | 7                   | 0.47     | 0.07                | 0.44       |
| (1,205) | 1:11:C:LYS:H    | 1:21:C:CYS:HB3  | 7                   | 0.32     | 0.08                | 0.35       |
| (3,23)  | 1:28:C:HIS:H    | 1:22:C:ARG:HG3  | 7                   | 0.31     | 0.09                | 0.33       |
| (3,23)  | 1:28:C:HIS:H    | 1:22:C:ARG:HG2  | 7                   | 0.31     | 0.09                | 0.33       |
| (4,24)  | 1:28:C:HIS:H    | 1:22:C:ARG:HG3  | 7                   | 0.3      | 0.08                | 0.33       |
| (4,24)  | 1:28:C:HIS:H    | 1:22:C:ARG:HG2  | 7                   | 0.3      | 0.08                | 0.33       |
| (3,33)  | 1:34:C:THR:H    | 1:35:C:VAL:HG23 | 7                   | 0.3      | 0.1                 | 0.28       |
| (3,33)  | 1:34:C:THR:H    | 1:35:C:VAL:HG11 | 7                   | 0.3      | 0.1                 | 0.28       |
| (3,33)  | 1:34:C:THR:H    | 1:35:C:VAL:HG12 | 7                   | 0.3      | 0.1                 | 0.28       |
| (4,35)  | 1:34:C:THR:H    | 1:35:C:VAL:HG23 | 7                   | 0.3      | 0.09                | 0.28       |
| (4,35)  | 1:34:C:THR:H    | 1:35:C:VAL:HG11 | 7                   | 0.3      | 0.09                | 0.28       |
| (4,35)  | 1:34:C:THR:H    | 1:35:C:VAL:HG12 | 7                   | 0.3      | 0.09                | 0.28       |
| (3,35)  | 1:25:C:ALA:H    | 1:24:C:LYS:HG2  | 7                   | 0.26     | 0.07                | 0.3        |
| (3,35)  | 1:25:C:ALA:H    | 1:24:C:LYS:HG3  | 7                   | 0.26     | 0.07                | 0.3        |
| (4,37)  | 1:25:C:ALA:H    | 1:24:C:LYS:HG2  | 7                   | 0.26     | 0.07                | 0.3        |
| (4,37)  | 1:25:C:ALA:H    | 1:24:C:LYS:HG3  | 7                   | 0.26     | 0.07                | 0.3        |
| (1,157) | 1:27:C:TYR:HD1  | 1:23:C:LYS:HA   | 7                   | 0.18     | 0.08                | 0.14       |
| (1,157) | 1:27:C:TYR:HD2  | 1:23:C:LYS:HA   | 7                   | 0.18     | 0.08                | 0.14       |
| (1,530) | 1:13:C:ALA:HB2  | 1:11:C:LYS:HE3  | 6                   | 0.32     | 0.05                | 0.34       |
| (1,530) | 1:13:C:ALA:HB1  | 1:11:C:LYS:HE3  | 6                   | 0.32     | 0.05                | 0.34       |
| (1,530) | 1:13:C:ALA:HB3  | 1:11:C:LYS:HE3  | 6                   | 0.32     | 0.05                | 0.34       |
| (3,2)   | 1:31:C:TRP:HE1  | 1:5:C:TRP:HZ3   | 6                   | 0.16     | 0.03                | 0.16       |
| (3,2)   | 1:31:C:TRP:HE1  | 1:31:C:TRP:HH2  | 6                   | 0.16     | 0.03                | 0.16       |
| (1,386) | 1:12:C:ASP:HA   | 1:20:C:GLU:HA   | 6                   | 0.16     | 0.06                | 0.13       |
| (4,2)   | 1:31:C:TRP:HE1  | 1:5:C:TRP:HZ3   | 6                   | 0.16     | 0.04                | 0.15       |
| (4,2)   | 1:31:C:TRP:HE1  | 1:31:C:TRP:HH2  | 6                   | 0.16     | 0.04                | 0.15       |
| (1,538) | 1:22:C:ARG:HB2  | 1:22:C:ARG:HD2  | 6                   | 0.12     | 0.01                | 0.12       |
| (1,285) | 1:23:C:LYS:H    | 1:23:C:LYS:HB2  | 5                   | 0.63     | 0.03                | 0.61       |
| (1,507) | 1:6:C:LEU:HD11  | 1:22:C:ARG:HD3  | 5                   | 0.58     | 0.69                | 0.23       |
| (1,507) | 1:6:C:LEU:HD12  | 1:22:C:ARG:HD3  | 5                   | 0.58     | 0.69                | 0.23       |
| (3,78)  | 1:30:C:VAL:HG22 | 1:22:C:ARG:HD3  | 5                   | 0.34     | 0.13                | 0.34       |
| (3,78)  | 1:30:C:VAL:HG23 | 1:22:C:ARG:HD3  | 5                   | 0.34     | 0.13                | 0.34       |
| (3,78)  | 1:30:C:VAL:HG21 | 1:22:C:ARG:HD3  | 5                   | 0.34     | 0.13                | 0.34       |
| (4,80)  | 1:30:C:VAL:HG22 | 1:22:C:ARG:HD3  | 5                   | 0.34     | 0.12                | 0.34       |
| (4,80)  | 1:30:C:VAL:HG23 | 1:22:C:ARG:HD3  | 5                   | 0.34     | 0.12                | 0.34       |

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| Key     | Atom-1          | Atom-2         | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|-----------------|----------------|---------------------|----------|---------------------|------------|
| (4,80)  | 1:30:C:VAL:HG21 | 1:22:C:ARG:HD3 | 5                   | 0.34     | 0.12                | 0.34       |
| (1,306) | 1:16:C:CYS:H    | 1:16:C:CYS:HB3 | 5                   | 0.32     | 0.25                | 0.22       |
| (3,21)  | 1:22:C:ARG:H    | 1:22:C:ARG:HG3 | 5                   | 0.28     | 0.07                | 0.27       |
| (4,22)  | 1:22:C:ARG:H    | 1:22:C:ARG:HG3 | 5                   | 0.28     | 0.07                | 0.27       |
| (3,45)  | 1:7:C:GLY:H     | 1:3:C:ARG:HB3  | 5                   | 0.23     | 0.03                | 0.23       |
| (4,47)  | 1:7:C:GLY:H     | 1:3:C:ARG:HB3  | 5                   | 0.22     | 0.03                | 0.23       |
| (3,102) | 1:23:C:LYS:H    | 1:23:C:LYS:HB3 | 5                   | 0.14     | 0.01                | 0.14       |
| (4,104) | 1:23:C:LYS:H    | 1:23:C:LYS:HB3 | 5                   | 0.14     | 0.01                | 0.14       |
| (1,202) | 1:11:C:LYS:H    | 1:11:C:LYS:HE3 | 4                   | 1.44     | 0.04                | 1.44       |
| (1,520) | 1:6:C:LEU:HD12  | 1:30:C:VAL:HB  | 4                   | 0.75     | 0.93                | 0.26       |
| (1,520) | 1:6:C:LEU:HD13  | 1:30:C:VAL:HB  | 4                   | 0.75     | 0.93                | 0.26       |
| (1,284) | 1:25:C:ALA:H    | 1:24:C:LYS:HB3 | 4                   | 0.53     | 0.01                | 0.54       |
| (1,256) | 1:24:C:LYS:H    | 1:24:C:LYS:HB2 | 4                   | 0.46     | 0.04                | 0.46       |
| (3,63)  | 1:23:C:LYS:HD2  | 1:23:C:LYS:HA  | 4                   | 0.38     | 0.16                | 0.41       |
| (3,63)  | 1:23:C:LYS:HD3  | 1:23:C:LYS:HA  | 4                   | 0.38     | 0.16                | 0.41       |
| (4,65)  | 1:23:C:LYS:HD2  | 1:23:C:LYS:HA  | 4                   | 0.38     | 0.16                | 0.4        |
| (4,65)  | 1:23:C:LYS:HD3  | 1:23:C:LYS:HA  | 4                   | 0.38     | 0.16                | 0.4        |
| (1,60)  | 1:24:C:LYS:H    | 1:27:C:TYR:HD2 | 4                   | 0.25     | 0.1                 | 0.24       |
| (1,60)  | 1:24:C:LYS:H    | 1:27:C:TYR:HD1 | 4                   | 0.25     | 0.1                 | 0.24       |
| (1,255) | 1:27:C:TYR:HE1  | 1:23:C:LYS:HB3 | 4                   | 0.23     | 0.12                | 0.17       |
| (1,255) | 1:27:C:TYR:HE2  | 1:23:C:LYS:HB3 | 4                   | 0.23     | 0.12                | 0.17       |
| (1,533) | 1:1:C:ALA:HB1   | 1:11:C:LYS:HE2 | 4                   | 0.14     | 0.02                | 0.14       |
| (1,533) | 1:1:C:ALA:HB3   | 1:11:C:LYS:HE2 | 4                   | 0.14     | 0.02                | 0.14       |
| (3,13)  | 1:15:C:CYS:H    | 1:9:C:CYS:HB2  | 3                   | 0.24     | 0.04                | 0.27       |
| (4,14)  | 1:15:C:CYS:H    | 1:9:C:CYS:HB2  | 3                   | 0.23     | 0.04                | 0.26       |
| (3,9)   | 1:4:C:GLU:H     | 1:3:C:ARG:HD3  | 3                   | 0.17     | 0.07                | 0.13       |
| (3,9)   | 1:4:C:GLU:H     | 1:3:C:ARG:HD2  | 3                   | 0.17     | 0.07                | 0.13       |
| (4,9)   | 1:4:C:GLU:H     | 1:3:C:ARG:HD3  | 3                   | 0.16     | 0.07                | 0.12       |
| (4,9)   | 1:4:C:GLU:H     | 1:3:C:ARG:HD2  | 3                   | 0.16     | 0.07                | 0.12       |
| (1,290) | 1:23:C:LYS:H    | 1:23:C:LYS:HG2 | 3                   | 0.16     | 0.04                | 0.18       |
| (3,98)  | 1:24:C:LYS:HG2  | 1:24:C:LYS:HB2 | 3                   | 0.12     | 0.02                | 0.11       |
| (3,98)  | 1:24:C:LYS:HG3  | 1:24:C:LYS:HB2 | 3                   | 0.12     | 0.02                | 0.11       |
| (4,100) | 1:24:C:LYS:HG2  | 1:24:C:LYS:HB2 | 3                   | 0.12     | 0.01                | 0.11       |
| (4,100) | 1:24:C:LYS:HG3  | 1:24:C:LYS:HB2 | 3                   | 0.12     | 0.01                | 0.11       |
| (1,242) | 1:5:C:TRP:H     | 1:4:C:GLU:HB3  | 3                   | 0.11     | 0.01                | 0.11       |
| (1,415) | 1:12:C:ASP:HB2  | 1:20:C:GLU:HA  | 2                   | 1.09     | 0.04                | 1.09       |
| (1,237) | 1:5:C:TRP:H     | 1:4:C:GLU:HG2  | 2                   | 0.76     | 0.06                | 0.76       |
| (1,304) | 1:12:C:ASP:H    | 1:12:C:ASP:HB3 | 2                   | 0.71     | 0.03                | 0.71       |
| (1,214) | 1:5:C:TRP:H     | 1:4:C:GLU:HG3  | 2                   | 0.34     | 0.01                | 0.34       |
| (1,528) | 1:19:C:LEU:HB3  | 1:14:C:ASP:HB2 | 2                   | 0.19     | 0.07                | 0.19       |
| (1,128) | 1:34:C:THR:H    | 1:34:C:THR:HB  | 2                   | 0.15     | 0.02                | 0.15       |
| (1,192) | 1:28:C:HIS:HD2  | 1:6:C:LEU:HA   | 2                   | 0.14     | 0.03                | 0.14       |

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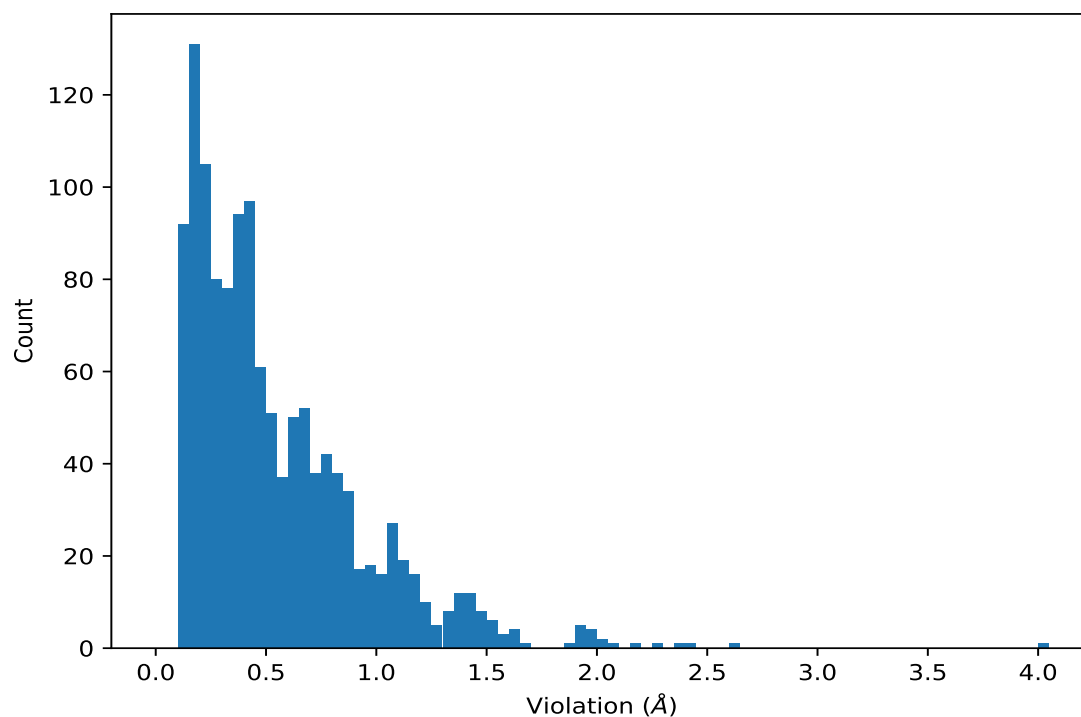
| Key     | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (3,30)  | 1:31:C:TRP:H    | 1:30:C:VAL:HG21 | 2                   | 0.14     | 0.02                | 0.14       |
| (3,30)  | 1:31:C:TRP:H    | 1:30:C:VAL:HG23 | 2                   | 0.14     | 0.02                | 0.14       |
| (4,32)  | 1:31:C:TRP:H    | 1:30:C:VAL:HG21 | 2                   | 0.14     | 0.02                | 0.14       |
| (4,32)  | 1:31:C:TRP:H    | 1:30:C:VAL:HG23 | 2                   | 0.14     | 0.02                | 0.14       |
| (1,516) | 1:30:C:VAL:HG11 | 1:6:C:LEU:HA    | 2                   | 0.13     | 0.02                | 0.13       |
| (1,516) | 1:30:C:VAL:HG13 | 1:6:C:LEU:HA    | 2                   | 0.13     | 0.02                | 0.13       |
| (1,402) | 1:35:C:VAL:HB   | 1:30:C:VAL:HA   | 2                   | 0.12     | 0.02                | 0.12       |

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

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

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

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



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

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

| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,521) | 1:6:C:LEU:HD13  | 1:29:C:CYS:HB3 | 4        | 4.02          |
| (1,366) | 1:5:C:TRP:HD1   | 1:6:C:LEU:HD13 | 4        | 2.64          |
| (1,540) | 1:3:C:ARG:HG3   | 1:11:C:LYS:HE3 | 7        | 2.4           |
| (1,520) | 1:6:C:LEU:HD13  | 1:30:C:VAL:HB  | 4        | 2.35          |
| (1,540) | 1:3:C:ARG:HG3   | 1:11:C:LYS:HE3 | 3        | 2.26          |
| (1,345) | 1:5:C:TRP:HE1   | 1:6:C:LEU:HD13 | 4        | 2.17          |
| (1,504) | 1:6:C:LEU:HD13  | 1:5:C:TRP:HA   | 4        | 2.05          |
| (1,506) | 1:19:C:LEU:HD22 | 1:14:C:ASP:HB3 | 5        | 2.03          |
| (1,365) | 1:28:C:HIS:HD2  | 1:6:C:LEU:HD11 | 4        | 2.02          |
| (1,351) | 1:6:C:LEU:H     | 1:6:C:LEU:HD11 | 4        | 1.98          |
| (1,506) | 1:19:C:LEU:HD22 | 1:14:C:ASP:HB3 | 3        | 1.97          |
| (1,507) | 1:6:C:LEU:HD11  | 1:22:C:ARG:HD3 | 4        | 1.96          |
| (1,506) | 1:19:C:LEU:HD21 | 1:14:C:ASP:HB3 | 8        | 1.96          |
| (1,506) | 1:19:C:LEU:HD22 | 1:14:C:ASP:HB3 | 4        | 1.92          |
| (1,506) | 1:19:C:LEU:HD21 | 1:14:C:ASP:HB3 | 7        | 1.92          |
| (1,506) | 1:19:C:LEU:HD23 | 1:14:C:ASP:HB3 | 10       | 1.91          |
| (1,540) | 1:3:C:ARG:HG3   | 1:11:C:LYS:HE3 | 8        | 1.9           |
| (1,506) | 1:19:C:LEU:HD23 | 1:14:C:ASP:HB3 | 1        | 1.9           |
| (1,506) | 1:19:C:LEU:HD21 | 1:14:C:ASP:HB3 | 2        | 1.89          |
| (1,412) | 1:6:C:LEU:HD13  | 1:30:C:VAL:HA  | 4        | 1.65          |
| (1,534) | 1:11:C:LYS:HD3  | 1:15:C:CYS:HB2 | 8        | 1.64          |
| (1,540) | 1:3:C:ARG:HG3   | 1:11:C:LYS:HE3 | 5        | 1.63          |
| (1,534) | 1:11:C:LYS:HD3  | 1:15:C:CYS:HB2 | 9        | 1.63          |
| (1,349) | 1:7:C:GLY:H     | 1:6:C:LEU:HD12 | 4        | 1.6           |
| (1,540) | 1:3:C:ARG:HG3   | 1:11:C:LYS:HE3 | 9        | 1.56          |
| (1,454) | 1:3:C:ARG:HG3   | 1:1:C:ALA:HA   | 2        | 1.55          |
| (1,454) | 1:3:C:ARG:HG3   | 1:1:C:ALA:HA   | 9        | 1.55          |
| (1,534) | 1:11:C:LYS:HD3  | 1:15:C:CYS:HB2 | 3        | 1.54          |
| (1,534) | 1:11:C:LYS:HD3  | 1:15:C:CYS:HB2 | 7        | 1.54          |
| (1,454) | 1:3:C:ARG:HG3   | 1:1:C:ALA:HA   | 6        | 1.54          |
| (1,454) | 1:3:C:ARG:HG3   | 1:1:C:ALA:HA   | 1        | 1.51          |
| (1,454) | 1:3:C:ARG:HG3   | 1:1:C:ALA:HA   | 4        | 1.5           |
| (1,202) | 1:11:C:LYS:H    | 1:11:C:LYS:HE3 | 8        | 1.5           |
| (1,534) | 1:11:C:LYS:HD3  | 1:15:C:CYS:HB2 | 4        | 1.49          |
| (1,534) | 1:11:C:LYS:HD3  | 1:15:C:CYS:HB2 | 10       | 1.48          |
| (1,454) | 1:3:C:ARG:HG3   | 1:1:C:ALA:HA   | 10       | 1.47          |
| (1,382) | 1:11:C:LYS:HD3  | 1:14:C:ASP:HA  | 4        | 1.47          |
| (1,534) | 1:11:C:LYS:HD3  | 1:15:C:CYS:HB2 | 1        | 1.45          |
| (1,382) | 1:11:C:LYS:HD3  | 1:14:C:ASP:HA  | 1        | 1.45          |
| (1,382) | 1:11:C:LYS:HD3  | 1:14:C:ASP:HA  | 6        | 1.45          |
| (1,202) | 1:11:C:LYS:H    | 1:11:C:LYS:HE3 | 3        | 1.45          |
| (1,503) | 1:17:C:ALA:HB1  | 1:16:C:CYS:HB2 | 2        | 1.44          |
| (1,503) | 1:17:C:ALA:HB1  | 1:16:C:CYS:HB2 | 7        | 1.43          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,301) | 1:3:C:ARG:H     | 1:15:C:CYS:HB3  | 2        | 1.43          |
| (1,301) | 1:3:C:ARG:H     | 1:15:C:CYS:HB3  | 7        | 1.43          |
| (4,49)  | 1:7:C:GLY:H     | 1:6:C:LEU:HD12  | 4        | 1.42          |
| (3,47)  | 1:7:C:GLY:H     | 1:6:C:LEU:HD12  | 4        | 1.42          |
| (1,202) | 1:11:C:LYS:H    | 1:11:C:LYS:HE3  | 7        | 1.42          |
| (1,534) | 1:11:C:LYS:HD3  | 1:15:C:CYS:HB2  | 2        | 1.41          |
| (1,503) | 1:17:C:ALA:HB1  | 1:16:C:CYS:HB2  | 1        | 1.4           |
| (1,503) | 1:17:C:ALA:HB2  | 1:16:C:CYS:HB2  | 3        | 1.4           |
| (1,354) | 1:31:C:TRP:HE1  | 1:6:C:LEU:HD13  | 4        | 1.4           |
| (1,311) | 1:10:C:SER:H    | 1:15:C:CYS:HB2  | 9        | 1.4           |
| (3,86)  | 1:20:C:GLU:HB2  | 1:32:C:ASP:HB2  | 9        | 1.39          |
| (1,503) | 1:17:C:ALA:HB2  | 1:16:C:CYS:HB2  | 8        | 1.39          |
| (1,503) | 1:17:C:ALA:HB3  | 1:16:C:CYS:HB2  | 9        | 1.39          |
| (1,503) | 1:17:C:ALA:HB3  | 1:16:C:CYS:HB2  | 10       | 1.39          |
| (1,382) | 1:11:C:LYS:HD3  | 1:14:C:ASP:HA   | 9        | 1.39          |
| (1,202) | 1:11:C:LYS:H    | 1:11:C:LYS:HE3  | 9        | 1.39          |
| (4,88)  | 1:20:C:GLU:HB2  | 1:32:C:ASP:HB2  | 9        | 1.38          |
| (1,155) | 1:31:C:TRP:HH2  | 1:18:C:HIS:HB3  | 1        | 1.38          |
| (1,382) | 1:11:C:LYS:HD3  | 1:14:C:ASP:HA   | 7        | 1.37          |
| (1,382) | 1:11:C:LYS:HD3  | 1:14:C:ASP:HA   | 10       | 1.36          |
| (4,93)  | 1:30:C:VAL:HG23 | 1:31:C:TRP:HB3  | 9        | 1.35          |
| (3,91)  | 1:30:C:VAL:HG23 | 1:31:C:TRP:HB3  | 9        | 1.35          |
| (1,590) | 1:6:C:LEU:HD13  | 1:30:C:VAL:HG13 | 4        | 1.34          |
| (1,503) | 1:17:C:ALA:HB1  | 1:16:C:CYS:HB2  | 4        | 1.34          |
| (1,382) | 1:11:C:LYS:HD3  | 1:14:C:ASP:HA   | 2        | 1.34          |
| (4,93)  | 1:30:C:VAL:HG21 | 1:31:C:TRP:HB3  | 1        | 1.32          |
| (3,91)  | 1:30:C:VAL:HG21 | 1:31:C:TRP:HB3  | 1        | 1.32          |
| (1,508) | 1:6:C:LEU:HD11  | 1:6:C:LEU:HA    | 4        | 1.32          |
| (1,382) | 1:11:C:LYS:HD3  | 1:14:C:ASP:HA   | 8        | 1.3           |
| (1,301) | 1:3:C:ARG:H     | 1:15:C:CYS:HB3  | 8        | 1.3           |
| (1,155) | 1:31:C:TRP:HH2  | 1:18:C:HIS:HB3  | 2        | 1.29          |
| (1,534) | 1:11:C:LYS:HD3  | 1:15:C:CYS:HB2  | 6        | 1.25          |
| (1,454) | 1:3:C:ARG:HG3   | 1:1:C:ALA:HA    | 7        | 1.25          |
| (1,171) | 1:33:C:TRP:HZ3  | 1:18:C:HIS:HB2  | 5        | 1.25          |
| (1,155) | 1:31:C:TRP:HH2  | 1:18:C:HIS:HB3  | 6        | 1.25          |
| (3,91)  | 1:30:C:VAL:HG21 | 1:31:C:TRP:HB3  | 6        | 1.24          |
| (1,454) | 1:3:C:ARG:HG3   | 1:1:C:ALA:HA    | 5        | 1.24          |
| (4,93)  | 1:30:C:VAL:HG21 | 1:31:C:TRP:HB3  | 6        | 1.23          |
| (1,301) | 1:3:C:ARG:H     | 1:15:C:CYS:HB3  | 1        | 1.23          |
| (1,301) | 1:3:C:ARG:H     | 1:15:C:CYS:HB3  | 9        | 1.23          |
| (1,155) | 1:31:C:TRP:HH2  | 1:18:C:HIS:HB3  | 3        | 1.22          |
| (1,513) | 1:19:C:LEU:HB3  | 1:14:C:ASP:HB3  | 7        | 1.21          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,382) | 1:11:C:LYS:HD3  | 1:14:C:ASP:HA  | 3        | 1.21          |
| (4,93)  | 1:30:C:VAL:HG21 | 1:31:C:TRP:HB3 | 8        | 1.2           |
| (3,91)  | 1:30:C:VAL:HG21 | 1:31:C:TRP:HB3 | 8        | 1.2           |
| (1,513) | 1:19:C:LEU:HB3  | 1:14:C:ASP:HB3 | 1        | 1.19          |
| (1,513) | 1:19:C:LEU:HB3  | 1:14:C:ASP:HB3 | 3        | 1.19          |
| (1,513) | 1:19:C:LEU:HB3  | 1:14:C:ASP:HB3 | 8        | 1.19          |
| (1,513) | 1:19:C:LEU:HB3  | 1:14:C:ASP:HB3 | 10       | 1.19          |
| (1,513) | 1:19:C:LEU:HB3  | 1:14:C:ASP:HB3 | 4        | 1.18          |
| (3,91)  | 1:30:C:VAL:HG21 | 1:31:C:TRP:HB3 | 4        | 1.17          |
| (1,524) | 1:19:C:LEU:HD21 | 1:5:C:TRP:HB3  | 5        | 1.17          |
| (1,513) | 1:19:C:LEU:HB3  | 1:14:C:ASP:HB3 | 2        | 1.17          |
| (4,93)  | 1:30:C:VAL:HG21 | 1:31:C:TRP:HB3 | 4        | 1.16          |
| (1,301) | 1:3:C:ARG:H     | 1:15:C:CYS:HB3 | 4        | 1.16          |
| (1,155) | 1:31:C:TRP:HH2  | 1:18:C:HIS:HB3 | 4        | 1.16          |
| (1,155) | 1:31:C:TRP:HH2  | 1:18:C:HIS:HB3 | 7        | 1.16          |
| (3,91)  | 1:30:C:VAL:HG22 | 1:31:C:TRP:HB3 | 10       | 1.15          |
| (1,524) | 1:19:C:LEU:HD21 | 1:5:C:TRP:HB3  | 3        | 1.15          |
| (1,513) | 1:19:C:LEU:HB3  | 1:14:C:ASP:HB3 | 5        | 1.15          |
| (1,311) | 1:10:C:SER:H    | 1:15:C:CYS:HB2 | 3        | 1.15          |
| (4,93)  | 1:30:C:VAL:HG22 | 1:31:C:TRP:HB3 | 10       | 1.14          |
| (4,30)  | 1:27:C:TYR:HE2  | 1:24:C:LYS:HB2 | 6        | 1.14          |
| (3,28)  | 1:27:C:TYR:HE2  | 1:24:C:LYS:HB2 | 6        | 1.14          |
| (1,524) | 1:19:C:LEU:HD22 | 1:5:C:TRP:HB3  | 10       | 1.14          |
| (1,155) | 1:31:C:TRP:HH2  | 1:18:C:HIS:HB3 | 9        | 1.14          |
| (3,91)  | 1:30:C:VAL:HG22 | 1:31:C:TRP:HB3 | 3        | 1.13          |
| (1,503) | 1:17:C:ALA:HB1  | 1:16:C:CYS:HB2 | 5        | 1.13          |
| (1,415) | 1:12:C:ASP:HB2  | 1:20:C:GLU:HA  | 8        | 1.13          |
| (4,93)  | 1:30:C:VAL:HG22 | 1:31:C:TRP:HB3 | 3        | 1.12          |
| (4,53)  | 1:21:C:CYS:HB3  | 1:29:C:CYS:HA  | 6        | 1.12          |
| (4,53)  | 1:21:C:CYS:HB3  | 1:29:C:CYS:HA  | 10       | 1.12          |
| (3,51)  | 1:21:C:CYS:HB3  | 1:29:C:CYS:HA  | 6        | 1.12          |
| (3,51)  | 1:21:C:CYS:HB3  | 1:29:C:CYS:HA  | 10       | 1.12          |
| (4,67)  | 1:35:C:VAL:HG12 | 1:34:C:THR:HB  | 9        | 1.11          |
| (3,65)  | 1:35:C:VAL:HG12 | 1:34:C:THR:HB  | 9        | 1.11          |
| (1,524) | 1:19:C:LEU:HD21 | 1:5:C:TRP:HB3  | 6        | 1.11          |
| (1,524) | 1:19:C:LEU:HD23 | 1:5:C:TRP:HB3  | 7        | 1.11          |
| (1,301) | 1:3:C:ARG:H     | 1:15:C:CYS:HB3 | 3        | 1.11          |
| (1,524) | 1:19:C:LEU:HD23 | 1:5:C:TRP:HB3  | 8        | 1.1           |
| (3,91)  | 1:30:C:VAL:HG23 | 1:31:C:TRP:HB3 | 5        | 1.09          |
| (1,524) | 1:19:C:LEU:HD23 | 1:5:C:TRP:HB3  | 2        | 1.09          |
| (1,524) | 1:19:C:LEU:HD21 | 1:5:C:TRP:HB3  | 4        | 1.09          |
| (1,301) | 1:3:C:ARG:H     | 1:15:C:CYS:HB3 | 6        | 1.09          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,200) | 1:15:C:CYS:H    | 1:15:C:CYS:HB2  | 6        | 1.09          |
| (1,175) | 1:17:C:ALA:H    | 1:16:C:CYS:HB2  | 7        | 1.09          |
| (1,155) | 1:31:C:TRP:HH2  | 1:18:C:HIS:HB3  | 10       | 1.09          |
| (4,93)  | 1:30:C:VAL:HG23 | 1:31:C:TRP:HB3  | 5        | 1.08          |
| (1,200) | 1:15:C:CYS:H    | 1:15:C:CYS:HB2  | 7        | 1.08          |
| (1,175) | 1:17:C:ALA:H    | 1:16:C:CYS:HB2  | 2        | 1.08          |
| (1,200) | 1:15:C:CYS:H    | 1:15:C:CYS:HB2  | 1        | 1.07          |
| (1,200) | 1:15:C:CYS:H    | 1:15:C:CYS:HB2  | 2        | 1.07          |
| (1,200) | 1:15:C:CYS:H    | 1:15:C:CYS:HB2  | 4        | 1.07          |
| (1,200) | 1:15:C:CYS:H    | 1:15:C:CYS:HB2  | 10       | 1.07          |
| (1,175) | 1:17:C:ALA:H    | 1:16:C:CYS:HB2  | 3        | 1.07          |
| (1,155) | 1:31:C:TRP:HH2  | 1:18:C:HIS:HB3  | 8        | 1.07          |
| (3,91)  | 1:30:C:VAL:HG21 | 1:31:C:TRP:HB3  | 2        | 1.06          |
| (1,311) | 1:10:C:SER:H    | 1:15:C:CYS:HB2  | 5        | 1.06          |
| (1,200) | 1:15:C:CYS:H    | 1:15:C:CYS:HB2  | 8        | 1.06          |
| (4,93)  | 1:30:C:VAL:HG21 | 1:31:C:TRP:HB3  | 2        | 1.05          |
| (3,65)  | 1:35:C:VAL:HG11 | 1:34:C:THR:HB   | 6        | 1.05          |
| (1,415) | 1:12:C:ASP:HB2  | 1:20:C:GLU:HA   | 4        | 1.05          |
| (1,200) | 1:15:C:CYS:H    | 1:15:C:CYS:HB2  | 3        | 1.05          |
| (1,200) | 1:15:C:CYS:H    | 1:15:C:CYS:HB2  | 5        | 1.05          |
| (1,200) | 1:15:C:CYS:H    | 1:15:C:CYS:HB2  | 9        | 1.05          |
| (1,175) | 1:17:C:ALA:H    | 1:16:C:CYS:HB2  | 1        | 1.05          |
| (1,175) | 1:17:C:ALA:H    | 1:16:C:CYS:HB2  | 8        | 1.05          |
| (4,93)  | 1:30:C:VAL:HG22 | 1:31:C:TRP:HB3  | 7        | 1.04          |
| (4,67)  | 1:35:C:VAL:HG11 | 1:34:C:THR:HB   | 6        | 1.04          |
| (3,91)  | 1:30:C:VAL:HG22 | 1:31:C:TRP:HB3  | 7        | 1.04          |
| (1,175) | 1:17:C:ALA:H    | 1:16:C:CYS:HB2  | 9        | 1.04          |
| (3,28)  | 1:27:C:TYR:HE1  | 1:23:C:LYS:HD2  | 2        | 1.02          |
| (1,175) | 1:17:C:ALA:H    | 1:16:C:CYS:HB2  | 4        | 1.02          |
| (1,155) | 1:31:C:TRP:HH2  | 1:18:C:HIS:HB3  | 5        | 1.02          |
| (4,82)  | 1:19:C:LEU:HD12 | 1:4:C:GLU:HB2   | 1        | 1.01          |
| (4,30)  | 1:27:C:TYR:HE1  | 1:23:C:LYS:HD2  | 2        | 1.01          |
| (3,80)  | 1:19:C:LEU:HD12 | 1:4:C:GLU:HB2   | 1        | 1.01          |
| (3,28)  | 1:27:C:TYR:HE2  | 1:23:C:LYS:HD3  | 4        | 1.01          |
| (1,524) | 1:19:C:LEU:HD22 | 1:5:C:TRP:HB3   | 1        | 1.01          |
| (4,30)  | 1:27:C:TYR:HE2  | 1:23:C:LYS:HD3  | 4        | 1.0           |
| (1,311) | 1:10:C:SER:H    | 1:15:C:CYS:HB2  | 4        | 1.0           |
| (1,296) | 1:28:C:HIS:HE1  | 1:30:C:VAL:HG12 | 2        | 1.0           |
| (1,293) | 1:13:C:ALA:H    | 1:11:C:LYS:HG2  | 7        | 1.0           |
| (3,49)  | 1:31:C:TRP:HD1  | 1:19:C:LEU:HD21 | 2        | 0.99          |
| (1,296) | 1:28:C:HIS:HE1  | 1:30:C:VAL:HG12 | 6        | 0.99          |
| (4,51)  | 1:31:C:TRP:HD1  | 1:19:C:LEU:HD21 | 2        | 0.98          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (4,51)  | 1:31:C:TRP:HD1  | 1:19:C:LEU:HD22 | 3        | 0.98          |
| (3,49)  | 1:31:C:TRP:HD1  | 1:19:C:LEU:HD22 | 3        | 0.98          |
| (1,296) | 1:28:C:HIS:HE1  | 1:30:C:VAL:HG12 | 4        | 0.98          |
| (4,51)  | 1:31:C:TRP:HD1  | 1:19:C:LEU:HD22 | 4        | 0.97          |
| (3,49)  | 1:31:C:TRP:HD1  | 1:19:C:LEU:HD22 | 4        | 0.97          |
| (3,49)  | 1:31:C:TRP:HD1  | 1:19:C:LEU:HD21 | 8        | 0.97          |
| (4,51)  | 1:31:C:TRP:HD1  | 1:19:C:LEU:HD21 | 8        | 0.96          |
| (3,49)  | 1:31:C:TRP:HD1  | 1:19:C:LEU:HD21 | 9        | 0.96          |
| (1,329) | 1:12:C:ASP:H    | 1:11:C:LYS:HB3  | 1        | 0.96          |
| (1,301) | 1:3:C:ARG:H     | 1:15:C:CYS:HB3  | 10       | 0.96          |
| (1,175) | 1:17:C:ALA:H    | 1:16:C:CYS:HB2  | 10       | 0.96          |
| (4,51)  | 1:31:C:TRP:HD1  | 1:19:C:LEU:HD21 | 9        | 0.95          |
| (3,49)  | 1:31:C:TRP:HD1  | 1:19:C:LEU:HD23 | 1        | 0.95          |
| (1,454) | 1:3:C:ARG:HG3   | 1:1:C:ALA:HA    | 8        | 0.95          |
| (1,329) | 1:12:C:ASP:H    | 1:11:C:LYS:HB3  | 4        | 0.95          |
| (4,53)  | 1:21:C:CYS:HB3  | 1:14:C:ASP:HA   | 4        | 0.94          |
| (4,51)  | 1:31:C:TRP:HD1  | 1:19:C:LEU:HD23 | 1        | 0.94          |
| (3,51)  | 1:21:C:CYS:HB3  | 1:14:C:ASP:HA   | 4        | 0.94          |
| (1,524) | 1:19:C:LEU:HD23 | 1:5:C:TRP:HB3   | 9        | 0.94          |
| (1,296) | 1:28:C:HIS:HE1  | 1:30:C:VAL:HG13 | 1        | 0.94          |
| (4,51)  | 1:31:C:TRP:HD1  | 1:19:C:LEU:HD21 | 7        | 0.93          |
| (3,49)  | 1:31:C:TRP:HD1  | 1:19:C:LEU:HD21 | 7        | 0.93          |
| (1,540) | 1:3:C:ARG:HG3   | 1:11:C:LYS:HE3  | 1        | 0.93          |
| (3,51)  | 1:21:C:CYS:HB3  | 1:14:C:ASP:HA   | 2        | 0.92          |
| (1,329) | 1:12:C:ASP:H    | 1:11:C:LYS:HB3  | 7        | 0.92          |
| (1,311) | 1:10:C:SER:H    | 1:15:C:CYS:HB2  | 8        | 0.92          |
| (4,53)  | 1:21:C:CYS:HB3  | 1:14:C:ASP:HA   | 2        | 0.91          |
| (1,296) | 1:28:C:HIS:HE1  | 1:30:C:VAL:HG13 | 7        | 0.91          |
| (4,82)  | 1:19:C:LEU:HD12 | 1:4:C:GLU:HB2   | 9        | 0.9           |
| (3,80)  | 1:19:C:LEU:HD12 | 1:4:C:GLU:HB2   | 9        | 0.9           |
| (1,296) | 1:28:C:HIS:HE1  | 1:30:C:VAL:HG11 | 10       | 0.9           |
| (1,224) | 1:31:C:TRP:HD1  | 1:31:C:TRP:HB3  | 5        | 0.9           |
| (4,53)  | 1:21:C:CYS:HB3  | 1:14:C:ASP:HA   | 3        | 0.89          |
| (3,51)  | 1:21:C:CYS:HB3  | 1:14:C:ASP:HA   | 3        | 0.89          |
| (1,323) | 1:21:C:CYS:H    | 1:20:C:GLU:HB3  | 7        | 0.89          |
| (1,296) | 1:28:C:HIS:HE1  | 1:30:C:VAL:HG12 | 3        | 0.89          |
| (3,49)  | 1:31:C:TRP:HD1  | 1:19:C:LEU:HD22 | 6        | 0.88          |
| (3,49)  | 1:31:C:TRP:HD1  | 1:19:C:LEU:HD23 | 10       | 0.88          |
| (1,522) | 1:6:C:LEU:HD11  | 1:28:C:HIS:HB2  | 4        | 0.88          |
| (1,323) | 1:21:C:CYS:H    | 1:20:C:GLU:HB3  | 8        | 0.88          |
| (1,301) | 1:3:C:ARG:H     | 1:15:C:CYS:HB3  | 5        | 0.88          |
| (1,224) | 1:31:C:TRP:HD1  | 1:31:C:TRP:HB3  | 4        | 0.88          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,224) | 1:31:C:TRP:HD1  | 1:31:C:TRP:HB3  | 6        | 0.88          |
| (4,51)  | 1:31:C:TRP:HD1  | 1:19:C:LEU:HD22 | 6        | 0.87          |
| (4,51)  | 1:31:C:TRP:HD1  | 1:19:C:LEU:HD23 | 10       | 0.87          |
| (4,41)  | 1:7:C:GLY:H     | 1:4:C:GLU:HB2   | 1        | 0.87          |
| (3,39)  | 1:7:C:GLY:H     | 1:4:C:GLU:HB2   | 1        | 0.87          |
| (3,28)  | 1:27:C:TYR:HE1  | 1:24:C:LYS:HB2  | 8        | 0.87          |
| (1,454) | 1:3:C:ARG:HG3   | 1:1:C:ALA:HA    | 3        | 0.87          |
| (1,293) | 1:13:C:ALA:H    | 1:11:C:LYS:HG2  | 3        | 0.87          |
| (1,224) | 1:31:C:TRP:HD1  | 1:31:C:TRP:HB3  | 10       | 0.87          |
| (4,30)  | 1:27:C:TYR:HE1  | 1:24:C:LYS:HB2  | 8        | 0.86          |
| (1,491) | 1:19:C:LEU:HB2  | 1:14:C:ASP:HB3  | 1        | 0.86          |
| (1,329) | 1:12:C:ASP:H    | 1:11:C:LYS:HB3  | 8        | 0.86          |
| (1,224) | 1:31:C:TRP:HD1  | 1:31:C:TRP:HB3  | 2        | 0.86          |
| (1,224) | 1:31:C:TRP:HD1  | 1:31:C:TRP:HB3  | 7        | 0.86          |
| (1,224) | 1:31:C:TRP:HD1  | 1:31:C:TRP:HB3  | 9        | 0.86          |
| (1,593) | 1:19:C:LEU:HD21 | 1:30:C:VAL:HG21 | 2        | 0.85          |
| (1,593) | 1:19:C:LEU:HD22 | 1:30:C:VAL:HG21 | 4        | 0.85          |
| (1,540) | 1:3:C:ARG:HG3   | 1:11:C:LYS:HE3  | 6        | 0.85          |
| (1,491) | 1:19:C:LEU:HB2  | 1:14:C:ASP:HB3  | 3        | 0.85          |
| (1,323) | 1:21:C:CYS:H    | 1:20:C:GLU:HB3  | 5        | 0.85          |
| (1,293) | 1:13:C:ALA:H    | 1:11:C:LYS:HG2  | 10       | 0.85          |
| (1,224) | 1:31:C:TRP:HD1  | 1:31:C:TRP:HB3  | 1        | 0.85          |
| (1,224) | 1:31:C:TRP:HD1  | 1:31:C:TRP:HB3  | 3        | 0.85          |
| (1,224) | 1:31:C:TRP:HD1  | 1:31:C:TRP:HB3  | 8        | 0.85          |
| (3,51)  | 1:21:C:CYS:HB3  | 1:14:C:ASP:HA   | 5        | 0.84          |
| (1,491) | 1:19:C:LEU:HB2  | 1:14:C:ASP:HB3  | 4        | 0.84          |
| (1,329) | 1:12:C:ASP:H    | 1:11:C:LYS:HB3  | 2        | 0.84          |
| (1,329) | 1:12:C:ASP:H    | 1:11:C:LYS:HB3  | 9        | 0.84          |
| (1,323) | 1:21:C:CYS:H    | 1:20:C:GLU:HB3  | 1        | 0.84          |
| (1,293) | 1:13:C:ALA:H    | 1:11:C:LYS:HG2  | 2        | 0.84          |
| (1,197) | 1:5:C:TRP:HE3   | 1:5:C:TRP:HB2   | 2        | 0.84          |
| (1,197) | 1:5:C:TRP:HE3   | 1:5:C:TRP:HB2   | 6        | 0.84          |
| (4,53)  | 1:21:C:CYS:HB3  | 1:14:C:ASP:HA   | 5        | 0.83          |
| (1,491) | 1:19:C:LEU:HB2  | 1:14:C:ASP:HB3  | 5        | 0.83          |
| (1,491) | 1:19:C:LEU:HB2  | 1:14:C:ASP:HB3  | 7        | 0.83          |
| (1,329) | 1:12:C:ASP:H    | 1:11:C:LYS:HB3  | 3        | 0.83          |
| (1,329) | 1:12:C:ASP:H    | 1:11:C:LYS:HB3  | 5        | 0.83          |
| (1,329) | 1:12:C:ASP:H    | 1:11:C:LYS:HB3  | 10       | 0.83          |
| (1,293) | 1:13:C:ALA:H    | 1:11:C:LYS:HG2  | 4        | 0.83          |
| (4,88)  | 1:20:C:GLU:HB2  | 1:32:C:ASP:HB2  | 1        | 0.82          |
| (3,86)  | 1:20:C:GLU:HB2  | 1:32:C:ASP:HB2  | 1        | 0.82          |
| (1,593) | 1:19:C:LEU:HD23 | 1:30:C:VAL:HG22 | 3        | 0.82          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,506) | 1:19:C:LEU:HD21 | 1:14:C:ASP:HB3  | 9        | 0.82          |
| (1,491) | 1:19:C:LEU:HB2  | 1:14:C:ASP:HB3  | 10       | 0.82          |
| (1,197) | 1:5:C:TRP:HE3   | 1:5:C:TRP:HB2   | 1        | 0.82          |
| (1,197) | 1:5:C:TRP:HE3   | 1:5:C:TRP:HB2   | 8        | 0.82          |
| (1,197) | 1:5:C:TRP:HE3   | 1:5:C:TRP:HB2   | 9        | 0.82          |
| (4,59)  | 1:34:C:THR:HG22 | 1:33:C:TRP:HA   | 9        | 0.81          |
| (3,57)  | 1:34:C:THR:HG22 | 1:33:C:TRP:HA   | 9        | 0.81          |
| (1,593) | 1:19:C:LEU:HD22 | 1:30:C:VAL:HG21 | 8        | 0.81          |
| (1,323) | 1:21:C:CYS:H    | 1:20:C:GLU:HB3  | 9        | 0.81          |
| (1,293) | 1:13:C:ALA:H    | 1:11:C:LYS:HG2  | 1        | 0.81          |
| (1,237) | 1:5:C:TRP:H     | 1:4:C:GLU:HG2   | 1        | 0.81          |
| (1,197) | 1:5:C:TRP:HE3   | 1:5:C:TRP:HB2   | 4        | 0.81          |
| (1,197) | 1:5:C:TRP:HE3   | 1:5:C:TRP:HB2   | 5        | 0.81          |
| (1,197) | 1:5:C:TRP:HE3   | 1:5:C:TRP:HB2   | 10       | 0.81          |
| (1,195) | 1:28:C:HIS:H    | 1:22:C:ARG:HD2  | 10       | 0.81          |
| (1,593) | 1:19:C:LEU:HD22 | 1:30:C:VAL:HG22 | 7        | 0.8           |
| (1,323) | 1:21:C:CYS:H    | 1:20:C:GLU:HB3  | 6        | 0.8           |
| (1,197) | 1:5:C:TRP:HE3   | 1:5:C:TRP:HB2   | 3        | 0.8           |
| (1,197) | 1:5:C:TRP:HE3   | 1:5:C:TRP:HB2   | 7        | 0.8           |
| (1,195) | 1:28:C:HIS:H    | 1:22:C:ARG:HD2  | 9        | 0.8           |
| (4,81)  | 1:19:C:LEU:HD13 | 1:16:C:CYS:HB3  | 6        | 0.79          |
| (3,79)  | 1:19:C:LEU:HD13 | 1:16:C:CYS:HB3  | 6        | 0.79          |
| (3,28)  | 1:27:C:TYR:HE2  | 1:24:C:LYS:HB2  | 5        | 0.79          |
| (1,491) | 1:19:C:LEU:HB2  | 1:14:C:ASP:HB3  | 2        | 0.79          |
| (1,491) | 1:19:C:LEU:HB2  | 1:14:C:ASP:HB3  | 8        | 0.79          |
| (1,201) | 1:22:C:ARG:H    | 1:22:C:ARG:HD2  | 3        | 0.79          |
| (1,195) | 1:28:C:HIS:H    | 1:22:C:ARG:HD2  | 3        | 0.79          |
| (4,88)  | 1:20:C:GLU:HB2  | 1:32:C:ASP:HB2  | 10       | 0.78          |
| (4,30)  | 1:27:C:TYR:HE2  | 1:24:C:LYS:HB2  | 5        | 0.78          |
| (3,86)  | 1:20:C:GLU:HB2  | 1:32:C:ASP:HB2  | 10       | 0.78          |
| (1,593) | 1:19:C:LEU:HD21 | 1:30:C:VAL:HG23 | 9        | 0.78          |
| (1,306) | 1:16:C:CYS:H    | 1:16:C:CYS:HB3  | 6        | 0.78          |
| (1,195) | 1:28:C:HIS:H    | 1:22:C:ARG:HD2  | 6        | 0.78          |
| (4,30)  | 1:27:C:TYR:HE2  | 1:23:C:LYS:HD3  | 3        | 0.77          |
| (3,28)  | 1:27:C:TYR:HE1  | 1:23:C:LYS:HD3  | 1        | 0.77          |
| (3,28)  | 1:27:C:TYR:HE2  | 1:23:C:LYS:HD3  | 3        | 0.77          |
| (1,593) | 1:19:C:LEU:HD23 | 1:30:C:VAL:HG21 | 1        | 0.77          |
| (1,593) | 1:19:C:LEU:HD22 | 1:30:C:VAL:HG23 | 5        | 0.77          |
| (1,274) | 1:11:C:LYS:H    | 1:11:C:LYS:HG3  | 5        | 0.77          |
| (1,199) | 1:33:C:TRP:H    | 1:32:C:ASP:HB2  | 10       | 0.77          |
| (1,195) | 1:28:C:HIS:H    | 1:22:C:ARG:HD2  | 1        | 0.77          |
| (4,30)  | 1:27:C:TYR:HE1  | 1:23:C:LYS:HD3  | 1        | 0.76          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,593) | 1:19:C:LEU:HD23 | 1:30:C:VAL:HG22 | 10       | 0.76          |
| (1,311) | 1:10:C:SER:H    | 1:15:C:CYS:HB2  | 2        | 0.76          |
| (1,293) | 1:13:C:ALA:H    | 1:11:C:LYS:HG2  | 8        | 0.76          |
| (1,234) | 1:31:C:TRP:HE3  | 1:31:C:TRP:HB2  | 8        | 0.76          |
| (1,195) | 1:28:C:HIS:H    | 1:22:C:ARG:HD2  | 4        | 0.76          |
| (1,175) | 1:17:C:ALA:H    | 1:16:C:CYS:HB2  | 5        | 0.76          |
| (4,88)  | 1:20:C:GLU:HB2  | 1:32:C:ASP:HB2  | 3        | 0.75          |
| (3,86)  | 1:20:C:GLU:HB2  | 1:32:C:ASP:HB2  | 3        | 0.75          |
| (1,329) | 1:12:C:ASP:H    | 1:11:C:LYS:HB3  | 6        | 0.75          |
| (1,323) | 1:21:C:CYS:H    | 1:20:C:GLU:HB3  | 3        | 0.75          |
| (1,311) | 1:10:C:SER:H    | 1:15:C:CYS:HB2  | 10       | 0.75          |
| (1,296) | 1:28:C:HIS:HE1  | 1:30:C:VAL:HG13 | 9        | 0.75          |
| (1,234) | 1:31:C:TRP:HE3  | 1:31:C:TRP:HB2  | 1        | 0.75          |
| (1,234) | 1:31:C:TRP:HE3  | 1:31:C:TRP:HB2  | 2        | 0.75          |
| (1,234) | 1:31:C:TRP:HE3  | 1:31:C:TRP:HB2  | 4        | 0.75          |
| (1,234) | 1:31:C:TRP:HE3  | 1:31:C:TRP:HB2  | 7        | 0.75          |
| (1,234) | 1:31:C:TRP:HE3  | 1:31:C:TRP:HB2  | 9        | 0.75          |
| (1,234) | 1:31:C:TRP:HE3  | 1:31:C:TRP:HB2  | 10       | 0.75          |
| (1,201) | 1:22:C:ARG:H    | 1:22:C:ARG:HD2  | 2        | 0.75          |
| (1,195) | 1:28:C:HIS:H    | 1:22:C:ARG:HD2  | 2        | 0.75          |
| (1,323) | 1:21:C:CYS:H    | 1:20:C:GLU:HB3  | 2        | 0.74          |
| (1,304) | 1:12:C:ASP:H    | 1:12:C:ASP:HB3  | 8        | 0.74          |
| (1,234) | 1:31:C:TRP:HE3  | 1:31:C:TRP:HB2  | 3        | 0.74          |
| (1,195) | 1:28:C:HIS:H    | 1:22:C:ARG:HD2  | 5        | 0.74          |
| (1,506) | 1:19:C:LEU:HD22 | 1:14:C:ASP:HB3  | 6        | 0.73          |
| (1,323) | 1:21:C:CYS:H    | 1:20:C:GLU:HB3  | 10       | 0.73          |
| (1,293) | 1:13:C:ALA:H    | 1:11:C:LYS:HG2  | 6        | 0.73          |
| (1,291) | 1:2:C:CYS:H     | 1:1:C:ALA:HB3   | 1        | 0.73          |
| (1,234) | 1:31:C:TRP:HE3  | 1:31:C:TRP:HB2  | 5        | 0.73          |
| (1,234) | 1:31:C:TRP:HE3  | 1:31:C:TRP:HB2  | 6        | 0.73          |
| (1,195) | 1:28:C:HIS:H    | 1:22:C:ARG:HD2  | 7        | 0.73          |
| (1,115) | 1:32:C:ASP:H    | 1:18:C:HIS:HB2  | 9        | 0.73          |
| (4,59)  | 1:34:C:THR:HG22 | 1:33:C:TRP:HA   | 2        | 0.72          |
| (3,57)  | 1:34:C:THR:HG22 | 1:33:C:TRP:HA   | 2        | 0.72          |
| (3,57)  | 1:34:C:THR:HG23 | 1:33:C:TRP:HA   | 6        | 0.72          |
| (1,503) | 1:17:C:ALA:HB2  | 1:16:C:CYS:HB2  | 6        | 0.72          |
| (1,323) | 1:21:C:CYS:H    | 1:20:C:GLU:HB3  | 4        | 0.72          |
| (1,296) | 1:28:C:HIS:HE1  | 1:30:C:VAL:HG11 | 5        | 0.72          |
| (1,218) | 1:31:C:TRP:HH2  | 1:5:C:TRP:HB3   | 5        | 0.72          |
| (1,195) | 1:28:C:HIS:H    | 1:22:C:ARG:HD2  | 8        | 0.72          |
| (1,153) | 1:18:C:HIS:HD2  | 1:18:C:HIS:HB3  | 3        | 0.72          |
| (1,153) | 1:18:C:HIS:HD2  | 1:18:C:HIS:HB3  | 6        | 0.72          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,153) | 1:18:C:HIS:HD2  | 1:18:C:HIS:HB3  | 7        | 0.72          |
| (4,59)  | 1:34:C:THR:HG23 | 1:33:C:TRP:HA   | 6        | 0.71          |
| (4,51)  | 1:31:C:TRP:HD1  | 1:19:C:LEU:HD22 | 5        | 0.71          |
| (3,93)  | 1:19:C:LEU:HB3  | 1:20:C:GLU:HG3  | 6        | 0.71          |
| (3,51)  | 1:21:C:CYS:HB3  | 1:14:C:ASP:HA   | 1        | 0.71          |
| (3,49)  | 1:31:C:TRP:HD1  | 1:19:C:LEU:HD22 | 5        | 0.71          |
| (1,241) | 1:13:C:ALA:H    | 1:11:C:LYS:HB3  | 2        | 0.71          |
| (1,218) | 1:31:C:TRP:HH2  | 1:5:C:TRP:HB3   | 10       | 0.71          |
| (1,201) | 1:22:C:ARG:H    | 1:22:C:ARG:HD2  | 10       | 0.71          |
| (1,199) | 1:33:C:TRP:H    | 1:32:C:ASP:HB2  | 6        | 0.71          |
| (1,153) | 1:18:C:HIS:HD2  | 1:18:C:HIS:HB3  | 4        | 0.71          |
| (4,95)  | 1:19:C:LEU:HB3  | 1:20:C:GLU:HG3  | 6        | 0.7           |
| (4,53)  | 1:21:C:CYS:HB3  | 1:14:C:ASP:HA   | 1        | 0.7           |
| (1,237) | 1:5:C:TRP:H     | 1:4:C:GLU:HG2   | 9        | 0.7           |
| (1,201) | 1:22:C:ARG:H    | 1:22:C:ARG:HD2  | 7        | 0.7           |
| (1,199) | 1:33:C:TRP:H    | 1:32:C:ASP:HB2  | 3        | 0.7           |
| (4,92)  | 1:19:C:LEU:HG   | 1:16:C:CYS:HB3  | 6        | 0.69          |
| (3,90)  | 1:19:C:LEU:HG   | 1:16:C:CYS:HB3  | 6        | 0.69          |
| (3,51)  | 1:21:C:CYS:HB3  | 1:14:C:ASP:HA   | 7        | 0.69          |
| (1,153) | 1:18:C:HIS:HD2  | 1:18:C:HIS:HB3  | 1        | 0.69          |
| (1,153) | 1:18:C:HIS:HD2  | 1:18:C:HIS:HB3  | 5        | 0.69          |
| (1,153) | 1:18:C:HIS:HD2  | 1:18:C:HIS:HB3  | 8        | 0.69          |
| (1,153) | 1:18:C:HIS:HD2  | 1:18:C:HIS:HB3  | 9        | 0.69          |
| (1,153) | 1:18:C:HIS:HD2  | 1:18:C:HIS:HB3  | 10       | 0.69          |
| (4,53)  | 1:21:C:CYS:HB3  | 1:14:C:ASP:HA   | 7        | 0.68          |
| (4,48)  | 1:16:C:CYS:H    | 1:19:C:LEU:HD23 | 3        | 0.68          |
| (3,65)  | 1:35:C:VAL:HG13 | 1:34:C:THR:HB   | 4        | 0.68          |
| (3,46)  | 1:16:C:CYS:H    | 1:19:C:LEU:HD23 | 3        | 0.68          |
| (1,567) | 1:25:C:ALA:HB3  | 1:26:C:PRO:HB2  | 3        | 0.68          |
| (1,567) | 1:25:C:ALA:HB3  | 1:26:C:PRO:HB2  | 9        | 0.68          |
| (1,304) | 1:12:C:ASP:H    | 1:12:C:ASP:HB3  | 4        | 0.68          |
| (1,291) | 1:2:C:CYS:H     | 1:1:C:ALA:HB1   | 6        | 0.68          |
| (1,115) | 1:32:C:ASP:H    | 1:18:C:HIS:HB2  | 6        | 0.68          |
| (4,95)  | 1:19:C:LEU:HB3  | 1:20:C:GLU:HG3  | 3        | 0.67          |
| (4,88)  | 1:20:C:GLU:HB2  | 1:32:C:ASP:HB2  | 2        | 0.67          |
| (4,88)  | 1:20:C:GLU:HB2  | 1:32:C:ASP:HB2  | 7        | 0.67          |
| (4,67)  | 1:35:C:VAL:HG13 | 1:34:C:THR:HB   | 4        | 0.67          |
| (4,67)  | 1:35:C:VAL:HG13 | 1:34:C:THR:HB   | 8        | 0.67          |
| (4,53)  | 1:21:C:CYS:HB3  | 1:14:C:ASP:HA   | 8        | 0.67          |
| (4,48)  | 1:16:C:CYS:H    | 1:19:C:LEU:HD22 | 7        | 0.67          |
| (3,93)  | 1:19:C:LEU:HB3  | 1:20:C:GLU:HG3  | 3        | 0.67          |
| (3,86)  | 1:20:C:GLU:HB2  | 1:32:C:ASP:HB2  | 2        | 0.67          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (3,86)  | 1:20:C:GLU:HB2  | 1:32:C:ASP:HB2  | 7        | 0.67          |
| (3,84)  | 1:24:C:LYS:HD3  | 1:23:C:LYS:HE2  | 2        | 0.67          |
| (3,84)  | 1:24:C:LYS:HD2  | 1:23:C:LYS:HE2  | 3        | 0.67          |
| (3,65)  | 1:35:C:VAL:HG13 | 1:34:C:THR:HB   | 8        | 0.67          |
| (3,51)  | 1:21:C:CYS:HB3  | 1:14:C:ASP:HA   | 8        | 0.67          |
| (3,46)  | 1:16:C:CYS:H    | 1:19:C:LEU:HD22 | 7        | 0.67          |
| (1,308) | 1:32:C:ASP:H    | 1:31:C:TRP:HB2  | 8        | 0.67          |
| (1,293) | 1:13:C:ALA:H    | 1:11:C:LYS:HG2  | 9        | 0.67          |
| (1,285) | 1:23:C:LYS:H    | 1:23:C:LYS:HB2  | 6        | 0.67          |
| (1,241) | 1:13:C:ALA:H    | 1:11:C:LYS:HB3  | 7        | 0.67          |
| (1,199) | 1:33:C:TRP:H    | 1:32:C:ASP:HB2  | 1        | 0.67          |
| (1,153) | 1:18:C:HIS:HD2  | 1:18:C:HIS:HB3  | 2        | 0.67          |
| (4,86)  | 1:24:C:LYS:HD3  | 1:23:C:LYS:HE2  | 2        | 0.66          |
| (4,86)  | 1:24:C:LYS:HD2  | 1:23:C:LYS:HE2  | 3        | 0.66          |
| (3,65)  | 1:35:C:VAL:HG12 | 1:34:C:THR:HB   | 10       | 0.66          |
| (3,46)  | 1:29:C:CYS:H    | 1:19:C:LEU:HD22 | 8        | 0.66          |
| (1,285) | 1:23:C:LYS:H    | 1:23:C:LYS:HB2  | 10       | 0.66          |
| (1,241) | 1:13:C:ALA:H    | 1:11:C:LYS:HB3  | 1        | 0.66          |
| (4,88)  | 1:20:C:GLU:HB2  | 1:32:C:ASP:HB2  | 5        | 0.65          |
| (4,67)  | 1:35:C:VAL:HG12 | 1:34:C:THR:HB   | 10       | 0.65          |
| (4,48)  | 1:29:C:CYS:H    | 1:19:C:LEU:HD22 | 8        | 0.65          |
| (3,86)  | 1:20:C:GLU:HB2  | 1:32:C:ASP:HB2  | 5        | 0.65          |
| (1,567) | 1:25:C:ALA:HB1  | 1:26:C:PRO:HB2  | 2        | 0.65          |
| (1,567) | 1:25:C:ALA:HB1  | 1:26:C:PRO:HB2  | 10       | 0.65          |
| (1,308) | 1:32:C:ASP:H    | 1:31:C:TRP:HB2  | 3        | 0.65          |
| (1,201) | 1:22:C:ARG:H    | 1:22:C:ARG:HD2  | 6        | 0.65          |
| (4,67)  | 1:35:C:VAL:HG11 | 1:34:C:THR:HB   | 2        | 0.64          |
| (4,67)  | 1:35:C:VAL:HG12 | 1:34:C:THR:HB   | 7        | 0.64          |
| (3,65)  | 1:35:C:VAL:HG11 | 1:34:C:THR:HB   | 2        | 0.64          |
| (3,65)  | 1:35:C:VAL:HG12 | 1:34:C:THR:HB   | 7        | 0.64          |
| (3,39)  | 1:7:C:GLY:H     | 1:4:C:GLU:HB2   | 9        | 0.64          |
| (1,291) | 1:2:C:CYS:H     | 1:1:C:ALA:HB2   | 2        | 0.64          |
| (1,201) | 1:22:C:ARG:H    | 1:22:C:ARG:HD2  | 1        | 0.64          |
| (4,48)  | 1:29:C:CYS:H    | 1:19:C:LEU:HD23 | 4        | 0.63          |
| (4,41)  | 1:7:C:GLY:H     | 1:4:C:GLU:HB2   | 9        | 0.63          |
| (3,48)  | 1:28:C:HIS:HE1  | 1:6:C:LEU:HD11  | 4        | 0.63          |
| (3,46)  | 1:29:C:CYS:H    | 1:19:C:LEU:HD22 | 2        | 0.63          |
| (3,46)  | 1:29:C:CYS:H    | 1:19:C:LEU:HD23 | 4        | 0.63          |
| (1,241) | 1:13:C:ALA:H    | 1:11:C:LYS:HB3  | 10       | 0.63          |
| (1,227) | 1:31:C:TRP:H    | 1:31:C:TRP:HB3  | 1        | 0.63          |
| (1,199) | 1:33:C:TRP:H    | 1:32:C:ASP:HB2  | 5        | 0.63          |
| (1,115) | 1:32:C:ASP:H    | 1:18:C:HIS:HB2  | 5        | 0.63          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,115) | 1:32:C:ASP:H   | 1:18:C:HIS:HB2  | 7        | 0.63          |
| (4,50)  | 1:28:C:HIS:HE1 | 1:6:C:LEU:HD11  | 4        | 0.62          |
| (4,48)  | 1:29:C:CYS:H   | 1:19:C:LEU:HD22 | 2        | 0.62          |
| (3,46)  | 1:16:C:CYS:H   | 1:19:C:LEU:HD23 | 5        | 0.62          |
| (1,521) | 1:6:C:LEU:HD11 | 1:29:C:CYS:HB3  | 3        | 0.62          |
| (1,521) | 1:6:C:LEU:HD11 | 1:29:C:CYS:HB3  | 7        | 0.62          |
| (1,308) | 1:32:C:ASP:H   | 1:31:C:TRP:HB2  | 4        | 0.62          |
| (1,241) | 1:13:C:ALA:H   | 1:11:C:LYS:HB3  | 8        | 0.62          |
| (1,227) | 1:31:C:TRP:H   | 1:31:C:TRP:HB3  | 6        | 0.62          |
| (1,227) | 1:31:C:TRP:H   | 1:31:C:TRP:HB3  | 7        | 0.62          |
| (1,201) | 1:22:C:ARG:H   | 1:22:C:ARG:HD2  | 4        | 0.62          |
| (1,199) | 1:33:C:TRP:H   | 1:32:C:ASP:HB2  | 4        | 0.62          |
| (4,48)  | 1:16:C:CYS:H   | 1:19:C:LEU:HD23 | 5        | 0.61          |
| (1,567) | 1:25:C:ALA:HB2 | 1:26:C:PRO:HB2  | 6        | 0.61          |
| (1,308) | 1:32:C:ASP:H   | 1:31:C:TRP:HB2  | 2        | 0.61          |
| (1,296) | 1:28:C:HIS:HE1 | 1:30:C:VAL:HG12 | 8        | 0.61          |
| (1,285) | 1:23:C:LYS:H   | 1:23:C:LYS:HB2  | 7        | 0.61          |
| (1,227) | 1:31:C:TRP:H   | 1:31:C:TRP:HB3  | 2        | 0.61          |
| (1,227) | 1:31:C:TRP:H   | 1:31:C:TRP:HB3  | 4        | 0.61          |
| (1,227) | 1:31:C:TRP:H   | 1:31:C:TRP:HB3  | 5        | 0.61          |
| (1,227) | 1:31:C:TRP:H   | 1:31:C:TRP:HB3  | 8        | 0.61          |
| (1,227) | 1:31:C:TRP:H   | 1:31:C:TRP:HB3  | 9        | 0.61          |
| (1,227) | 1:31:C:TRP:H   | 1:31:C:TRP:HB3  | 10       | 0.61          |
| (1,199) | 1:33:C:TRP:H   | 1:32:C:ASP:HB2  | 2        | 0.61          |
| (1,115) | 1:32:C:ASP:H   | 1:18:C:HIS:HB2  | 10       | 0.61          |
| (4,30)  | 1:27:C:TYR:HE1 | 1:24:C:LYS:HB2  | 10       | 0.6           |
| (4,8)   | 1:2:C:CYS:H    | 1:3:C:ARG:HD3   | 10       | 0.6           |
| (3,28)  | 1:27:C:TYR:HE1 | 1:24:C:LYS:HB2  | 10       | 0.6           |
| (3,8)   | 1:2:C:CYS:H    | 1:3:C:ARG:HD3   | 10       | 0.6           |
| (1,567) | 1:25:C:ALA:HB1 | 1:26:C:PRO:HB2  | 5        | 0.6           |
| (1,521) | 1:6:C:LEU:HD11 | 1:29:C:CYS:HB3  | 6        | 0.6           |
| (1,285) | 1:23:C:LYS:H   | 1:23:C:LYS:HB2  | 2        | 0.6           |
| (1,227) | 1:31:C:TRP:H   | 1:31:C:TRP:HB3  | 3        | 0.6           |
| (1,156) | 1:31:C:TRP:HZ3 | 1:18:C:HIS:HB3  | 1        | 0.6           |
| (1,285) | 1:23:C:LYS:H   | 1:23:C:LYS:HB2  | 5        | 0.59          |
| (1,241) | 1:13:C:ALA:H   | 1:11:C:LYS:HB3  | 6        | 0.59          |
| (1,201) | 1:22:C:ARG:H   | 1:22:C:ARG:HD2  | 5        | 0.59          |
| (1,201) | 1:22:C:ARG:H   | 1:22:C:ARG:HD2  | 8        | 0.59          |
| (4,31)  | 1:31:C:TRP:H   | 1:30:C:VAL:HG13 | 5        | 0.58          |
| (3,29)  | 1:31:C:TRP:H   | 1:30:C:VAL:HG13 | 5        | 0.58          |
| (1,297) | 1:18:C:HIS:HE1 | 1:17:C:ALA:HB3  | 5        | 0.58          |
| (1,291) | 1:2:C:CYS:H    | 1:1:C:ALA:HB1   | 10       | 0.58          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (4,43)  | 1:20:C:GLU:H    | 1:30:C:VAL:HB   | 2        | 0.57          |
| (3,41)  | 1:20:C:GLU:H    | 1:30:C:VAL:HB   | 2        | 0.57          |
| (1,593) | 1:19:C:LEU:HD22 | 1:30:C:VAL:HG21 | 6        | 0.57          |
| (1,241) | 1:13:C:ALA:H    | 1:11:C:LYS:HB3  | 3        | 0.57          |
| (1,241) | 1:13:C:ALA:H    | 1:11:C:LYS:HB3  | 4        | 0.57          |
| (1,199) | 1:33:C:TRP:H    | 1:32:C:ASP:HB2  | 7        | 0.57          |
| (1,191) | 1:27:C:TYR:HE1  | 1:27:C:TYR:HB2  | 4        | 0.57          |
| (1,115) | 1:32:C:ASP:H    | 1:18:C:HIS:HB2  | 4        | 0.57          |
| (4,65)  | 1:23:C:LYS:HD3  | 1:23:C:LYS:HA   | 10       | 0.56          |
| (3,86)  | 1:20:C:GLU:HB2  | 1:32:C:ASP:HB2  | 4        | 0.56          |
| (3,78)  | 1:30:C:VAL:HG23 | 1:22:C:ARG:HD3  | 7        | 0.56          |
| (3,63)  | 1:23:C:LYS:HD3  | 1:23:C:LYS:HA   | 10       | 0.56          |
| (1,218) | 1:31:C:TRP:HH2  | 1:5:C:TRP:HB3   | 8        | 0.56          |
| (1,199) | 1:33:C:TRP:H    | 1:32:C:ASP:HB2  | 8        | 0.56          |
| (1,115) | 1:32:C:ASP:H    | 1:18:C:HIS:HB2  | 2        | 0.56          |
| (4,88)  | 1:20:C:GLU:HB2  | 1:32:C:ASP:HB2  | 4        | 0.55          |
| (4,82)  | 1:19:C:LEU:HD13 | 1:4:C:GLU:HG2   | 7        | 0.55          |
| (4,82)  | 1:19:C:LEU:HD11 | 1:4:C:GLU:HG2   | 8        | 0.55          |
| (4,80)  | 1:30:C:VAL:HG23 | 1:22:C:ARG:HD3  | 7        | 0.55          |
| (4,31)  | 1:31:C:TRP:H    | 1:30:C:VAL:HG11 | 1        | 0.55          |
| (4,31)  | 1:31:C:TRP:H    | 1:30:C:VAL:HG12 | 6        | 0.55          |
| (3,80)  | 1:19:C:LEU:HD13 | 1:4:C:GLU:HG2   | 7        | 0.55          |
| (3,80)  | 1:19:C:LEU:HD11 | 1:4:C:GLU:HG2   | 8        | 0.55          |
| (3,29)  | 1:31:C:TRP:H    | 1:30:C:VAL:HG11 | 1        | 0.55          |
| (3,29)  | 1:31:C:TRP:H    | 1:30:C:VAL:HG12 | 6        | 0.55          |
| (1,521) | 1:6:C:LEU:HD13  | 1:29:C:CYS:HB3  | 2        | 0.55          |
| (1,521) | 1:6:C:LEU:HD13  | 1:29:C:CYS:HB3  | 10       | 0.55          |
| (1,291) | 1:2:C:CYS:H     | 1:1:C:ALA:HB1   | 5        | 0.55          |
| (1,291) | 1:2:C:CYS:H     | 1:1:C:ALA:HB3   | 9        | 0.55          |
| (4,48)  | 1:29:C:CYS:H    | 1:19:C:LEU:HD22 | 9        | 0.54          |
| (3,86)  | 1:20:C:GLU:HB2  | 1:32:C:ASP:HB2  | 6        | 0.54          |
| (3,46)  | 1:29:C:CYS:H    | 1:19:C:LEU:HD22 | 9        | 0.54          |
| (1,521) | 1:6:C:LEU:HD11  | 1:29:C:CYS:HB3  | 1        | 0.54          |
| (1,353) | 1:31:C:TRP:HE1  | 1:19:C:LEU:HD23 | 2        | 0.54          |
| (1,353) | 1:31:C:TRP:HE1  | 1:19:C:LEU:HD21 | 4        | 0.54          |
| (1,353) | 1:31:C:TRP:HE1  | 1:19:C:LEU:HD23 | 8        | 0.54          |
| (1,308) | 1:32:C:ASP:H    | 1:31:C:TRP:HB2  | 1        | 0.54          |
| (1,284) | 1:25:C:ALA:H    | 1:24:C:LYS:HB3  | 1        | 0.54          |
| (1,284) | 1:25:C:ALA:H    | 1:24:C:LYS:HB3  | 5        | 0.54          |
| (1,218) | 1:31:C:TRP:HH2  | 1:5:C:TRP:HB3   | 6        | 0.54          |
| (4,88)  | 1:20:C:GLU:HB2  | 1:32:C:ASP:HB2  | 6        | 0.53          |
| (4,59)  | 1:34:C:THR:HG21 | 1:33:C:TRP:HA   | 8        | 0.53          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (4,53)  | 1:21:C:CYS:HB3  | 1:14:C:ASP:HA   | 9        | 0.53          |
| (3,57)  | 1:34:C:THR:HG21 | 1:33:C:TRP:HA   | 8        | 0.53          |
| (3,51)  | 1:21:C:CYS:HB3  | 1:14:C:ASP:HA   | 9        | 0.53          |
| (1,353) | 1:31:C:TRP:HE1  | 1:19:C:LEU:HD22 | 1        | 0.53          |
| (1,353) | 1:31:C:TRP:HE1  | 1:19:C:LEU:HD21 | 3        | 0.53          |
| (1,353) | 1:31:C:TRP:HE1  | 1:19:C:LEU:HD23 | 7        | 0.53          |
| (1,311) | 1:10:C:SER:H    | 1:15:C:CYS:HB2  | 7        | 0.53          |
| (1,308) | 1:32:C:ASP:H    | 1:31:C:TRP:HB2  | 6        | 0.53          |
| (1,308) | 1:32:C:ASP:H    | 1:31:C:TRP:HB2  | 7        | 0.53          |
| (1,308) | 1:32:C:ASP:H    | 1:31:C:TRP:HB2  | 9        | 0.53          |
| (1,308) | 1:32:C:ASP:H    | 1:31:C:TRP:HB2  | 10       | 0.53          |
| (1,284) | 1:25:C:ALA:H    | 1:24:C:LYS:HB3  | 8        | 0.53          |
| (1,241) | 1:13:C:ALA:H    | 1:11:C:LYS:HB3  | 9        | 0.53          |
| (1,218) | 1:31:C:TRP:HH2  | 1:5:C:TRP:HB3   | 3        | 0.53          |
| (1,115) | 1:32:C:ASP:H    | 1:18:C:HIS:HB2  | 8        | 0.53          |
| (3,8)   | 1:2:C:CYS:H     | 1:3:C:ARG:HD3   | 6        | 0.52          |
| (1,300) | 1:16:C:CYS:H    | 1:15:C:CYS:HB3  | 6        | 0.52          |
| (1,256) | 1:24:C:LYS:H    | 1:24:C:LYS:HB2  | 7        | 0.52          |
| (4,82)  | 1:19:C:LEU:HD11 | 1:4:C:GLU:HG2   | 6        | 0.51          |
| (4,31)  | 1:31:C:TRP:H    | 1:30:C:VAL:HG13 | 2        | 0.51          |
| (4,8)   | 1:2:C:CYS:H     | 1:3:C:ARG:HD3   | 6        | 0.51          |
| (3,80)  | 1:19:C:LEU:HD11 | 1:4:C:GLU:HG2   | 6        | 0.51          |
| (3,39)  | 1:7:C:GLY:H     | 1:4:C:GLU:HG2   | 2        | 0.51          |
| (3,29)  | 1:31:C:TRP:H    | 1:30:C:VAL:HG13 | 2        | 0.51          |
| (1,521) | 1:6:C:LEU:HD13  | 1:29:C:CYS:HB3  | 8        | 0.51          |
| (1,353) | 1:31:C:TRP:HE1  | 1:19:C:LEU:HD23 | 9        | 0.51          |
| (1,284) | 1:25:C:ALA:H    | 1:24:C:LYS:HB3  | 7        | 0.51          |
| (4,48)  | 1:29:C:CYS:H    | 1:19:C:LEU:HD21 | 10       | 0.5           |
| (4,41)  | 1:7:C:GLY:H     | 1:4:C:GLU:HG2   | 2        | 0.5           |
| (3,63)  | 1:23:C:LYS:HD3  | 1:23:C:LYS:HA   | 7        | 0.5           |
| (3,57)  | 1:34:C:THR:HG21 | 1:33:C:TRP:HA   | 7        | 0.5           |
| (3,46)  | 1:29:C:CYS:H    | 1:19:C:LEU:HD21 | 10       | 0.5           |
| (1,567) | 1:25:C:ALA:HB1  | 1:26:C:PRO:HB2  | 1        | 0.5           |
| (1,300) | 1:16:C:CYS:H    | 1:15:C:CYS:HB3  | 5        | 0.5           |
| (1,300) | 1:16:C:CYS:H    | 1:15:C:CYS:HB3  | 10       | 0.5           |
| (1,291) | 1:2:C:CYS:H     | 1:1:C:ALA:HB3   | 4        | 0.5           |
| (1,191) | 1:27:C:TYR:HE2  | 1:27:C:TYR:HB2  | 2        | 0.5           |
| (1,191) | 1:27:C:TYR:HE1  | 1:27:C:TYR:HB2  | 10       | 0.5           |
| (4,65)  | 1:23:C:LYS:HD3  | 1:23:C:LYS:HA   | 7        | 0.49          |
| (4,59)  | 1:34:C:THR:HG21 | 1:33:C:TRP:HA   | 7        | 0.49          |
| (4,43)  | 1:20:C:GLU:H    | 1:30:C:VAL:HB   | 1        | 0.49          |
| (3,41)  | 1:20:C:GLU:H    | 1:30:C:VAL:HB   | 1        | 0.49          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,570) | 1:30:C:VAL:HG13 | 1:22:C:ARG:HB3  | 9        | 0.49          |
| (1,521) | 1:6:C:LEU:HD13  | 1:29:C:CYS:HB3  | 5        | 0.49          |
| (1,521) | 1:6:C:LEU:HD11  | 1:29:C:CYS:HB3  | 9        | 0.49          |
| (1,300) | 1:16:C:CYS:H    | 1:15:C:CYS:HB3  | 2        | 0.49          |
| (1,300) | 1:16:C:CYS:H    | 1:15:C:CYS:HB3  | 3        | 0.49          |
| (1,300) | 1:16:C:CYS:H    | 1:15:C:CYS:HB3  | 7        | 0.49          |
| (1,300) | 1:16:C:CYS:H    | 1:15:C:CYS:HB3  | 8        | 0.49          |
| (1,218) | 1:31:C:TRP:HH2  | 1:5:C:TRP:HB3   | 2        | 0.49          |
| (4,86)  | 1:24:C:LYS:HD3  | 1:23:C:LYS:HE2  | 9        | 0.48          |
| (3,84)  | 1:24:C:LYS:HD3  | 1:23:C:LYS:HE2  | 9        | 0.48          |
| (3,39)  | 1:7:C:GLY:H     | 1:4:C:GLU:HG2   | 6        | 0.48          |
| (1,291) | 1:2:C:CYS:H     | 1:1:C:ALA:HB2   | 7        | 0.48          |
| (1,256) | 1:24:C:LYS:H    | 1:24:C:LYS:HB2  | 5        | 0.48          |
| (1,218) | 1:31:C:TRP:HH2  | 1:5:C:TRP:HB3   | 7        | 0.48          |
| (1,156) | 1:31:C:TRP:HZ3  | 1:18:C:HIS:HB3  | 2        | 0.48          |
| (1,115) | 1:32:C:ASP:H    | 1:18:C:HIS:HB2  | 1        | 0.48          |
| (4,41)  | 1:7:C:GLY:H     | 1:4:C:GLU:HG2   | 4        | 0.47          |
| (4,41)  | 1:7:C:GLY:H     | 1:4:C:GLU:HG2   | 6        | 0.47          |
| (4,31)  | 1:31:C:TRP:H    | 1:30:C:VAL:HG11 | 9        | 0.47          |
| (4,30)  | 1:27:C:TYR:HE1  | 1:24:C:LYS:HB2  | 7        | 0.47          |
| (4,8)   | 1:2:C:CYS:H     | 1:3:C:ARG:HD3   | 2        | 0.47          |
| (4,8)   | 1:2:C:CYS:H     | 1:3:C:ARG:HD3   | 8        | 0.47          |
| (3,39)  | 1:7:C:GLY:H     | 1:4:C:GLU:HG2   | 4        | 0.47          |
| (3,39)  | 1:7:C:GLY:H     | 1:4:C:GLU:HG2   | 7        | 0.47          |
| (3,29)  | 1:31:C:TRP:H    | 1:30:C:VAL:HG11 | 9        | 0.47          |
| (3,28)  | 1:27:C:TYR:HE1  | 1:24:C:LYS:HB2  | 7        | 0.47          |
| (3,8)   | 1:2:C:CYS:H     | 1:3:C:ARG:HD3   | 8        | 0.47          |
| (1,262) | 1:5:C:TRP:HD1   | 1:30:C:VAL:HG11 | 10       | 0.47          |
| (4,43)  | 1:20:C:GLU:H    | 1:30:C:VAL:HB   | 10       | 0.46          |
| (4,41)  | 1:7:C:GLY:H     | 1:4:C:GLU:HG2   | 7        | 0.46          |
| (4,41)  | 1:7:C:GLY:H     | 1:4:C:GLU:HG2   | 10       | 0.46          |
| (4,31)  | 1:31:C:TRP:H    | 1:30:C:VAL:HG11 | 8        | 0.46          |
| (3,41)  | 1:20:C:GLU:H    | 1:30:C:VAL:HB   | 10       | 0.46          |
| (3,39)  | 1:7:C:GLY:H     | 1:4:C:GLU:HG2   | 3        | 0.46          |
| (3,39)  | 1:7:C:GLY:H     | 1:4:C:GLU:HG2   | 10       | 0.46          |
| (3,29)  | 1:31:C:TRP:H    | 1:30:C:VAL:HG11 | 8        | 0.46          |
| (1,354) | 1:31:C:TRP:HE1  | 1:6:C:LEU:HD12  | 5        | 0.46          |
| (1,353) | 1:31:C:TRP:HE1  | 1:19:C:LEU:HD21 | 6        | 0.46          |
| (1,300) | 1:16:C:CYS:H    | 1:15:C:CYS:HB3  | 4        | 0.46          |
| (1,241) | 1:13:C:ALA:H    | 1:11:C:LYS:HB3  | 5        | 0.46          |
| (4,95)  | 1:19:C:LEU:HB3  | 1:20:C:GLU:HG3  | 5        | 0.45          |
| (4,48)  | 1:29:C:CYS:H    | 1:19:C:LEU:HD21 | 1        | 0.45          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (4,41)  | 1:7:C:GLY:H     | 1:4:C:GLU:HG2   | 3        | 0.45          |
| (3,93)  | 1:19:C:LEU:HB3  | 1:20:C:GLU:HG3  | 5        | 0.45          |
| (3,93)  | 1:19:C:LEU:HB3  | 1:20:C:GLU:HG3  | 9        | 0.45          |
| (3,80)  | 1:19:C:LEU:HD12 | 1:4:C:GLU:HG2   | 3        | 0.45          |
| (3,46)  | 1:29:C:CYS:H    | 1:19:C:LEU:HD21 | 1        | 0.45          |
| (1,598) | 1:11:C:LYS:H    | 1:10:C:SER:HB3  | 9        | 0.45          |
| (1,570) | 1:30:C:VAL:HG13 | 1:22:C:ARG:HB3  | 8        | 0.45          |
| (1,308) | 1:32:C:ASP:H    | 1:31:C:TRP:HB2  | 5        | 0.45          |
| (1,280) | 1:31:C:TRP:HE3  | 1:19:C:LEU:HD11 | 8        | 0.45          |
| (1,264) | 1:28:C:HIS:HD2  | 1:30:C:VAL:HG22 | 4        | 0.45          |
| (1,262) | 1:5:C:TRP:HD1   | 1:30:C:VAL:HG12 | 3        | 0.45          |
| (1,262) | 1:5:C:TRP:HD1   | 1:30:C:VAL:HG12 | 6        | 0.45          |
| (1,262) | 1:5:C:TRP:HD1   | 1:30:C:VAL:HG13 | 7        | 0.45          |
| (1,191) | 1:27:C:TYR:HE1  | 1:27:C:TYR:HB2  | 8        | 0.45          |
| (1,115) | 1:32:C:ASP:H    | 1:18:C:HIS:HB2  | 3        | 0.45          |
| (4,95)  | 1:19:C:LEU:HB3  | 1:20:C:GLU:HG3  | 9        | 0.44          |
| (4,82)  | 1:19:C:LEU:HD11 | 1:4:C:GLU:HG2   | 2        | 0.44          |
| (4,82)  | 1:19:C:LEU:HD12 | 1:4:C:GLU:HG2   | 3        | 0.44          |
| (4,35)  | 1:34:C:THR:H    | 1:35:C:VAL:HG23 | 1        | 0.44          |
| (3,80)  | 1:19:C:LEU:HD11 | 1:4:C:GLU:HG2   | 2        | 0.44          |
| (3,39)  | 1:7:C:GLY:H     | 1:4:C:GLU:HG2   | 8        | 0.44          |
| (3,33)  | 1:34:C:THR:H    | 1:35:C:VAL:HG23 | 1        | 0.44          |
| (3,8)   | 1:2:C:CYS:H     | 1:3:C:ARG:HD2   | 5        | 0.44          |
| (1,598) | 1:11:C:LYS:H    | 1:10:C:SER:HB3  | 8        | 0.44          |
| (1,567) | 1:25:C:ALA:HB1  | 1:26:C:PRO:HB2  | 7        | 0.44          |
| (1,300) | 1:16:C:CYS:H    | 1:15:C:CYS:HB3  | 1        | 0.44          |
| (1,300) | 1:16:C:CYS:H    | 1:15:C:CYS:HB3  | 9        | 0.44          |
| (1,297) | 1:18:C:HIS:HE1  | 1:17:C:ALA:HB1  | 3        | 0.44          |
| (1,297) | 1:18:C:HIS:HE1  | 1:17:C:ALA:HB2  | 9        | 0.44          |
| (1,264) | 1:28:C:HIS:HD2  | 1:30:C:VAL:HG22 | 1        | 0.44          |
| (1,264) | 1:28:C:HIS:HD2  | 1:30:C:VAL:HG23 | 3        | 0.44          |
| (1,264) | 1:28:C:HIS:HD2  | 1:30:C:VAL:HG21 | 5        | 0.44          |
| (1,256) | 1:24:C:LYS:H    | 1:24:C:LYS:HB2  | 8        | 0.44          |
| (1,193) | 1:28:C:HIS:HD2  | 1:22:C:ARG:HD2  | 2        | 0.44          |
| (1,191) | 1:27:C:TYR:HE1  | 1:27:C:TYR:HB2  | 3        | 0.44          |
| (4,82)  | 1:19:C:LEU:HD13 | 1:4:C:GLU:HG2   | 5        | 0.43          |
| (4,43)  | 1:20:C:GLU:H    | 1:30:C:VAL:HB   | 4        | 0.43          |
| (4,41)  | 1:7:C:GLY:H     | 1:4:C:GLU:HG2   | 8        | 0.43          |
| (4,8)   | 1:2:C:CYS:H     | 1:3:C:ARG:HD2   | 5        | 0.43          |
| (3,80)  | 1:19:C:LEU:HD13 | 1:4:C:GLU:HG2   | 5        | 0.43          |
| (3,41)  | 1:20:C:GLU:H    | 1:30:C:VAL:HB   | 4        | 0.43          |
| (3,33)  | 1:34:C:THR:H    | 1:35:C:VAL:HG12 | 9        | 0.43          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (3,8)   | 1:2:C:CYS:H    | 1:3:C:ARG:HD2   | 4        | 0.43          |
| (1,343) | 1:32:C:ASP:H   | 1:30:C:VAL:HG21 | 1        | 0.43          |
| (1,297) | 1:18:C:HIS:HE1 | 1:17:C:ALA:HB3  | 7        | 0.43          |
| (1,255) | 1:27:C:TYR:HE2 | 1:23:C:LYS:HB3  | 4        | 0.43          |
| (1,222) | 1:5:C:TRP:HD1  | 1:5:C:TRP:HB3   | 2        | 0.43          |
| (1,222) | 1:5:C:TRP:HD1  | 1:5:C:TRP:HB3   | 4        | 0.43          |
| (1,222) | 1:5:C:TRP:HD1  | 1:5:C:TRP:HB3   | 7        | 0.43          |
| (1,222) | 1:5:C:TRP:HD1  | 1:5:C:TRP:HB3   | 8        | 0.43          |
| (1,222) | 1:5:C:TRP:HD1  | 1:5:C:TRP:HB3   | 10       | 0.43          |
| (1,191) | 1:27:C:TYR:HE1 | 1:27:C:TYR:HB2  | 9        | 0.43          |
| (1,156) | 1:31:C:TRP:HZ3 | 1:18:C:HIS:HB3  | 6        | 0.43          |
| (4,35)  | 1:34:C:THR:H   | 1:35:C:VAL:HG12 | 9        | 0.42          |
| (4,31)  | 1:31:C:TRP:H   | 1:34:C:THR:HG22 | 4        | 0.42          |
| (4,8)   | 1:2:C:CYS:H    | 1:3:C:ARG:HD2   | 4        | 0.42          |
| (4,8)   | 1:2:C:CYS:H    | 1:3:C:ARG:HD2   | 9        | 0.42          |
| (3,29)  | 1:31:C:TRP:H   | 1:34:C:THR:HG22 | 4        | 0.42          |
| (3,8)   | 1:2:C:CYS:H    | 1:3:C:ARG:HD2   | 9        | 0.42          |
| (1,354) | 1:31:C:TRP:HE1 | 1:6:C:LEU:HD12  | 8        | 0.42          |
| (1,345) | 1:5:C:TRP:HE1  | 1:6:C:LEU:HD12  | 5        | 0.42          |
| (1,311) | 1:10:C:SER:H   | 1:15:C:CYS:HB2  | 1        | 0.42          |
| (1,297) | 1:18:C:HIS:HE1 | 1:17:C:ALA:HB2  | 10       | 0.42          |
| (1,291) | 1:2:C:CYS:H    | 1:1:C:ALA:HB1   | 3        | 0.42          |
| (1,280) | 1:31:C:TRP:HE3 | 1:19:C:LEU:HD13 | 7        | 0.42          |
| (1,264) | 1:28:C:HIS:HD2 | 1:30:C:VAL:HG23 | 7        | 0.42          |
| (1,262) | 1:5:C:TRP:HD1  | 1:30:C:VAL:HG13 | 2        | 0.42          |
| (1,256) | 1:24:C:LYS:H   | 1:24:C:LYS:HB2  | 1        | 0.42          |
| (1,222) | 1:5:C:TRP:HD1  | 1:5:C:TRP:HB3   | 3        | 0.42          |
| (1,222) | 1:5:C:TRP:HD1  | 1:5:C:TRP:HB3   | 5        | 0.42          |
| (1,222) | 1:5:C:TRP:HD1  | 1:5:C:TRP:HB3   | 6        | 0.42          |
| (1,222) | 1:5:C:TRP:HD1  | 1:5:C:TRP:HB3   | 9        | 0.42          |
| (1,193) | 1:28:C:HIS:HD2 | 1:22:C:ARG:HD2  | 9        | 0.42          |
| (1,191) | 1:27:C:TYR:HE2 | 1:27:C:TYR:HB2  | 5        | 0.42          |
| (1,191) | 1:27:C:TYR:HE2 | 1:27:C:TYR:HB2  | 6        | 0.42          |
| (1,156) | 1:31:C:TRP:HZ3 | 1:18:C:HIS:HB3  | 3        | 0.42          |
| (4,8)   | 1:2:C:CYS:H    | 1:3:C:ARG:HD3   | 7        | 0.41          |
| (3,23)  | 1:28:C:HIS:H   | 1:22:C:ARG:HG3  | 6        | 0.41          |
| (3,23)  | 1:28:C:HIS:H   | 1:22:C:ARG:HG3  | 7        | 0.41          |
| (1,354) | 1:31:C:TRP:HE1 | 1:6:C:LEU:HD12  | 2        | 0.41          |
| (1,354) | 1:31:C:TRP:HE1 | 1:6:C:LEU:HD13  | 9        | 0.41          |
| (1,343) | 1:32:C:ASP:H   | 1:30:C:VAL:HG21 | 2        | 0.41          |
| (1,343) | 1:32:C:ASP:H   | 1:30:C:VAL:HG22 | 7        | 0.41          |
| (1,297) | 1:18:C:HIS:HE1 | 1:17:C:ALA:HB1  | 6        | 0.41          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,291) | 1:2:C:CYS:H     | 1:1:C:ALA:HB1   | 8        | 0.41          |
| (1,280) | 1:31:C:TRP:HE3  | 1:19:C:LEU:HD13 | 4        | 0.41          |
| (1,280) | 1:31:C:TRP:HE3  | 1:19:C:LEU:HD12 | 10       | 0.41          |
| (1,264) | 1:28:C:HIS:HD2  | 1:30:C:VAL:HG22 | 2        | 0.41          |
| (1,222) | 1:5:C:TRP:HD1   | 1:5:C:TRP:HB3   | 1        | 0.41          |
| (1,193) | 1:28:C:HIS:HD2  | 1:22:C:ARG:HD2  | 3        | 0.41          |
| (1,191) | 1:27:C:TYR:HE1  | 1:27:C:TYR:HB2  | 7        | 0.41          |
| (4,24)  | 1:28:C:HIS:H    | 1:22:C:ARG:HG3  | 6        | 0.4           |
| (4,24)  | 1:28:C:HIS:H    | 1:22:C:ARG:HG3  | 7        | 0.4           |
| (4,22)  | 1:22:C:ARG:H    | 1:22:C:ARG:HG3  | 3        | 0.4           |
| (3,21)  | 1:22:C:ARG:H    | 1:22:C:ARG:HG3  | 3        | 0.4           |
| (1,598) | 1:11:C:LYS:H    | 1:10:C:SER:HB3  | 10       | 0.4           |
| (1,570) | 1:30:C:VAL:HG13 | 1:22:C:ARG:HB3  | 1        | 0.4           |
| (1,567) | 1:25:C:ALA:HB3  | 1:26:C:PRO:HB2  | 4        | 0.4           |
| (1,564) | 1:34:C:THR:HG22 | 1:31:C:TRP:HB3  | 9        | 0.4           |
| (1,354) | 1:31:C:TRP:HE1  | 1:6:C:LEU:HD12  | 10       | 0.4           |
| (1,343) | 1:32:C:ASP:H    | 1:30:C:VAL:HG21 | 4        | 0.4           |
| (1,343) | 1:32:C:ASP:H    | 1:30:C:VAL:HG21 | 6        | 0.4           |
| (1,343) | 1:32:C:ASP:H    | 1:30:C:VAL:HG23 | 9        | 0.4           |
| (1,341) | 1:12:C:ASP:H    | 1:11:C:LYS:HG2  | 4        | 0.4           |
| (1,341) | 1:12:C:ASP:H    | 1:11:C:LYS:HG2  | 7        | 0.4           |
| (1,280) | 1:31:C:TRP:HE3  | 1:19:C:LEU:HD11 | 2        | 0.4           |
| (1,280) | 1:31:C:TRP:HE3  | 1:19:C:LEU:HD12 | 3        | 0.4           |
| (1,264) | 1:28:C:HIS:HD2  | 1:30:C:VAL:HG23 | 10       | 0.4           |
| (1,262) | 1:5:C:TRP:HD1   | 1:30:C:VAL:HG11 | 1        | 0.4           |
| (1,193) | 1:28:C:HIS:HD2  | 1:22:C:ARG:HD2  | 1        | 0.4           |
| (1,193) | 1:28:C:HIS:HD2  | 1:22:C:ARG:HD2  | 5        | 0.4           |
| (1,193) | 1:28:C:HIS:HD2  | 1:22:C:ARG:HD2  | 8        | 0.4           |
| (4,80)  | 1:30:C:VAL:HG22 | 1:22:C:ARG:HD3  | 2        | 0.39          |
| (3,78)  | 1:30:C:VAL:HG22 | 1:22:C:ARG:HD3  | 2        | 0.39          |
| (3,39)  | 1:7:C:GLY:H     | 1:4:C:GLU:HG2   | 5        | 0.39          |
| (1,464) | 1:25:C:ALA:HB2  | 1:24:C:LYS:HA   | 9        | 0.39          |
| (1,437) | 1:16:C:CYS:HB3  | 1:4:C:GLU:HA    | 6        | 0.39          |
| (1,354) | 1:31:C:TRP:HE1  | 1:6:C:LEU:HD13  | 1        | 0.39          |
| (1,354) | 1:31:C:TRP:HE1  | 1:6:C:LEU:HD13  | 7        | 0.39          |
| (1,353) | 1:31:C:TRP:HE1  | 1:19:C:LEU:HD22 | 10       | 0.39          |
| (1,352) | 1:6:C:LEU:H     | 1:19:C:LEU:HD23 | 6        | 0.39          |
| (1,346) | 1:5:C:TRP:HE1   | 1:19:C:LEU:HD22 | 9        | 0.39          |
| (1,267) | 1:31:C:TRP:HZ3  | 1:19:C:LEU:HD12 | 10       | 0.39          |
| (1,156) | 1:31:C:TRP:HZ3  | 1:18:C:HIS:HB3  | 7        | 0.39          |
| (4,86)  | 1:24:C:LYS:HD2  | 1:23:C:LYS:HE3  | 8        | 0.38          |
| (4,41)  | 1:7:C:GLY:H     | 1:4:C:GLU:HG2   | 5        | 0.38          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (4,8)   | 1:2:C:CYS:H     | 1:3:C:ARG:HD3   | 1        | 0.38          |
| (3,84)  | 1:24:C:LYS:HD2  | 1:23:C:LYS:HE3  | 8        | 0.38          |
| (3,8)   | 1:2:C:CYS:H     | 1:3:C:ARG:HD3   | 1        | 0.38          |
| (1,464) | 1:25:C:ALA:HB2  | 1:24:C:LYS:HA   | 3        | 0.38          |
| (1,464) | 1:25:C:ALA:HB3  | 1:24:C:LYS:HA   | 10       | 0.38          |
| (1,343) | 1:32:C:ASP:H    | 1:30:C:VAL:HG22 | 3        | 0.38          |
| (1,306) | 1:16:C:CYS:H    | 1:16:C:CYS:HB3  | 5        | 0.38          |
| (1,297) | 1:18:C:HIS:HE1  | 1:17:C:ALA:HB3  | 2        | 0.38          |
| (1,297) | 1:18:C:HIS:HE1  | 1:17:C:ALA:HB3  | 4        | 0.38          |
| (1,297) | 1:18:C:HIS:HE1  | 1:17:C:ALA:HB1  | 8        | 0.38          |
| (1,267) | 1:31:C:TRP:HZ3  | 1:19:C:LEU:HD13 | 5        | 0.38          |
| (1,267) | 1:31:C:TRP:HZ3  | 1:19:C:LEU:HD13 | 7        | 0.38          |
| (1,267) | 1:31:C:TRP:HZ3  | 1:19:C:LEU:HD11 | 8        | 0.38          |
| (1,262) | 1:5:C:TRP:HD1   | 1:30:C:VAL:HG13 | 4        | 0.38          |
| (1,262) | 1:5:C:TRP:HD1   | 1:30:C:VAL:HG13 | 5        | 0.38          |
| (1,262) | 1:5:C:TRP:HD1   | 1:30:C:VAL:HG11 | 8        | 0.38          |
| (1,191) | 1:27:C:TYR:HE2  | 1:27:C:TYR:HB2  | 1        | 0.38          |
| (4,82)  | 1:19:C:LEU:HD12 | 1:4:C:GLU:HG2   | 10       | 0.37          |
| (4,8)   | 1:2:C:CYS:H     | 1:3:C:ARG:HD3   | 3        | 0.37          |
| (3,80)  | 1:19:C:LEU:HD12 | 1:4:C:GLU:HG2   | 10       | 0.37          |
| (1,598) | 1:11:C:LYS:H    | 1:10:C:SER:HB3  | 7        | 0.37          |
| (1,354) | 1:31:C:TRP:HE1  | 1:6:C:LEU:HD13  | 3        | 0.37          |
| (1,353) | 1:31:C:TRP:HE1  | 1:19:C:LEU:HD21 | 5        | 0.37          |
| (1,343) | 1:32:C:ASP:H    | 1:30:C:VAL:HG23 | 5        | 0.37          |
| (1,343) | 1:32:C:ASP:H    | 1:30:C:VAL:HG22 | 10       | 0.37          |
| (1,341) | 1:12:C:ASP:H    | 1:11:C:LYS:HG2  | 3        | 0.37          |
| (1,341) | 1:12:C:ASP:H    | 1:11:C:LYS:HG2  | 9        | 0.37          |
| (1,311) | 1:10:C:SER:H    | 1:15:C:CYS:HB2  | 6        | 0.37          |
| (1,193) | 1:28:C:HIS:HD2  | 1:22:C:ARG:HD2  | 4        | 0.37          |
| (1,60)  | 1:24:C:LYS:H    | 1:27:C:TYR:HD2  | 1        | 0.37          |
| (4,82)  | 1:19:C:LEU:HD13 | 1:4:C:GLU:HG2   | 4        | 0.36          |
| (4,59)  | 1:34:C:THR:HG21 | 1:31:C:TRP:HA   | 10       | 0.36          |
| (3,80)  | 1:19:C:LEU:HD13 | 1:4:C:GLU:HG2   | 4        | 0.36          |
| (3,57)  | 1:34:C:THR:HG21 | 1:31:C:TRP:HA   | 10       | 0.36          |
| (3,46)  | 1:29:C:CYS:H    | 1:19:C:LEU:HD23 | 6        | 0.36          |
| (3,41)  | 1:20:C:GLU:H    | 1:30:C:VAL:HB   | 7        | 0.36          |
| (3,23)  | 1:28:C:HIS:H    | 1:22:C:ARG:HG2  | 10       | 0.36          |
| (1,600) | 1:5:C:TRP:HH2   | 1:6:C:LEU:HD12  | 5        | 0.36          |
| (1,354) | 1:31:C:TRP:HE1  | 1:6:C:LEU:HD13  | 6        | 0.36          |
| (1,345) | 1:5:C:TRP:HE1   | 1:6:C:LEU:HD12  | 10       | 0.36          |
| (1,297) | 1:18:C:HIS:HE1  | 1:17:C:ALA:HB3  | 1        | 0.36          |
| (1,262) | 1:5:C:TRP:HD1   | 1:30:C:VAL:HG11 | 9        | 0.36          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,205) | 1:11:C:LYS:H    | 1:21:C:CYS:HB3  | 1        | 0.36          |
| (1,205) | 1:11:C:LYS:H    | 1:21:C:CYS:HB3  | 6        | 0.36          |
| (1,205) | 1:11:C:LYS:H    | 1:21:C:CYS:HB3  | 7        | 0.36          |
| (1,201) | 1:22:C:ARG:H    | 1:22:C:ARG:HD2  | 9        | 0.36          |
| (4,88)  | 1:20:C:GLU:HB2  | 1:32:C:ASP:HB2  | 8        | 0.35          |
| (4,86)  | 1:24:C:LYS:HD3  | 1:23:C:LYS:HE2  | 1        | 0.35          |
| (4,59)  | 1:34:C:THR:HG23 | 1:33:C:TRP:HA   | 4        | 0.35          |
| (4,48)  | 1:29:C:CYS:H    | 1:19:C:LEU:HD23 | 6        | 0.35          |
| (4,43)  | 1:20:C:GLU:H    | 1:30:C:VAL:HB   | 7        | 0.35          |
| (4,24)  | 1:28:C:HIS:H    | 1:22:C:ARG:HG2  | 10       | 0.35          |
| (3,86)  | 1:20:C:GLU:HB2  | 1:32:C:ASP:HB2  | 8        | 0.35          |
| (3,84)  | 1:24:C:LYS:HD3  | 1:23:C:LYS:HE2  | 1        | 0.35          |
| (3,57)  | 1:34:C:THR:HG23 | 1:33:C:TRP:HA   | 4        | 0.35          |
| (1,600) | 1:5:C:TRP:HH2   | 1:6:C:LEU:HD13  | 3        | 0.35          |
| (1,598) | 1:11:C:LYS:H    | 1:10:C:SER:HB3  | 2        | 0.35          |
| (1,598) | 1:11:C:LYS:H    | 1:10:C:SER:HB3  | 4        | 0.35          |
| (1,530) | 1:13:C:ALA:HB2  | 1:11:C:LYS:HE3  | 1        | 0.35          |
| (1,530) | 1:13:C:ALA:HB1  | 1:11:C:LYS:HE3  | 4        | 0.35          |
| (1,530) | 1:13:C:ALA:HB3  | 1:11:C:LYS:HE3  | 10       | 0.35          |
| (1,360) | 1:31:C:TRP:H    | 1:19:C:LEU:HD21 | 7        | 0.35          |
| (1,346) | 1:5:C:TRP:HE1   | 1:19:C:LEU:HD21 | 1        | 0.35          |
| (1,280) | 1:31:C:TRP:HE3  | 1:19:C:LEU:HD12 | 9        | 0.35          |
| (1,267) | 1:31:C:TRP:HZ3  | 1:19:C:LEU:HD11 | 2        | 0.35          |
| (1,267) | 1:31:C:TRP:HZ3  | 1:19:C:LEU:HD13 | 4        | 0.35          |
| (1,264) | 1:28:C:HIS:HD2  | 1:30:C:VAL:HG22 | 6        | 0.35          |
| (1,205) | 1:11:C:LYS:H    | 1:21:C:CYS:HB3  | 2        | 0.35          |
| (1,205) | 1:11:C:LYS:H    | 1:21:C:CYS:HB3  | 10       | 0.35          |
| (1,156) | 1:31:C:TRP:HZ3  | 1:18:C:HIS:HB3  | 9        | 0.35          |
| (1,62)  | 1:27:C:TYR:HD1  | 1:27:C:TYR:HE1  | 1        | 0.35          |
| (1,62)  | 1:27:C:TYR:HD1  | 1:27:C:TYR:HE1  | 2        | 0.35          |
| (1,62)  | 1:27:C:TYR:HD1  | 1:27:C:TYR:HE1  | 3        | 0.35          |
| (1,62)  | 1:27:C:TYR:HD2  | 1:27:C:TYR:HE2  | 4        | 0.35          |
| (1,62)  | 1:27:C:TYR:HD2  | 1:27:C:TYR:HE2  | 5        | 0.35          |
| (1,62)  | 1:27:C:TYR:HD1  | 1:27:C:TYR:HE1  | 6        | 0.35          |
| (1,62)  | 1:27:C:TYR:HD1  | 1:27:C:TYR:HE1  | 7        | 0.35          |
| (1,62)  | 1:27:C:TYR:HD1  | 1:27:C:TYR:HE1  | 8        | 0.35          |
| (1,62)  | 1:27:C:TYR:HD2  | 1:27:C:TYR:HE2  | 9        | 0.35          |
| (1,62)  | 1:27:C:TYR:HD1  | 1:27:C:TYR:HE1  | 10       | 0.35          |
| (4,80)  | 1:30:C:VAL:HG22 | 1:22:C:ARG:HD3  | 6        | 0.34          |
| (4,43)  | 1:20:C:GLU:H    | 1:30:C:VAL:HB   | 6        | 0.34          |
| (4,11)  | 1:31:C:TRP:HD1  | 1:31:C:TRP:HA   | 1        | 0.34          |
| (3,78)  | 1:30:C:VAL:HG22 | 1:22:C:ARG:HD3  | 6        | 0.34          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (3,41)  | 1:20:C:GLU:H    | 1:30:C:VAL:HB   | 6        | 0.34          |
| (3,10)  | 1:31:C:TRP:HD1  | 1:31:C:TRP:HA   | 1        | 0.34          |
| (1,600) | 1:5:C:TRP:HH2   | 1:6:C:LEU:HD12  | 8        | 0.34          |
| (1,600) | 1:5:C:TRP:HH2   | 1:6:C:LEU:HD12  | 10       | 0.34          |
| (1,570) | 1:30:C:VAL:HG12 | 1:22:C:ARG:HB3  | 5        | 0.34          |
| (1,530) | 1:13:C:ALA:HB2  | 1:11:C:LYS:HE3  | 2        | 0.34          |
| (1,464) | 1:25:C:ALA:HB3  | 1:24:C:LYS:HA   | 5        | 0.34          |
| (1,360) | 1:31:C:TRP:H    | 1:19:C:LEU:HD21 | 2        | 0.34          |
| (1,322) | 1:21:C:CYS:H    | 1:20:C:GLU:HG2  | 1        | 0.34          |
| (1,322) | 1:21:C:CYS:H    | 1:20:C:GLU:HG2  | 7        | 0.34          |
| (1,280) | 1:31:C:TRP:HE3  | 1:19:C:LEU:HD13 | 5        | 0.34          |
| (1,267) | 1:31:C:TRP:HZ3  | 1:19:C:LEU:HD12 | 3        | 0.34          |
| (1,214) | 1:5:C:TRP:H     | 1:4:C:GLU:HG3   | 9        | 0.34          |
| (1,157) | 1:27:C:TYR:HD2  | 1:23:C:LYS:HA   | 10       | 0.34          |
| (4,37)  | 1:25:C:ALA:H    | 1:24:C:LYS:HG2  | 3        | 0.33          |
| (4,37)  | 1:25:C:ALA:H    | 1:24:C:LYS:HG2  | 8        | 0.33          |
| (4,24)  | 1:28:C:HIS:H    | 1:22:C:ARG:HG2  | 2        | 0.33          |
| (4,11)  | 1:31:C:TRP:HD1  | 1:31:C:TRP:HA   | 9        | 0.33          |
| (3,35)  | 1:25:C:ALA:H    | 1:24:C:LYS:HG2  | 3        | 0.33          |
| (3,35)  | 1:25:C:ALA:H    | 1:24:C:LYS:HG2  | 8        | 0.33          |
| (3,23)  | 1:28:C:HIS:H    | 1:22:C:ARG:HG2  | 2        | 0.33          |
| (3,10)  | 1:31:C:TRP:HD1  | 1:31:C:TRP:HA   | 8        | 0.33          |
| (3,10)  | 1:31:C:TRP:HD1  | 1:31:C:TRP:HA   | 9        | 0.33          |
| (1,360) | 1:31:C:TRP:H    | 1:19:C:LEU:HD22 | 4        | 0.33          |
| (1,343) | 1:32:C:ASP:H    | 1:30:C:VAL:HG21 | 8        | 0.33          |
| (1,341) | 1:12:C:ASP:H    | 1:11:C:LYS:HG2  | 1        | 0.33          |
| (1,264) | 1:28:C:HIS:HD2  | 1:30:C:VAL:HG22 | 8        | 0.33          |
| (1,214) | 1:5:C:TRP:H     | 1:4:C:GLU:HG3   | 1        | 0.33          |
| (1,193) | 1:28:C:HIS:HD2  | 1:22:C:ARG:HD2  | 10       | 0.33          |
| (1,60)  | 1:24:C:LYS:H    | 1:27:C:TYR:HD1  | 9        | 0.33          |
| (4,65)  | 1:23:C:LYS:HD2  | 1:23:C:LYS:HA   | 8        | 0.32          |
| (4,37)  | 1:25:C:ALA:H    | 1:24:C:LYS:HG3  | 5        | 0.32          |
| (4,11)  | 1:31:C:TRP:HD1  | 1:31:C:TRP:HA   | 8        | 0.32          |
| (3,63)  | 1:23:C:LYS:HD2  | 1:23:C:LYS:HA   | 8        | 0.32          |
| (3,35)  | 1:25:C:ALA:H    | 1:24:C:LYS:HG3  | 5        | 0.32          |
| (3,10)  | 1:31:C:TRP:HD1  | 1:31:C:TRP:HA   | 10       | 0.32          |
| (1,600) | 1:5:C:TRP:HH2   | 1:6:C:LEU:HD13  | 1        | 0.32          |
| (1,540) | 1:3:C:ARG:HG3   | 1:11:C:LYS:HE3  | 2        | 0.32          |
| (1,464) | 1:25:C:ALA:HB3  | 1:24:C:LYS:HA   | 1        | 0.32          |
| (1,464) | 1:25:C:ALA:HB1  | 1:24:C:LYS:HA   | 6        | 0.32          |
| (1,464) | 1:25:C:ALA:HB3  | 1:24:C:LYS:HA   | 7        | 0.32          |
| (1,205) | 1:11:C:LYS:H    | 1:21:C:CYS:HB3  | 5        | 0.32          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,193) | 1:28:C:HIS:HD2  | 1:22:C:ARG:HD2  | 6        | 0.32          |
| (1,156) | 1:31:C:TRP:HZ3  | 1:18:C:HIS:HB3  | 4        | 0.32          |
| (4,86)  | 1:24:C:LYS:HD2  | 1:23:C:LYS:HE2  | 6        | 0.31          |
| (4,43)  | 1:20:C:GLU:H    | 1:30:C:VAL:HB   | 3        | 0.31          |
| (4,11)  | 1:31:C:TRP:HD1  | 1:31:C:TRP:HA   | 3        | 0.31          |
| (4,11)  | 1:31:C:TRP:HD1  | 1:31:C:TRP:HA   | 7        | 0.31          |
| (4,11)  | 1:31:C:TRP:HD1  | 1:31:C:TRP:HA   | 10       | 0.31          |
| (3,84)  | 1:24:C:LYS:HD2  | 1:23:C:LYS:HE2  | 6        | 0.31          |
| (3,41)  | 1:20:C:GLU:H    | 1:30:C:VAL:HB   | 3        | 0.31          |
| (3,33)  | 1:34:C:THR:H    | 1:35:C:VAL:HG11 | 2        | 0.31          |
| (3,10)  | 1:31:C:TRP:HD1  | 1:31:C:TRP:HA   | 3        | 0.31          |
| (3,10)  | 1:31:C:TRP:HD1  | 1:31:C:TRP:HA   | 7        | 0.31          |
| (1,600) | 1:5:C:TRP:HH2   | 1:6:C:LEU:HD13  | 6        | 0.31          |
| (1,464) | 1:25:C:ALA:HB3  | 1:24:C:LYS:HA   | 2        | 0.31          |
| (1,345) | 1:5:C:TRP:HE1   | 1:6:C:LEU:HD13  | 3        | 0.31          |
| (1,341) | 1:12:C:ASP:H    | 1:11:C:LYS:HG2  | 8        | 0.31          |
| (1,193) | 1:28:C:HIS:HD2  | 1:22:C:ARG:HD2  | 7        | 0.31          |
| (4,95)  | 1:19:C:LEU:HB3  | 1:20:C:GLU:HG3  | 10       | 0.3           |
| (4,37)  | 1:25:C:ALA:H    | 1:24:C:LYS:HG3  | 7        | 0.3           |
| (4,35)  | 1:34:C:THR:H    | 1:35:C:VAL:HG11 | 2        | 0.3           |
| (3,93)  | 1:19:C:LEU:HB3  | 1:20:C:GLU:HG3  | 10       | 0.3           |
| (3,35)  | 1:25:C:ALA:H    | 1:24:C:LYS:HG3  | 7        | 0.3           |
| (3,10)  | 1:31:C:TRP:HD1  | 1:31:C:TRP:HA   | 6        | 0.3           |
| (1,600) | 1:5:C:TRP:HH2   | 1:6:C:LEU:HD13  | 7        | 0.3           |
| (1,600) | 1:5:C:TRP:HH2   | 1:6:C:LEU:HD13  | 9        | 0.3           |
| (1,530) | 1:13:C:ALA:HB1  | 1:11:C:LYS:HE3  | 6        | 0.3           |
| (1,520) | 1:6:C:LEU:HD12  | 1:30:C:VAL:HB   | 9        | 0.3           |
| (1,464) | 1:25:C:ALA:HB2  | 1:24:C:LYS:HA   | 4        | 0.3           |
| (1,360) | 1:31:C:TRP:H    | 1:19:C:LEU:HD22 | 3        | 0.3           |
| (1,352) | 1:6:C:LEU:H     | 1:19:C:LEU:HD23 | 4        | 0.3           |
| (1,352) | 1:6:C:LEU:H     | 1:19:C:LEU:HD21 | 10       | 0.3           |
| (1,273) | 1:15:C:CYS:H    | 1:13:C:ALA:HB1  | 6        | 0.3           |
| (4,11)  | 1:31:C:TRP:HD1  | 1:31:C:TRP:HA   | 5        | 0.29          |
| (4,11)  | 1:31:C:TRP:HD1  | 1:31:C:TRP:HA   | 6        | 0.29          |
| (3,10)  | 1:31:C:TRP:HD1  | 1:31:C:TRP:HA   | 5        | 0.29          |
| (1,600) | 1:5:C:TRP:HH2   | 1:6:C:LEU:HD12  | 2        | 0.29          |
| (1,598) | 1:11:C:LYS:H    | 1:10:C:SER:HB3  | 6        | 0.29          |
| (1,570) | 1:30:C:VAL:HG11 | 1:22:C:ARG:HB3  | 6        | 0.29          |
| (1,507) | 1:6:C:LEU:HD11  | 1:22:C:ARG:HD3  | 5        | 0.29          |
| (1,411) | 1:19:C:LEU:HD13 | 1:16:C:CYS:HA   | 6        | 0.29          |
| (1,352) | 1:6:C:LEU:H     | 1:19:C:LEU:HD22 | 2        | 0.29          |
| (1,352) | 1:6:C:LEU:H     | 1:19:C:LEU:HD23 | 5        | 0.29          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (4,95)  | 1:19:C:LEU:HB3  | 1:20:C:GLU:HG3  | 8        | 0.28          |
| (4,35)  | 1:34:C:THR:H    | 1:35:C:VAL:HG23 | 3        | 0.28          |
| (4,27)  | 1:28:C:HIS:HD2  | 1:22:C:ARG:HG3  | 10       | 0.28          |
| (4,11)  | 1:31:C:TRP:HD1  | 1:31:C:TRP:HA   | 2        | 0.28          |
| (3,93)  | 1:19:C:LEU:HB3  | 1:20:C:GLU:HG3  | 8        | 0.28          |
| (3,33)  | 1:34:C:THR:H    | 1:35:C:VAL:HG23 | 3        | 0.28          |
| (3,25)  | 1:28:C:HIS:HD2  | 1:22:C:ARG:HG3  | 6        | 0.28          |
| (3,25)  | 1:28:C:HIS:HD2  | 1:22:C:ARG:HG3  | 10       | 0.28          |
| (3,21)  | 1:22:C:ARG:H    | 1:22:C:ARG:HG3  | 10       | 0.28          |
| (3,13)  | 1:15:C:CYS:H    | 1:9:C:CYS:HB2   | 6        | 0.28          |
| (3,10)  | 1:31:C:TRP:HD1  | 1:31:C:TRP:HA   | 2        | 0.28          |
| (1,573) | 1:30:C:VAL:HG21 | 1:22:C:ARG:HB2  | 9        | 0.28          |
| (1,464) | 1:25:C:ALA:HB3  | 1:24:C:LYS:HA   | 8        | 0.28          |
| (1,355) | 1:5:C:TRP:H     | 1:19:C:LEU:HD21 | 6        | 0.28          |
| (1,352) | 1:6:C:LEU:H     | 1:19:C:LEU:HD22 | 8        | 0.28          |
| (1,273) | 1:15:C:CYS:H    | 1:13:C:ALA:HB2  | 1        | 0.28          |
| (1,156) | 1:31:C:TRP:HZ3  | 1:18:C:HIS:HB3  | 10       | 0.28          |
| (4,86)  | 1:24:C:LYS:HD2  | 1:23:C:LYS:HE2  | 10       | 0.27          |
| (4,47)  | 1:7:C:GLY:H     | 1:3:C:ARG:HB3   | 9        | 0.27          |
| (4,27)  | 1:28:C:HIS:HD2  | 1:22:C:ARG:HG3  | 4        | 0.27          |
| (4,27)  | 1:28:C:HIS:HD2  | 1:22:C:ARG:HG3  | 6        | 0.27          |
| (4,22)  | 1:22:C:ARG:H    | 1:22:C:ARG:HG3  | 7        | 0.27          |
| (4,22)  | 1:22:C:ARG:H    | 1:22:C:ARG:HG3  | 10       | 0.27          |
| (4,14)  | 1:15:C:CYS:H    | 1:9:C:CYS:HB2   | 6        | 0.27          |
| (3,84)  | 1:24:C:LYS:HD2  | 1:23:C:LYS:HE2  | 10       | 0.27          |
| (3,45)  | 1:7:C:GLY:H     | 1:3:C:ARG:HB3   | 9        | 0.27          |
| (3,41)  | 1:20:C:GLU:H    | 1:30:C:VAL:HB   | 8        | 0.27          |
| (3,29)  | 1:31:C:TRP:H    | 1:34:C:THR:HG23 | 7        | 0.27          |
| (3,28)  | 1:27:C:TYR:HE2  | 1:23:C:LYS:HD2  | 9        | 0.27          |
| (3,25)  | 1:28:C:HIS:HD2  | 1:22:C:ARG:HG3  | 4        | 0.27          |
| (3,21)  | 1:22:C:ARG:H    | 1:22:C:ARG:HG3  | 7        | 0.27          |
| (3,13)  | 1:15:C:CYS:H    | 1:9:C:CYS:HB2   | 1        | 0.27          |
| (1,591) | 1:6:C:LEU:HG    | 1:6:C:LEU:HB3   | 4        | 0.27          |
| (1,567) | 1:25:C:ALA:HB1  | 1:26:C:PRO:HB2  | 8        | 0.27          |
| (1,471) | 1:19:C:LEU:HD11 | 1:4:C:GLU:HA    | 6        | 0.27          |
| (1,386) | 1:12:C:ASP:HA   | 1:20:C:GLU:HA   | 2        | 0.27          |
| (1,352) | 1:6:C:LEU:H     | 1:19:C:LEU:HD21 | 1        | 0.27          |
| (1,267) | 1:31:C:TRP:HZ3  | 1:19:C:LEU:HD12 | 9        | 0.27          |
| (1,218) | 1:31:C:TRP:HH2  | 1:5:C:TRP:HB3   | 9        | 0.27          |
| (1,156) | 1:31:C:TRP:HZ3  | 1:18:C:HIS:HB3  | 8        | 0.27          |
| (4,86)  | 1:24:C:LYS:HD3  | 1:23:C:LYS:HE2  | 7        | 0.26          |
| (4,43)  | 1:20:C:GLU:H    | 1:30:C:VAL:HB   | 8        | 0.26          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (4,31)  | 1:31:C:TRP:H    | 1:34:C:THR:HG23 | 7        | 0.26          |
| (4,30)  | 1:27:C:TYR:HE2  | 1:23:C:LYS:HD2  | 9        | 0.26          |
| (4,27)  | 1:28:C:HIS:HD2  | 1:22:C:ARG:HG3  | 2        | 0.26          |
| (4,14)  | 1:15:C:CYS:H    | 1:9:C:CYS:HB2   | 1        | 0.26          |
| (4,11)  | 1:31:C:TRP:HD1  | 1:31:C:TRP:HA   | 4        | 0.26          |
| (4,9)   | 1:4:C:GLU:H     | 1:3:C:ARG:HD3   | 1        | 0.26          |
| (3,84)  | 1:24:C:LYS:HD3  | 1:23:C:LYS:HE2  | 7        | 0.26          |
| (3,41)  | 1:20:C:GLU:H    | 1:30:C:VAL:HB   | 5        | 0.26          |
| (3,25)  | 1:28:C:HIS:HD2  | 1:22:C:ARG:HG3  | 2        | 0.26          |
| (3,21)  | 1:22:C:ARG:H    | 1:22:C:ARG:HG3  | 2        | 0.26          |
| (3,10)  | 1:31:C:TRP:HD1  | 1:31:C:TRP:HA   | 4        | 0.26          |
| (3,9)   | 1:4:C:GLU:H     | 1:3:C:ARG:HD3   | 1        | 0.26          |
| (1,573) | 1:30:C:VAL:HG22 | 1:22:C:ARG:HB2  | 1        | 0.26          |
| (1,528) | 1:19:C:LEU:HB3  | 1:14:C:ASP:HB2  | 6        | 0.26          |
| (1,366) | 1:5:C:TRP:HD1   | 1:6:C:LEU:HD13  | 5        | 0.26          |
| (1,366) | 1:5:C:TRP:HD1   | 1:6:C:LEU:HD13  | 9        | 0.26          |
| (1,358) | 1:5:C:TRP:HZ2   | 1:6:C:LEU:HD13  | 4        | 0.26          |
| (1,273) | 1:15:C:CYS:H    | 1:13:C:ALA:HB2  | 7        | 0.26          |
| (4,43)  | 1:20:C:GLU:H    | 1:30:C:VAL:HB   | 5        | 0.25          |
| (4,35)  | 1:34:C:THR:H    | 1:35:C:VAL:HG23 | 5        | 0.25          |
| (4,22)  | 1:22:C:ARG:H    | 1:22:C:ARG:HG3  | 2        | 0.25          |
| (3,33)  | 1:34:C:THR:H    | 1:35:C:VAL:HG23 | 5        | 0.25          |
| (1,570) | 1:30:C:VAL:HG12 | 1:22:C:ARG:HB3  | 4        | 0.25          |
| (1,352) | 1:6:C:LEU:H     | 1:19:C:LEU:HD23 | 3        | 0.25          |
| (1,289) | 1:13:C:ALA:H    | 1:13:C:ALA:HB3  | 9        | 0.25          |
| (1,273) | 1:15:C:CYS:H    | 1:13:C:ALA:HB2  | 2        | 0.25          |
| (1,273) | 1:15:C:CYS:H    | 1:13:C:ALA:HB1  | 4        | 0.25          |
| (1,218) | 1:31:C:TRP:HH2  | 1:5:C:TRP:HB3   | 4        | 0.25          |
| (4,35)  | 1:34:C:THR:H    | 1:35:C:VAL:HG12 | 10       | 0.24          |
| (4,2)   | 1:31:C:TRP:HE1  | 1:31:C:TRP:HH2  | 5        | 0.24          |
| (3,93)  | 1:19:C:LEU:HB3  | 1:20:C:GLU:HG3  | 7        | 0.24          |
| (3,45)  | 1:7:C:GLY:H     | 1:3:C:ARG:HB3   | 2        | 0.24          |
| (3,33)  | 1:34:C:THR:H    | 1:35:C:VAL:HG12 | 10       | 0.24          |
| (3,23)  | 1:28:C:HIS:H    | 1:22:C:ARG:HG2  | 3        | 0.24          |
| (3,2)   | 1:31:C:TRP:HE1  | 1:31:C:TRP:HH2  | 5        | 0.24          |
| (1,366) | 1:5:C:TRP:HD1   | 1:6:C:LEU:HD13  | 3        | 0.24          |
| (1,366) | 1:5:C:TRP:HD1   | 1:6:C:LEU:HD13  | 7        | 0.24          |
| (1,352) | 1:6:C:LEU:H     | 1:19:C:LEU:HD22 | 7        | 0.24          |
| (1,345) | 1:5:C:TRP:HE1   | 1:6:C:LEU:HD13  | 1        | 0.24          |
| (1,345) | 1:5:C:TRP:HE1   | 1:6:C:LEU:HD13  | 9        | 0.24          |
| (1,322) | 1:21:C:CYS:H    | 1:20:C:GLU:HG2  | 8        | 0.24          |
| (1,264) | 1:28:C:HIS:HD2  | 1:30:C:VAL:HG21 | 9        | 0.24          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (4,95)  | 1:19:C:LEU:HB3  | 1:20:C:GLU:HG3  | 7        | 0.23          |
| (4,70)  | 1:15:C:CYS:HB2  | 1:9:C:CYS:HB3   | 6        | 0.23          |
| (4,47)  | 1:7:C:GLY:H     | 1:3:C:ARG:HB3   | 2        | 0.23          |
| (4,47)  | 1:7:C:GLY:H     | 1:3:C:ARG:HB3   | 8        | 0.23          |
| (4,27)  | 1:28:C:HIS:HD2  | 1:22:C:ARG:HG3  | 1        | 0.23          |
| (4,24)  | 1:28:C:HIS:H    | 1:22:C:ARG:HG2  | 3        | 0.23          |
| (3,68)  | 1:15:C:CYS:HB2  | 1:9:C:CYS:HB3   | 6        | 0.23          |
| (3,45)  | 1:7:C:GLY:H     | 1:3:C:ARG:HB3   | 8        | 0.23          |
| (3,45)  | 1:7:C:GLY:H     | 1:3:C:ARG:HB3   | 10       | 0.23          |
| (3,25)  | 1:28:C:HIS:HD2  | 1:22:C:ARG:HG3  | 1        | 0.23          |
| (3,23)  | 1:28:C:HIS:H    | 1:22:C:ARG:HG3  | 4        | 0.23          |
| (1,573) | 1:30:C:VAL:HG23 | 1:22:C:ARG:HB2  | 7        | 0.23          |
| (1,570) | 1:30:C:VAL:HG12 | 1:22:C:ARG:HB3  | 2        | 0.23          |
| (1,570) | 1:30:C:VAL:HG12 | 1:22:C:ARG:HB3  | 7        | 0.23          |
| (1,520) | 1:6:C:LEU:HD12  | 1:30:C:VAL:HB   | 3        | 0.23          |
| (1,507) | 1:6:C:LEU:HD11  | 1:22:C:ARG:HD3  | 8        | 0.23          |
| (1,355) | 1:5:C:TRP:H     | 1:19:C:LEU:HD23 | 8        | 0.23          |
| (1,338) | 1:20:C:GLU:H    | 1:30:C:VAL:HG21 | 2        | 0.23          |
| (1,322) | 1:21:C:CYS:H    | 1:20:C:GLU:HG2  | 9        | 0.23          |
| (1,289) | 1:13:C:ALA:H    | 1:13:C:ALA:HB3  | 8        | 0.23          |
| (1,273) | 1:15:C:CYS:H    | 1:13:C:ALA:HB3  | 10       | 0.23          |
| (1,157) | 1:27:C:TYR:HD1  | 1:23:C:LYS:HA   | 5        | 0.23          |
| (4,80)  | 1:30:C:VAL:HG22 | 1:22:C:ARG:HD3  | 4        | 0.22          |
| (4,70)  | 1:15:C:CYS:HB2  | 1:9:C:CYS:HB3   | 1        | 0.22          |
| (4,47)  | 1:7:C:GLY:H     | 1:3:C:ARG:HB3   | 10       | 0.22          |
| (4,27)  | 1:28:C:HIS:HD2  | 1:22:C:ARG:HG3  | 3        | 0.22          |
| (4,24)  | 1:28:C:HIS:H    | 1:22:C:ARG:HG3  | 4        | 0.22          |
| (4,12)  | 1:33:C:TRP:HZ3  | 1:33:C:TRP:HB3  | 1        | 0.22          |
| (4,12)  | 1:22:C:ARG:HE   | 1:26:C:PRO:HD3  | 7        | 0.22          |
| (3,78)  | 1:30:C:VAL:HG22 | 1:22:C:ARG:HD3  | 4        | 0.22          |
| (3,68)  | 1:15:C:CYS:HB2  | 1:9:C:CYS:HB3   | 1        | 0.22          |
| (3,25)  | 1:28:C:HIS:HD2  | 1:22:C:ARG:HG3  | 3        | 0.22          |
| (3,25)  | 1:28:C:HIS:HD2  | 1:22:C:ARG:HG3  | 8        | 0.22          |
| (3,11)  | 1:33:C:TRP:HZ3  | 1:33:C:TRP:HB3  | 1        | 0.22          |
| (3,11)  | 1:22:C:ARG:HE   | 1:26:C:PRO:HD3  | 7        | 0.22          |
| (1,530) | 1:13:C:ALA:HB1  | 1:11:C:LYS:HE3  | 5        | 0.22          |
| (1,507) | 1:6:C:LEU:HD12  | 1:22:C:ARG:HD3  | 7        | 0.22          |
| (1,507) | 1:6:C:LEU:HD12  | 1:22:C:ARG:HD3  | 9        | 0.22          |
| (1,355) | 1:5:C:TRP:H     | 1:19:C:LEU:HD23 | 2        | 0.22          |
| (1,341) | 1:12:C:ASP:H    | 1:11:C:LYS:HG2  | 10       | 0.22          |
| (1,306) | 1:16:C:CYS:H    | 1:16:C:CYS:HB3  | 10       | 0.22          |
| (1,273) | 1:15:C:CYS:H    | 1:13:C:ALA:HB3  | 3        | 0.22          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,266) | 1:31:C:TRP:HH2  | 1:19:C:LEU:HD13 | 5        | 0.22          |
| (1,266) | 1:31:C:TRP:HH2  | 1:19:C:LEU:HD13 | 7        | 0.22          |
| (1,162) | 1:18:C:HIS:HD2  | 1:18:C:HIS:HA   | 2        | 0.22          |
| (1,157) | 1:27:C:TYR:HD2  | 1:23:C:LYS:HA   | 4        | 0.22          |
| (4,80)  | 1:30:C:VAL:HG21 | 1:22:C:ARG:HD3  | 10       | 0.21          |
| (4,55)  | 1:19:C:LEU:HD12 | 1:29:C:CYS:HA   | 6        | 0.21          |
| (4,27)  | 1:28:C:HIS:HD2  | 1:22:C:ARG:HG3  | 8        | 0.21          |
| (4,10)  | 1:18:C:HIS:HD2  | 1:18:C:HIS:HA   | 2        | 0.21          |
| (4,10)  | 1:18:C:HIS:HD2  | 1:18:C:HIS:HA   | 9        | 0.21          |
| (3,93)  | 1:19:C:LEU:HB3  | 1:20:C:GLU:HG3  | 2        | 0.21          |
| (3,78)  | 1:30:C:VAL:HG21 | 1:22:C:ARG:HD3  | 10       | 0.21          |
| (3,53)  | 1:19:C:LEU:HD12 | 1:29:C:CYS:HA   | 6        | 0.21          |
| (3,11)  | 1:33:C:TRP:HZ3  | 1:33:C:TRP:HB3  | 10       | 0.21          |
| (1,366) | 1:5:C:TRP:HD1   | 1:6:C:LEU:HD12  | 2        | 0.21          |
| (1,366) | 1:5:C:TRP:HD1   | 1:6:C:LEU:HD13  | 10       | 0.21          |
| (1,355) | 1:5:C:TRP:H     | 1:19:C:LEU:HD21 | 4        | 0.21          |
| (1,355) | 1:5:C:TRP:H     | 1:19:C:LEU:HD22 | 10       | 0.21          |
| (1,352) | 1:6:C:LEU:H     | 1:19:C:LEU:HD22 | 9        | 0.21          |
| (1,273) | 1:15:C:CYS:H    | 1:13:C:ALA:HB1  | 5        | 0.21          |
| (1,199) | 1:33:C:TRP:H    | 1:32:C:ASP:HB2  | 9        | 0.21          |
| (1,162) | 1:18:C:HIS:HD2  | 1:18:C:HIS:HA   | 8        | 0.21          |
| (1,162) | 1:18:C:HIS:HD2  | 1:18:C:HIS:HA   | 9        | 0.21          |
| (1,156) | 1:31:C:TRP:HZ3  | 1:18:C:HIS:HB3  | 5        | 0.21          |
| (4,95)  | 1:19:C:LEU:HB3  | 1:20:C:GLU:HG3  | 2        | 0.2           |
| (4,12)  | 1:33:C:TRP:HZ3  | 1:33:C:TRP:HB3  | 10       | 0.2           |
| (4,10)  | 1:18:C:HIS:HD2  | 1:18:C:HIS:HA   | 1        | 0.2           |
| (4,10)  | 1:18:C:HIS:HD2  | 1:18:C:HIS:HA   | 8        | 0.2           |
| (3,35)  | 1:25:C:ALA:H    | 1:24:C:LYS:HG2  | 1        | 0.2           |
| (3,25)  | 1:28:C:HIS:HD2  | 1:22:C:ARG:HG3  | 5        | 0.2           |
| (3,25)  | 1:28:C:HIS:HD2  | 1:22:C:ARG:HG3  | 7        | 0.2           |
| (1,573) | 1:30:C:VAL:HG22 | 1:22:C:ARG:HB2  | 4        | 0.2           |
| (1,573) | 1:30:C:VAL:HG21 | 1:22:C:ARG:HB2  | 5        | 0.2           |
| (1,573) | 1:30:C:VAL:HG22 | 1:22:C:ARG:HB2  | 6        | 0.2           |
| (1,386) | 1:12:C:ASP:HA   | 1:20:C:GLU:HA   | 9        | 0.2           |
| (1,366) | 1:5:C:TRP:HD1   | 1:6:C:LEU:HD12  | 8        | 0.2           |
| (1,360) | 1:31:C:TRP:H    | 1:19:C:LEU:HD21 | 8        | 0.2           |
| (1,355) | 1:5:C:TRP:H     | 1:19:C:LEU:HD23 | 7        | 0.2           |
| (1,346) | 1:5:C:TRP:HE1   | 1:19:C:LEU:HD22 | 6        | 0.2           |
| (1,345) | 1:5:C:TRP:HE1   | 1:6:C:LEU:HD12  | 8        | 0.2           |
| (1,322) | 1:21:C:CYS:H    | 1:20:C:GLU:HG2  | 2        | 0.2           |
| (1,289) | 1:13:C:ALA:H    | 1:13:C:ALA:HB3  | 2        | 0.2           |
| (1,283) | 1:5:C:TRP:H     | 1:19:C:LEU:HD11 | 6        | 0.2           |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,283) | 1:5:C:TRP:H     | 1:19:C:LEU:HD13 | 7        | 0.2           |
| (1,273) | 1:15:C:CYS:H    | 1:13:C:ALA:HB2  | 8        | 0.2           |
| (1,266) | 1:31:C:TRP:HH2  | 1:19:C:LEU:HD13 | 4        | 0.2           |
| (1,218) | 1:31:C:TRP:HH2  | 1:5:C:TRP:HB3   | 1        | 0.2           |
| (1,162) | 1:18:C:HIS:HD2  | 1:18:C:HIS:HA   | 1        | 0.2           |
| (1,162) | 1:18:C:HIS:HD2  | 1:18:C:HIS:HA   | 10       | 0.2           |
| (1,2)   | 1:5:C:TRP:H     | 1:5:C:TRP:HB3   | 1        | 0.2           |
| (4,37)  | 1:25:C:ALA:H    | 1:24:C:LYS:HG2  | 1        | 0.19          |
| (4,27)  | 1:28:C:HIS:HD2  | 1:22:C:ARG:HG3  | 5        | 0.19          |
| (4,27)  | 1:28:C:HIS:HD2  | 1:22:C:ARG:HG3  | 7        | 0.19          |
| (4,22)  | 1:22:C:ARG:H    | 1:22:C:ARG:HG3  | 6        | 0.19          |
| (4,10)  | 1:18:C:HIS:HD2  | 1:18:C:HIS:HA   | 10       | 0.19          |
| (3,93)  | 1:19:C:LEU:HB3  | 1:20:C:GLU:HG3  | 1        | 0.19          |
| (3,35)  | 1:25:C:ALA:H    | 1:24:C:LYS:HG3  | 9        | 0.19          |
| (3,21)  | 1:22:C:ARG:H    | 1:22:C:ARG:HG3  | 6        | 0.19          |
| (1,346) | 1:5:C:TRP:HE1   | 1:19:C:LEU:HD22 | 2        | 0.19          |
| (1,290) | 1:23:C:LYS:H    | 1:23:C:LYS:HG2  | 4        | 0.19          |
| (1,289) | 1:13:C:ALA:H    | 1:13:C:ALA:HB3  | 1        | 0.19          |
| (1,289) | 1:13:C:ALA:H    | 1:13:C:ALA:HB2  | 4        | 0.19          |
| (1,283) | 1:5:C:TRP:H     | 1:19:C:LEU:HD13 | 5        | 0.19          |
| (1,266) | 1:31:C:TRP:HH2  | 1:19:C:LEU:HD11 | 8        | 0.19          |
| (4,95)  | 1:19:C:LEU:HB3  | 1:20:C:GLU:HG3  | 1        | 0.18          |
| (4,95)  | 1:19:C:LEU:HB3  | 1:20:C:GLU:HG3  | 4        | 0.18          |
| (4,37)  | 1:25:C:ALA:H    | 1:24:C:LYS:HG3  | 9        | 0.18          |
| (4,37)  | 1:25:C:ALA:H    | 1:24:C:LYS:HG2  | 10       | 0.18          |
| (4,27)  | 1:28:C:HIS:HD2  | 1:22:C:ARG:HG3  | 9        | 0.18          |
| (4,24)  | 1:28:C:HIS:H    | 1:22:C:ARG:HG3  | 1        | 0.18          |
| (3,93)  | 1:19:C:LEU:HB3  | 1:20:C:GLU:HG3  | 4        | 0.18          |
| (3,45)  | 1:7:C:GLY:H     | 1:3:C:ARG:HB3   | 7        | 0.18          |
| (3,35)  | 1:25:C:ALA:H    | 1:24:C:LYS:HG2  | 10       | 0.18          |
| (3,25)  | 1:28:C:HIS:HD2  | 1:22:C:ARG:HG3  | 9        | 0.18          |
| (3,23)  | 1:28:C:HIS:H    | 1:22:C:ARG:HG3  | 1        | 0.18          |
| (3,13)  | 1:15:C:CYS:H    | 1:9:C:CYS:HB2   | 7        | 0.18          |
| (1,573) | 1:30:C:VAL:HG22 | 1:22:C:ARG:HB2  | 2        | 0.18          |
| (1,540) | 1:3:C:ARG:HG3   | 1:11:C:LYS:HE3  | 4        | 0.18          |
| (1,366) | 1:5:C:TRP:HD1   | 1:6:C:LEU:HD13  | 6        | 0.18          |
| (1,346) | 1:5:C:TRP:HE1   | 1:19:C:LEU:HD23 | 3        | 0.18          |
| (1,322) | 1:21:C:CYS:H    | 1:20:C:GLU:HG2  | 4        | 0.18          |
| (1,322) | 1:21:C:CYS:H    | 1:20:C:GLU:HG2  | 10       | 0.18          |
| (1,290) | 1:23:C:LYS:H    | 1:23:C:LYS:HG2  | 1        | 0.18          |
| (1,283) | 1:5:C:TRP:H     | 1:19:C:LEU:HD12 | 3        | 0.18          |
| (1,266) | 1:31:C:TRP:HH2  | 1:19:C:LEU:HD11 | 2        | 0.18          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,255) | 1:27:C:TYR:HE2  | 1:23:C:LYS:HB3  | 3        | 0.18          |
| (1,2)   | 1:5:C:TRP:H     | 1:5:C:TRP:HB3   | 5        | 0.18          |
| (4,59)  | 1:34:C:THR:HG23 | 1:33:C:TRP:HA   | 1        | 0.17          |
| (4,47)  | 1:7:C:GLY:H     | 1:3:C:ARG:HB3   | 7        | 0.17          |
| (4,40)  | 1:29:C:CYS:H    | 1:29:C:CYS:HB3  | 9        | 0.17          |
| (4,14)  | 1:15:C:CYS:H    | 1:9:C:CYS:HB2   | 7        | 0.17          |
| (4,12)  | 1:33:C:TRP:HZ3  | 1:33:C:TRP:HB3  | 2        | 0.17          |
| (4,12)  | 1:33:C:TRP:HZ3  | 1:33:C:TRP:HB3  | 4        | 0.17          |
| (4,10)  | 1:18:C:HIS:HD2  | 1:18:C:HIS:HA   | 6        | 0.17          |
| (3,57)  | 1:34:C:THR:HG23 | 1:33:C:TRP:HA   | 1        | 0.17          |
| (3,38)  | 1:29:C:CYS:H    | 1:29:C:CYS:HB3  | 9        | 0.17          |
| (3,11)  | 1:33:C:TRP:HZ3  | 1:33:C:TRP:HB3  | 2        | 0.17          |
| (3,11)  | 1:33:C:TRP:HZ3  | 1:33:C:TRP:HB3  | 3        | 0.17          |
| (3,11)  | 1:33:C:TRP:HZ3  | 1:33:C:TRP:HB3  | 4        | 0.17          |
| (3,11)  | 1:33:C:TRP:HZ3  | 1:33:C:TRP:HB3  | 8        | 0.17          |
| (1,605) | 1:5:C:TRP:HZ2   | 1:30:C:VAL:HA   | 9        | 0.17          |
| (1,598) | 1:11:C:LYS:H    | 1:10:C:SER:HB3  | 1        | 0.17          |
| (1,355) | 1:5:C:TRP:H     | 1:19:C:LEU:HD21 | 5        | 0.17          |
| (1,346) | 1:5:C:TRP:HE1   | 1:19:C:LEU:HD21 | 10       | 0.17          |
| (1,345) | 1:5:C:TRP:HE1   | 1:6:C:LEU:HD13  | 7        | 0.17          |
| (1,341) | 1:12:C:ASP:H    | 1:11:C:LYS:HG2  | 2        | 0.17          |
| (1,289) | 1:13:C:ALA:H    | 1:13:C:ALA:HB2  | 6        | 0.17          |
| (1,283) | 1:5:C:TRP:H     | 1:19:C:LEU:HD11 | 2        | 0.17          |
| (1,283) | 1:5:C:TRP:H     | 1:19:C:LEU:HD11 | 8        | 0.17          |
| (1,273) | 1:15:C:CYS:H    | 1:13:C:ALA:HB3  | 9        | 0.17          |
| (1,266) | 1:31:C:TRP:HH2  | 1:19:C:LEU:HD12 | 3        | 0.17          |
| (1,192) | 1:28:C:HIS:HD2  | 1:6:C:LEU:HA    | 9        | 0.17          |
| (1,162) | 1:18:C:HIS:HD2  | 1:18:C:HIS:HA   | 4        | 0.17          |
| (1,162) | 1:18:C:HIS:HD2  | 1:18:C:HIS:HA   | 6        | 0.17          |
| (1,128) | 1:34:C:THR:H    | 1:34:C:THR:HB   | 5        | 0.17          |
| (1,2)   | 1:5:C:TRP:H     | 1:5:C:TRP:HB3   | 10       | 0.17          |
| (4,40)  | 1:29:C:CYS:H    | 1:29:C:CYS:HB3  | 1        | 0.16          |
| (4,40)  | 1:29:C:CYS:H    | 1:29:C:CYS:HB3  | 5        | 0.16          |
| (4,40)  | 1:29:C:CYS:H    | 1:29:C:CYS:HB3  | 7        | 0.16          |
| (4,12)  | 1:33:C:TRP:HZ3  | 1:33:C:TRP:HB3  | 3        | 0.16          |
| (4,12)  | 1:33:C:TRP:HZ3  | 1:33:C:TRP:HB3  | 8        | 0.16          |
| (4,10)  | 1:18:C:HIS:HD2  | 1:18:C:HIS:HA   | 4        | 0.16          |
| (4,2)   | 1:31:C:TRP:HE1  | 1:5:C:TRP:HZ3   | 8        | 0.16          |
| (3,102) | 1:23:C:LYS:H    | 1:23:C:LYS:HB3  | 3        | 0.16          |
| (3,68)  | 1:15:C:CYS:HB2  | 1:9:C:CYS:HB3   | 7        | 0.16          |
| (3,38)  | 1:29:C:CYS:H    | 1:29:C:CYS:HB3  | 1        | 0.16          |
| (3,38)  | 1:29:C:CYS:H    | 1:29:C:CYS:HB3  | 3        | 0.16          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (3,38)  | 1:29:C:CYS:H    | 1:29:C:CYS:HB3  | 5        | 0.16          |
| (3,38)  | 1:29:C:CYS:H    | 1:29:C:CYS:HB3  | 7        | 0.16          |
| (3,38)  | 1:29:C:CYS:H    | 1:29:C:CYS:HB3  | 8        | 0.16          |
| (3,30)  | 1:31:C:TRP:H    | 1:30:C:VAL:HG23 | 9        | 0.16          |
| (3,2)   | 1:31:C:TRP:HE1  | 1:5:C:TRP:HZ3   | 6        | 0.16          |
| (3,2)   | 1:31:C:TRP:HE1  | 1:5:C:TRP:HZ3   | 8        | 0.16          |
| (1,533) | 1:1:C:ALA:HB1   | 1:11:C:LYS:HE2  | 4        | 0.16          |
| (1,382) | 1:11:C:LYS:HD3  | 1:14:C:ASP:HA   | 5        | 0.16          |
| (1,360) | 1:31:C:TRP:H    | 1:19:C:LEU:HD21 | 9        | 0.16          |
| (1,346) | 1:5:C:TRP:HE1   | 1:19:C:LEU:HD22 | 7        | 0.16          |
| (1,341) | 1:12:C:ASP:H    | 1:11:C:LYS:HG2  | 6        | 0.16          |
| (1,322) | 1:21:C:CYS:H    | 1:20:C:GLU:HG2  | 5        | 0.16          |
| (1,283) | 1:5:C:TRP:H     | 1:19:C:LEU:HD12 | 10       | 0.16          |
| (1,255) | 1:27:C:TYR:HE2  | 1:23:C:LYS:HB3  | 10       | 0.16          |
| (1,60)  | 1:24:C:LYS:H    | 1:27:C:TYR:HD1  | 4        | 0.16          |
| (1,2)   | 1:5:C:TRP:H     | 1:5:C:TRP:HB3   | 3        | 0.16          |
| (1,2)   | 1:5:C:TRP:H     | 1:5:C:TRP:HB3   | 6        | 0.16          |
| (4,104) | 1:23:C:LYS:H    | 1:23:C:LYS:HB3  | 3        | 0.15          |
| (4,104) | 1:23:C:LYS:H    | 1:23:C:LYS:HB3  | 9        | 0.15          |
| (4,70)  | 1:15:C:CYS:HB2  | 1:9:C:CYS:HB3   | 3        | 0.15          |
| (4,70)  | 1:15:C:CYS:HB2  | 1:9:C:CYS:HB3   | 7        | 0.15          |
| (4,70)  | 1:15:C:CYS:HB2  | 1:9:C:CYS:HB3   | 10       | 0.15          |
| (4,40)  | 1:29:C:CYS:H    | 1:29:C:CYS:HB3  | 3        | 0.15          |
| (4,40)  | 1:29:C:CYS:H    | 1:29:C:CYS:HB3  | 4        | 0.15          |
| (4,40)  | 1:29:C:CYS:H    | 1:29:C:CYS:HB3  | 8        | 0.15          |
| (4,35)  | 1:34:C:THR:H    | 1:35:C:VAL:HG12 | 7        | 0.15          |
| (4,32)  | 1:31:C:TRP:H    | 1:30:C:VAL:HG23 | 9        | 0.15          |
| (4,10)  | 1:18:C:HIS:HD2  | 1:18:C:HIS:HA   | 3        | 0.15          |
| (4,10)  | 1:18:C:HIS:HD2  | 1:18:C:HIS:HA   | 7        | 0.15          |
| (4,2)   | 1:31:C:TRP:HE1  | 1:5:C:TRP:HZ3   | 6        | 0.15          |
| (4,2)   | 1:31:C:TRP:HE1  | 1:5:C:TRP:HZ3   | 10       | 0.15          |
| (3,102) | 1:23:C:LYS:H    | 1:23:C:LYS:HB3  | 9        | 0.15          |
| (3,98)  | 1:24:C:LYS:HG2  | 1:24:C:LYS:HB2  | 9        | 0.15          |
| (3,68)  | 1:15:C:CYS:HB2  | 1:9:C:CYS:HB3   | 3        | 0.15          |
| (3,68)  | 1:15:C:CYS:HB2  | 1:9:C:CYS:HB3   | 10       | 0.15          |
| (3,38)  | 1:29:C:CYS:H    | 1:29:C:CYS:HB3  | 4        | 0.15          |
| (3,33)  | 1:34:C:THR:H    | 1:35:C:VAL:HG12 | 7        | 0.15          |
| (3,2)   | 1:31:C:TRP:HE1  | 1:5:C:TRP:HZ3   | 9        | 0.15          |
| (3,2)   | 1:31:C:TRP:HE1  | 1:5:C:TRP:HZ3   | 10       | 0.15          |
| (1,533) | 1:1:C:ALA:HB3   | 1:11:C:LYS:HE2  | 2        | 0.15          |
| (1,516) | 1:30:C:VAL:HG13 | 1:6:C:LEU:HA    | 9        | 0.15          |
| (1,363) | 1:31:C:TRP:HZ2  | 1:19:C:LEU:HD21 | 6        | 0.15          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,360) | 1:31:C:TRP:H   | 1:19:C:LEU:HD23 | 10       | 0.15          |
| (1,355) | 1:5:C:TRP:H    | 1:19:C:LEU:HD21 | 3        | 0.15          |
| (1,346) | 1:5:C:TRP:HE1  | 1:19:C:LEU:HD23 | 4        | 0.15          |
| (1,289) | 1:13:C:ALA:H   | 1:13:C:ALA:HB1  | 5        | 0.15          |
| (1,283) | 1:5:C:TRP:H    | 1:19:C:LEU:HD13 | 4        | 0.15          |
| (1,280) | 1:31:C:TRP:HE3 | 1:19:C:LEU:HD12 | 1        | 0.15          |
| (1,255) | 1:27:C:TYR:HE1 | 1:23:C:LYS:HB3  | 1        | 0.15          |
| (1,162) | 1:18:C:HIS:HD2 | 1:18:C:HIS:HA   | 3        | 0.15          |
| (1,162) | 1:18:C:HIS:HD2 | 1:18:C:HIS:HA   | 7        | 0.15          |
| (1,2)   | 1:5:C:TRP:H    | 1:5:C:TRP:HB3   | 4        | 0.15          |
| (1,2)   | 1:5:C:TRP:H    | 1:5:C:TRP:HB3   | 7        | 0.15          |
| (1,2)   | 1:5:C:TRP:H    | 1:5:C:TRP:HB3   | 9        | 0.15          |
| (4,104) | 1:23:C:LYS:H   | 1:23:C:LYS:HB3  | 4        | 0.14          |
| (4,100) | 1:24:C:LYS:HG2 | 1:24:C:LYS:HB2  | 9        | 0.14          |
| (4,70)  | 1:15:C:CYS:HB2 | 1:9:C:CYS:HB3   | 5        | 0.14          |
| (4,70)  | 1:15:C:CYS:HB2 | 1:9:C:CYS:HB3   | 8        | 0.14          |
| (4,65)  | 1:23:C:LYS:HD2 | 1:23:C:LYS:HA   | 9        | 0.14          |
| (4,40)  | 1:29:C:CYS:H   | 1:29:C:CYS:HB3  | 2        | 0.14          |
| (4,40)  | 1:29:C:CYS:H   | 1:29:C:CYS:HB3  | 6        | 0.14          |
| (4,40)  | 1:29:C:CYS:H   | 1:29:C:CYS:HB3  | 10       | 0.14          |
| (4,12)  | 1:22:C:ARG:HE  | 1:26:C:PRO:HD3  | 6        | 0.14          |
| (4,2)   | 1:31:C:TRP:HE1 | 1:5:C:TRP:HZ3   | 9        | 0.14          |
| (3,102) | 1:23:C:LYS:H   | 1:23:C:LYS:HB3  | 1        | 0.14          |
| (3,102) | 1:23:C:LYS:H   | 1:23:C:LYS:HB3  | 4        | 0.14          |
| (3,68)  | 1:15:C:CYS:HB2 | 1:9:C:CYS:HB3   | 5        | 0.14          |
| (3,68)  | 1:15:C:CYS:HB2 | 1:9:C:CYS:HB3   | 8        | 0.14          |
| (3,63)  | 1:23:C:LYS:HD2 | 1:23:C:LYS:HA   | 9        | 0.14          |
| (3,38)  | 1:29:C:CYS:H   | 1:29:C:CYS:HB3  | 2        | 0.14          |
| (3,38)  | 1:29:C:CYS:H   | 1:29:C:CYS:HB3  | 6        | 0.14          |
| (3,38)  | 1:29:C:CYS:H   | 1:29:C:CYS:HB3  | 10       | 0.14          |
| (3,11)  | 1:22:C:ARG:HE  | 1:26:C:PRO:HD3  | 6        | 0.14          |
| (1,605) | 1:5:C:TRP:HZ2  | 1:30:C:VAL:HA   | 8        | 0.14          |
| (1,402) | 1:35:C:VAL:HB  | 1:30:C:VAL:HA   | 1        | 0.14          |
| (1,366) | 1:5:C:TRP:HD1  | 1:6:C:LEU:HD11  | 1        | 0.14          |
| (1,289) | 1:13:C:ALA:H   | 1:13:C:ALA:HB1  | 3        | 0.14          |
| (1,281) | 1:19:C:LEU:H   | 1:19:C:LEU:HD13 | 6        | 0.14          |
| (1,266) | 1:31:C:TRP:HH2 | 1:19:C:LEU:HD12 | 10       | 0.14          |
| (1,157) | 1:27:C:TYR:HD1 | 1:23:C:LYS:HA   | 1        | 0.14          |
| (1,157) | 1:27:C:TYR:HD2 | 1:23:C:LYS:HA   | 7        | 0.14          |
| (1,60)  | 1:24:C:LYS:H   | 1:27:C:TYR:HD2  | 2        | 0.14          |
| (1,2)   | 1:5:C:TRP:H    | 1:5:C:TRP:HB3   | 2        | 0.14          |
| (1,2)   | 1:5:C:TRP:H    | 1:5:C:TRP:HB3   | 8        | 0.14          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (4,104) | 1:23:C:LYS:H    | 1:23:C:LYS:HB3  | 1        | 0.13          |
| (4,104) | 1:23:C:LYS:H    | 1:23:C:LYS:HB3  | 8        | 0.13          |
| (4,70)  | 1:15:C:CYS:HB2  | 1:9:C:CYS:HB3   | 2        | 0.13          |
| (3,102) | 1:23:C:LYS:H    | 1:23:C:LYS:HB3  | 8        | 0.13          |
| (3,68)  | 1:15:C:CYS:HB2  | 1:9:C:CYS:HB3   | 2        | 0.13          |
| (3,9)   | 1:4:C:GLU:H     | 1:3:C:ARG:HD3   | 7        | 0.13          |
| (3,2)   | 1:31:C:TRP:HE1  | 1:5:C:TRP:HZ3   | 2        | 0.13          |
| (1,605) | 1:5:C:TRP:HZ2   | 1:30:C:VAL:HA   | 1        | 0.13          |
| (1,605) | 1:5:C:TRP:HZ2   | 1:30:C:VAL:HA   | 3        | 0.13          |
| (1,605) | 1:5:C:TRP:HZ2   | 1:30:C:VAL:HA   | 7        | 0.13          |
| (1,599) | 1:14:C:ASP:H    | 1:14:C:ASP:HB3  | 6        | 0.13          |
| (1,573) | 1:30:C:VAL:HG22 | 1:22:C:ARG:HB2  | 8        | 0.13          |
| (1,538) | 1:22:C:ARG:HB2  | 1:22:C:ARG:HD2  | 1        | 0.13          |
| (1,538) | 1:22:C:ARG:HB2  | 1:22:C:ARG:HD2  | 2        | 0.13          |
| (1,538) | 1:22:C:ARG:HB2  | 1:22:C:ARG:HD2  | 8        | 0.13          |
| (1,533) | 1:1:C:ALA:HB1   | 1:11:C:LYS:HE2  | 9        | 0.13          |
| (1,386) | 1:12:C:ASP:HA   | 1:20:C:GLU:HA   | 7        | 0.13          |
| (1,386) | 1:12:C:ASP:HA   | 1:20:C:GLU:HA   | 8        | 0.13          |
| (1,386) | 1:12:C:ASP:HA   | 1:20:C:GLU:HA   | 10       | 0.13          |
| (1,289) | 1:13:C:ALA:H    | 1:13:C:ALA:HB1  | 10       | 0.13          |
| (1,205) | 1:11:C:LYS:H    | 1:21:C:CYS:HB3  | 4        | 0.13          |
| (1,128) | 1:34:C:THR:H    | 1:34:C:THR:HB   | 1        | 0.13          |
| (4,46)  | 1:29:C:CYS:H    | 1:22:C:ARG:HB2  | 9        | 0.12          |
| (4,32)  | 1:31:C:TRP:H    | 1:30:C:VAL:HG21 | 1        | 0.12          |
| (4,13)  | 1:9:C:CYS:H     | 1:9:C:CYS:HB3   | 1        | 0.12          |
| (4,9)   | 1:4:C:GLU:H     | 1:3:C:ARG:HD3   | 7        | 0.12          |
| (4,2)   | 1:31:C:TRP:HE1  | 1:5:C:TRP:HZ3   | 2        | 0.12          |
| (3,44)  | 1:29:C:CYS:H    | 1:22:C:ARG:HB2  | 9        | 0.12          |
| (3,30)  | 1:31:C:TRP:H    | 1:30:C:VAL:HG21 | 1        | 0.12          |
| (3,12)  | 1:9:C:CYS:H     | 1:9:C:CYS:HB3   | 1        | 0.12          |
| (1,605) | 1:5:C:TRP:HZ2   | 1:30:C:VAL:HA   | 2        | 0.12          |
| (1,605) | 1:5:C:TRP:HZ2   | 1:30:C:VAL:HA   | 6        | 0.12          |
| (1,538) | 1:22:C:ARG:HB2  | 1:22:C:ARG:HD2  | 4        | 0.12          |
| (1,538) | 1:22:C:ARG:HB2  | 1:22:C:ARG:HD2  | 9        | 0.12          |
| (1,533) | 1:1:C:ALA:HB1   | 1:11:C:LYS:HE2  | 1        | 0.12          |
| (1,528) | 1:19:C:LEU:HB3  | 1:14:C:ASP:HB2  | 9        | 0.12          |
| (1,520) | 1:6:C:LEU:HD12  | 1:30:C:VAL:HB   | 7        | 0.12          |
| (1,345) | 1:5:C:TRP:HE1   | 1:6:C:LEU:HD13  | 6        | 0.12          |
| (1,242) | 1:5:C:TRP:H     | 1:4:C:GLU:HB3   | 3        | 0.12          |
| (1,230) | 1:33:C:TRP:H    | 1:31:C:TRP:HB2  | 8        | 0.12          |
| (1,157) | 1:27:C:TYR:HD2  | 1:23:C:LYS:HA   | 3        | 0.12          |
| (4,100) | 1:24:C:LYS:HG3  | 1:24:C:LYS:HB2  | 3        | 0.11          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (4,100) | 1:24:C:LYS:HG2  | 1:24:C:LYS:HB2  | 4        | 0.11          |
| (4,9)   | 1:4:C:GLU:H     | 1:3:C:ARG:HD2   | 5        | 0.11          |
| (3,98)  | 1:24:C:LYS:HG3  | 1:24:C:LYS:HB2  | 3        | 0.11          |
| (3,98)  | 1:24:C:LYS:HG2  | 1:24:C:LYS:HB2  | 4        | 0.11          |
| (3,9)   | 1:4:C:GLU:H     | 1:3:C:ARG:HD2   | 5        | 0.11          |
| (1,605) | 1:5:C:TRP:HZ2   | 1:30:C:VAL:HA   | 10       | 0.11          |
| (1,538) | 1:22:C:ARG:HB2  | 1:22:C:ARG:HD2  | 5        | 0.11          |
| (1,516) | 1:30:C:VAL:HG11 | 1:6:C:LEU:HA    | 1        | 0.11          |
| (1,416) | 1:20:C:GLU:HG2  | 1:20:C:GLU:HA   | 8        | 0.11          |
| (1,402) | 1:35:C:VAL:HB   | 1:30:C:VAL:HA   | 6        | 0.11          |
| (1,360) | 1:31:C:TRP:H    | 1:19:C:LEU:HD23 | 1        | 0.11          |
| (1,306) | 1:16:C:CYS:H    | 1:16:C:CYS:HB3  | 1        | 0.11          |
| (1,306) | 1:16:C:CYS:H    | 1:16:C:CYS:HB3  | 3        | 0.11          |
| (1,290) | 1:23:C:LYS:H    | 1:23:C:LYS:HG2  | 3        | 0.11          |
| (1,266) | 1:31:C:TRP:HH2  | 1:19:C:LEU:HD12 | 9        | 0.11          |
| (1,242) | 1:5:C:TRP:H     | 1:4:C:GLU:HB3   | 5        | 0.11          |
| (1,192) | 1:28:C:HIS:HD2  | 1:6:C:LEU:HA    | 1        | 0.11          |
| (1,386) | 1:12:C:ASP:HA   | 1:20:C:GLU:HA   | 3        | 0.1           |
| (1,242) | 1:5:C:TRP:H     | 1:4:C:GLU:HB3   | 6        | 0.1           |
| (1,157) | 1:27:C:TYR:HD1  | 1:23:C:LYS:HA   | 6        | 0.1           |

## 10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found