



# Full wwPDB NMR Structure Validation Report ⓘ

Mar 6, 2026 – 01:19 PM UTC

PDB ID : 6R28 / pdb\_00006r28  
BMRB ID : 34380  
Title : Structure of peptide P7, which binds Cdc42 and inhibits effector interactions.  
Authors : Murphy, N.P.; Mott, H.R.; Owen, D.  
Deposited on : 2019-03-15

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

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
wwPDB-RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
wwPDB-ShiftChecker : v1.2  
BMRB Restraints Analysis : v1.2  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

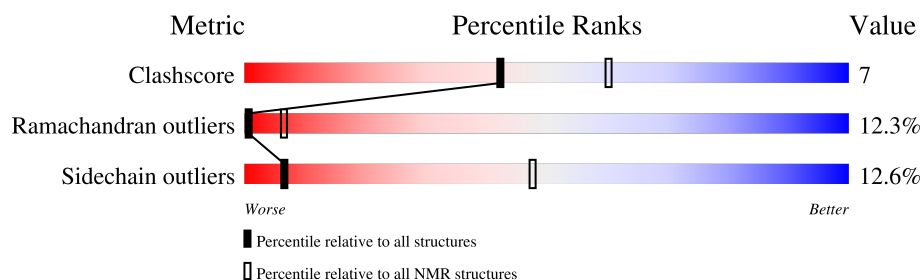
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 48%.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



| Metric                | Whole archive<br>(#Entries) | NMR archive<br>(#Entries) |
|-----------------------|-----------------------------|---------------------------|
| Clashscore            | 229148                      | 14424                     |
| Ramachandran outliers | 224038                      | 12848                     |
| Sidechain outliers    | 223484                      | 12823                     |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$

| Mol | Chain | Length | Quality of chain                                          |
|-----|-------|--------|-----------------------------------------------------------|
| 1   | A     | 16     | <div> <div>38%</div> <div>25%</div> <div>38%</div> </div> |

## 2 Ensemble composition and analysis

This entry contains 35 models. Model 15 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

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

| Well-defined (core) protein residues |                       |                   |              |
|--------------------------------------|-----------------------|-------------------|--------------|
| Well-defined core                    | Residue range (total) | Backbone RMSD (Å) | Medoid model |
| 1                                    | A:6-A:15 (10)         | 0.13              | 15           |

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 6 clusters. No single-model clusters were found.

| Cluster number | Models                                                  |
|----------------|---------------------------------------------------------|
| 1              | 1, 2, 7, 14, 15, 18, 22, 24, 26, 28, 30, 31, 32, 33, 34 |
| 2              | 9, 10, 13, 17, 23, 27, 35                               |
| 3              | 6, 8, 11, 21                                            |
| 4              | 4, 5, 20                                                |
| 5              | 3, 12, 19                                               |
| 6              | 16, 25, 29                                              |

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

There is only 1 type of molecule in this entry. The entry contains 278 atoms, of which 133 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called peptide P7.

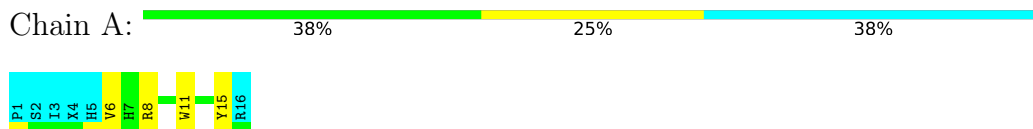
| Mol | Chain | Residues | Atoms |    |     |    |    |   | Trace |
|-----|-------|----------|-------|----|-----|----|----|---|-------|
| 1   | A     | 16       | Total | C  | H   | N  | O  | S | 0     |
|     |       |          | 278   | 95 | 133 | 28 | 20 | 2 |       |

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

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

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

- Molecule 1: peptide P7

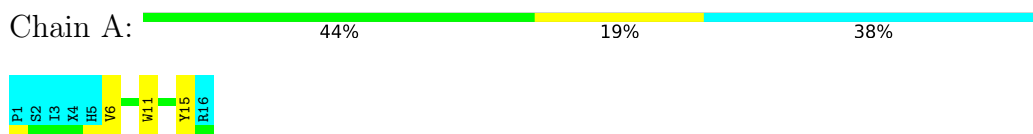


### 4.2 Scores per residue for each member of the ensemble

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

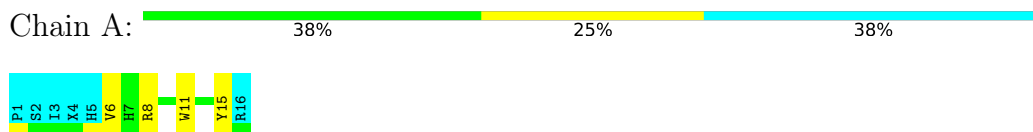
#### 4.2.1 Score per residue for model 1

- Molecule 1: peptide P7



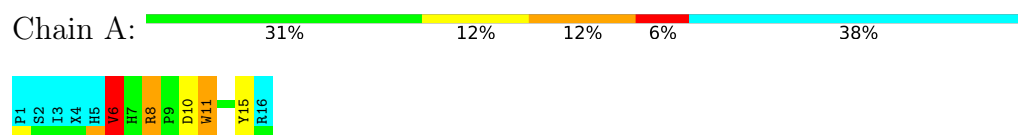
#### 4.2.2 Score per residue for model 2

- Molecule 1: peptide P7



### 4.2.3 Score per residue for model 3

- Molecule 1: peptide P7



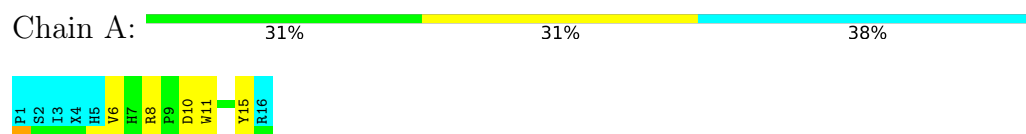
### 4.2.4 Score per residue for model 4

- Molecule 1: peptide P7



### 4.2.5 Score per residue for model 5

- Molecule 1: peptide P7



### 4.2.6 Score per residue for model 6

- Molecule 1: peptide P7



### 4.2.7 Score per residue for model 7

- Molecule 1: peptide P7



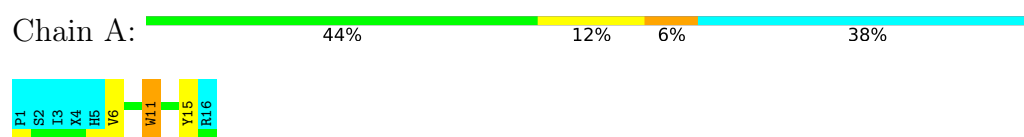
### 4.2.8 Score per residue for model 8

- Molecule 1: peptide P7



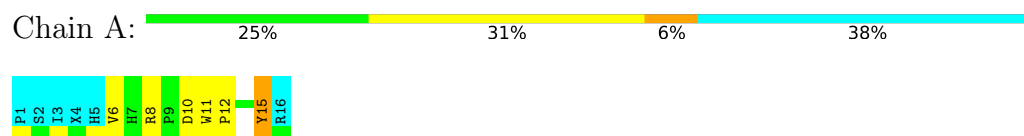
### 4.2.9 Score per residue for model 9

- Molecule 1: peptide P7



### 4.2.10 Score per residue for model 10

- Molecule 1: peptide P7



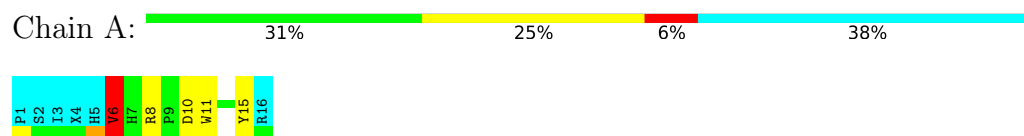
### 4.2.11 Score per residue for model 11

- Molecule 1: peptide P7



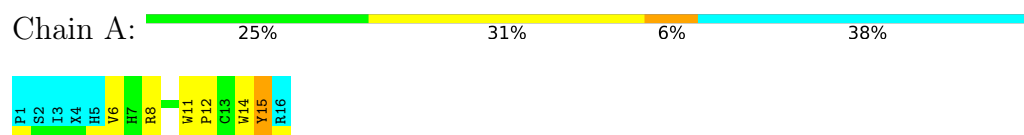
### 4.2.12 Score per residue for model 12

- Molecule 1: peptide P7



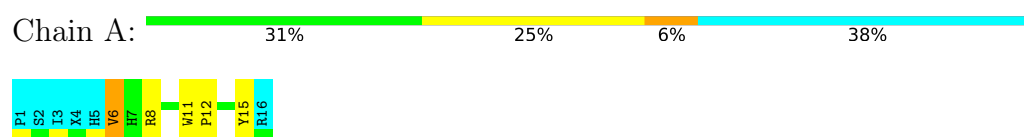
#### 4.2.13 Score per residue for model 13

- Molecule 1: peptide P7



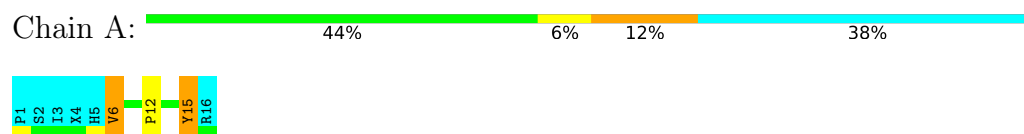
#### 4.2.14 Score per residue for model 14

- Molecule 1: peptide P7



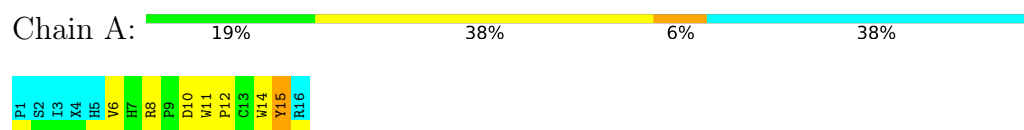
#### 4.2.15 Score per residue for model 15 (medoid)

- Molecule 1: peptide P7



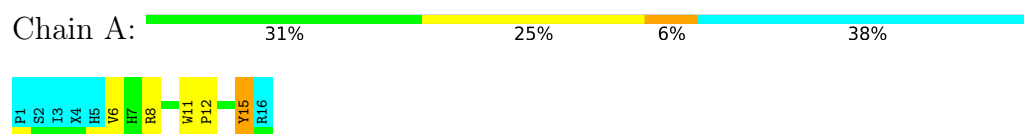
#### 4.2.16 Score per residue for model 16

- Molecule 1: peptide P7



#### 4.2.17 Score per residue for model 17

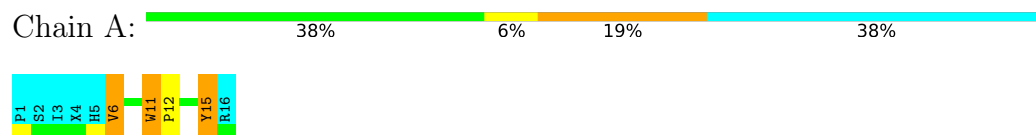
- Molecule 1: peptide P7





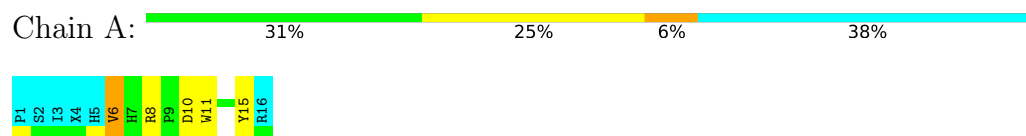
#### 4.2.18 Score per residue for model 18

- Molecule 1: peptide P7



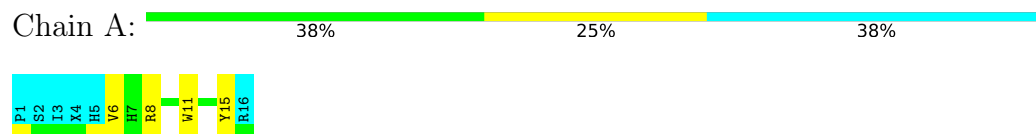
#### 4.2.19 Score per residue for model 19

- Molecule 1: peptide P7



#### 4.2.20 Score per residue for model 20

- Molecule 1: peptide P7



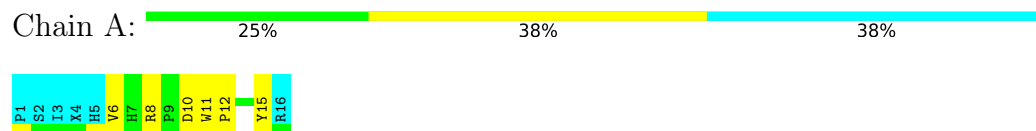
#### 4.2.21 Score per residue for model 21

- Molecule 1: peptide P7



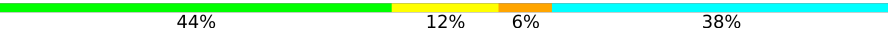
#### 4.2.22 Score per residue for model 22

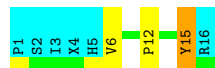
- Molecule 1: peptide P7



#### 4.2.23 Score per residue for model 23

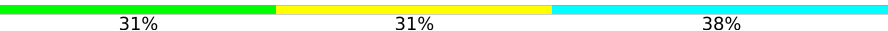
- Molecule 1: peptide P7

Chain A: 



#### 4.2.24 Score per residue for model 24

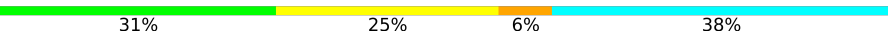
- Molecule 1: peptide P7

Chain A: 



#### 4.2.25 Score per residue for model 25

- Molecule 1: peptide P7

Chain A: 



#### 4.2.26 Score per residue for model 26

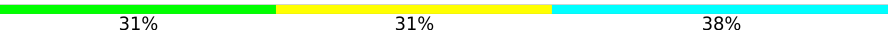
- Molecule 1: peptide P7

Chain A: 



#### 4.2.27 Score per residue for model 27

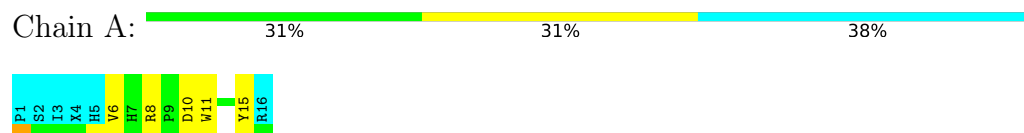
- Molecule 1: peptide P7

Chain A: 



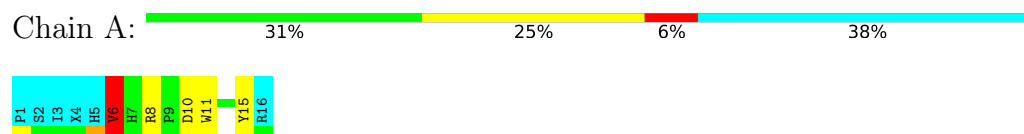
#### 4.2.28 Score per residue for model 28

- Molecule 1: peptide P7



#### 4.2.29 Score per residue for model 29

- Molecule 1: peptide P7



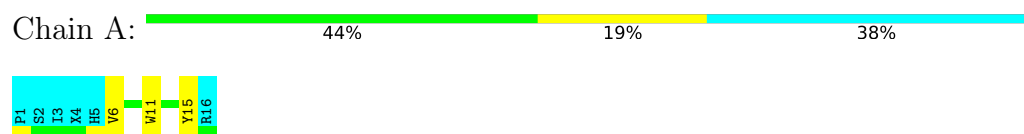
#### 4.2.30 Score per residue for model 30

- Molecule 1: peptide P7



#### 4.2.31 Score per residue for model 31

- Molecule 1: peptide P7



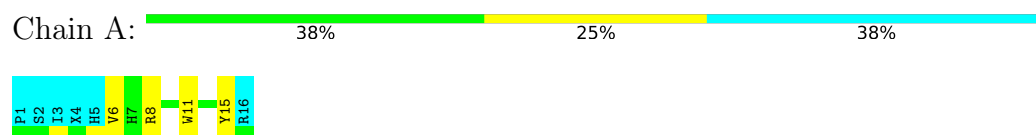
#### 4.2.32 Score per residue for model 32

- Molecule 1: peptide P7



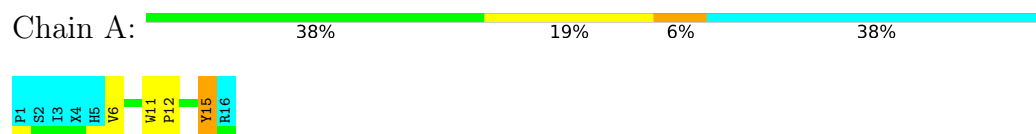
#### 4.2.33 Score per residue for model 33

- Molecule 1: peptide P7



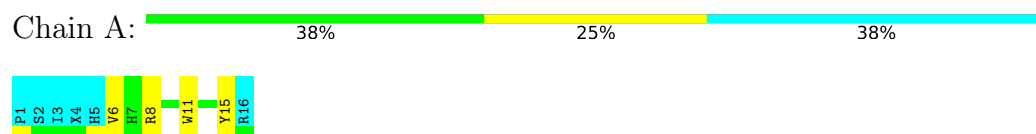
#### 4.2.34 Score per residue for model 34

- Molecule 1: peptide P7



#### 4.2.35 Score per residue for model 35

- Molecule 1: peptide P7



## 5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 35 were deposited, based on the following criterion: *structures with the lowest energy*.

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

| Software name | Classification        | Version |
|---------------|-----------------------|---------|
| ARIA          | structure calculation | 1.2     |
| CNS           | structure calculation |         |
| CNS           | refinement            |         |

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

|                                              |                |
|----------------------------------------------|----------------|
| Chemical shift file(s)                       | working_cs.cif |
| Number of chemical shift lists               | 1              |
| Total number of shifts                       | 112            |
| Number of shifts mapped to atoms             | 112            |
| Number of unparsed shifts                    | 0              |
| Number of shifts with mapping errors         | 0              |
| Number of shifts with mapping warnings       | 0              |
| Assignment completeness (well-defined parts) | 48%            |

## 6 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: HCS

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes |
|-----|-------|-------|----------|----------|---------|
| 1   | A     | 96    | 81       | 80       | 1±1     |
| All | All   | 3360  | 2835     | 2800     | 41      |

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 7.

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

| Atom-1         | Atom-2         | Clash(Å) | Distance(Å) | Models |       |
|----------------|----------------|----------|-------------|--------|-------|
|                |                |          |             | Worst  | Total |
| 1:A:8:ARG:HB2  | 1:A:11:TRP:CD1 | 0.61     | 2.31        | 16     | 18    |
| 1:A:8:ARG:HG3  | 1:A:11:TRP:CD2 | 0.57     | 2.35        | 3      | 1     |
| 1:A:8:ARG:HB3  | 1:A:10:ASP:OD1 | 0.47     | 2.09        | 19     | 5     |
| 1:A:12:PRO:HG2 | 1:A:15:TYR:H   | 0.44     | 1.72        | 25     | 9     |
| 1:A:6:VAL:HG11 | 1:A:12:PRO:O   | 0.43     | 2.14        | 14     | 3     |
| 1:A:11:TRP:C   | 1:A:11:TRP:CD1 | 0.42     | 2.98        | 9      | 2     |
| 1:A:11:TRP:HB2 | 1:A:12:PRO:HD2 | 0.41     | 1.92        | 22     | 1     |
| 1:A:8:ARG:H    | 1:A:11:TRP:NE1 | 0.41     | 2.14        | 35     | 1     |
| 1:A:11:TRP:CD1 | 1:A:11:TRP:C   | 0.40     | 3.00        | 18     | 1     |

## 6.3 Torsion angles [i](#)

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

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

| Mol | Chain | Analysed      | Favoured    | Allowed     | Outliers    | Percentiles |          |
|-----|-------|---------------|-------------|-------------|-------------|-------------|----------|
| 1   | A     | 10/16 (62%)   | 5±1 (53±7%) | 3±1 (35±6%) | 1±0 (12±4%) | <b>1</b>    | <b>6</b> |
| All | All   | 350/560 (62%) | 186 (53%)   | 121 (35%)   | 43 (12%)    | <b>1</b>    | <b>6</b> |

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

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 15  | TYR  | 35             |
| 1   | A     | 6   | VAL  | 8              |

### 6.3.2 Protein sidechains [i](#)

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

| Mol | Chain | Analysed      | Rotameric   | Outliers    | Percentiles |    |
|-----|-------|---------------|-------------|-------------|-------------|----|
| 1   | A     | 10/15 (67%)   | 9±1 (87±6%) | 1±1 (13±6%) | <b>6</b>    | 48 |
| All | All   | 350/525 (67%) | 306 (87%)   | 44 (13%)    | <b>6</b>    | 48 |

All 4 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 6   | VAL  | 35             |
| 1   | A     | 11  | TRP  | 5              |
| 1   | A     | 10  | ASP  | 3              |
| 1   | A     | 8   | ARG  | 1              |

### 6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

| Mol | Type | Chain | Res | Link | Bond lengths |           |            |
|-----|------|-------|-----|------|--------------|-----------|------------|
|     |      |       |     |      | Counts       | RMSZ      | #Z>2       |
| 1   | HCS  | A     | 4   | 1    | 5,6,7        | 0.60±0.03 | 0±0 (0±0%) |

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

| Mol | Type | Chain | Res | Link | Bond angles |           |            |
|-----|------|-------|-----|------|-------------|-----------|------------|
|     |      |       |     |      | Counts      | RMSZ      | #Z>2       |
| 1   | HCS  | A     | 4   | 1    | 2,6,8       | 0.69±0.23 | 0±0 (0±0%) |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions  | Rings |
|-----|------|-------|-----|------|---------|-----------|-------|
| 1   | HCS  | A     | 4   | 1    | -       | 0±0,4,5,7 | -     |

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no torsion outliers.



There are no ring outliers.

## 6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 6.7 Other polymers [i](#)

There are no such molecules in this entry.

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

There are no chain breaks in this entry.

## 7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 48% for the well-defined parts and 46% for the entire structure.

### 7.1 Chemical shift list 1

File name: working\_cs.cif

Chemical shift list name: *peptide7.csv4*

#### 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                  | 112 |
| Number of shifts mapped to atoms        | 112 |
| 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

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

#### 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 48%, i.e. 73 atoms were assigned a chemical shift out of a possible 152. 0 out of 1 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total        | <sup>1</sup> H | <sup>13</sup> C | <sup>15</sup> N |
|-----------|--------------|----------------|-----------------|-----------------|
| Backbone  | 18/46 (39%)  | 18/18 (100%)   | 0/20 (0%)       | 0/8 (0%)        |
| Sidechain | 37/65 (57%)  | 37/42 (88%)    | 0/20 (0%)       | 0/3 (0%)        |
| Aromatic  | 18/41 (44%)  | 18/20 (90%)    | 0/17 (0%)       | 0/4 (0%)        |
| Overall   | 73/152 (48%) | 73/80 (91%)    | 0/57 (0%)       | 0/15 (0%)       |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 46%, i.e. 106 atoms were assigned a chemical shift out of a possible 229. 0 out of 1 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total         | $^1\text{H}$  | $^{13}\text{C}$ | $^{15}\text{N}$ |
|-----------|---------------|---------------|-----------------|-----------------|
| Backbone  | 26/69 (38%)   | 26/27 (96%)   | 0/30 (0%)       | 0/12 (0%)       |
| Sidechain | 60/111 (54%)  | 60/72 (83%)   | 0/33 (0%)       | 0/6 (0%)        |
| Aromatic  | 20/49 (41%)   | 20/24 (83%)   | 0/19 (0%)       | 0/6 (0%)        |
| Overall   | 106/229 (46%) | 106/123 (86%) | 0/82 (0%)       | 0/24 (0%)       |

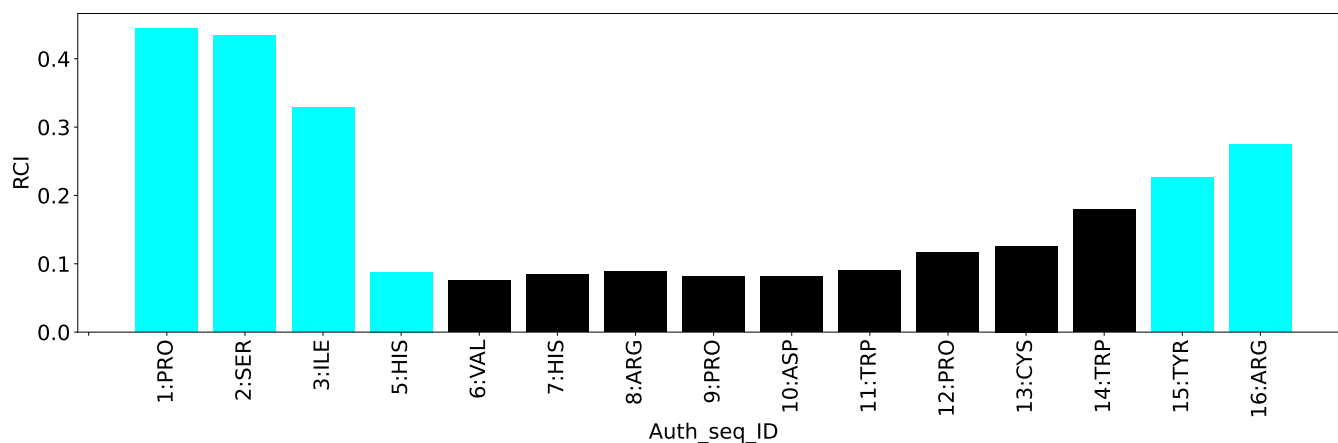
### 7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

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

Random coil index (RCI) for chain A:



## 8 NMR restraints analysis

### 8.1 Conformationally restricting restraints

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

| Description                                              | Value |
|----------------------------------------------------------|-------|
| Total distance restraints                                | 440   |
| Intra-residue ( $ i-j =0$ )                              | 170   |
| Sequential ( $ i-j =1$ )                                 | 114   |
| Medium range ( $ i-j >1$ and $ i-j <5$ )                 | 108   |
| Long range ( $ i-j \geq 5$ )                             | 48    |
| 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                         | 27.5  |
| Number of long range restraints per residue <sup>1</sup> | 3.0   |

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

### 8.2 Residual restraint violations

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

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

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

| Bins (Å)         | Average number of violations per model | Max (Å) |
|------------------|----------------------------------------|---------|
| 0.1-0.2 (Small)  | 9.0                                    | 0.2     |
| 0.2-0.5 (Medium) | 20.4                                   | 0.5     |
| >0.5 (Large)     | 23.9                                   | 2.4     |

### 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 ⓘ

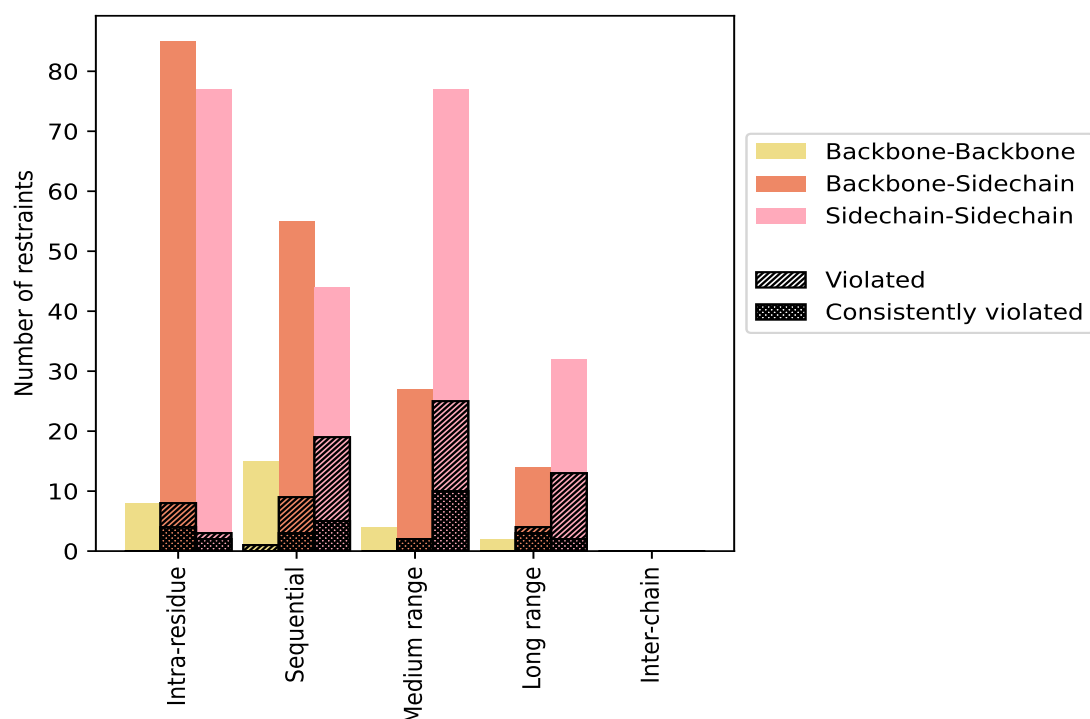
### 9.1 Summary of distance violations ⓘ

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> |
| <b>Intra-residue (<math> i-j =0</math>)</b>                                 | <b>170</b> | <b>38.6</b>    | <b>11</b>             | <b>6.5</b>     | <b>2.5</b>     | <b>6</b>                           | <b>3.5</b>     | <b>1.4</b>     |
| Backbone-Backbone                                                           | 8          | 1.8            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 85         | 19.3           | 8                     | 9.4            | 1.8            | 4                                  | 4.7            | 0.9            |
| Sidechain-Sidechain                                                         | 77         | 17.5           | 3                     | 3.9            | 0.7            | 2                                  | 2.6            | 0.5            |
| <b>Sequential (<math> i-j =1</math>)</b>                                    | <b>114</b> | <b>25.9</b>    | <b>29</b>             | <b>25.4</b>    | <b>6.6</b>     | <b>8</b>                           | <b>7.0</b>     | <b>1.8</b>     |
| Backbone-Backbone                                                           | 15         | 3.4            | 1                     | 6.7            | 0.2            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 55         | 12.5           | 9                     | 16.4           | 2.0            | 3                                  | 5.5            | 0.7            |
| Sidechain-Sidechain                                                         | 44         | 10.0           | 19                    | 43.2           | 4.3            | 5                                  | 11.4           | 1.1            |
| <b>Medium range (<math> i-j &gt;1</math> &amp; <math> i-j &lt;5</math>)</b> | <b>108</b> | <b>24.5</b>    | <b>27</b>             | <b>25.0</b>    | <b>6.1</b>     | <b>12</b>                          | <b>11.1</b>    | <b>2.7</b>     |
| Backbone-Backbone                                                           | 4          | 0.9            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 27         | 6.1            | 2                     | 7.4            | 0.5            | 2                                  | 7.4            | 0.5            |
| Sidechain-Sidechain                                                         | 77         | 17.5           | 25                    | 32.5           | 5.7            | 10                                 | 13.0           | 2.3            |
| <b>Long range (<math> i-j \geq 5</math>)</b>                                | <b>48</b>  | <b>10.9</b>    | <b>17</b>             | <b>35.4</b>    | <b>3.9</b>     | <b>5</b>                           | <b>10.4</b>    | <b>1.1</b>     |
| Backbone-Backbone                                                           | 2          | 0.5            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 14         | 3.2            | 4                     | 28.6           | 0.9            | 3                                  | 21.4           | 0.7            |
| Sidechain-Sidechain                                                         | 32         | 7.3            | 13                    | 40.6           | 3.0            | 2                                  | 6.2            | 0.5            |
| <b>Inter-chain</b>                                                          | <b>0</b>   | <b>0.0</b>     | <b>0</b>              | <b>0.0</b>     | <b>0.0</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| Backbone-Backbone                                                           | 0          | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 0          | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Sidechain-Sidechain                                                         | 0          | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| <b>Hydrogen bond</b>                                                        | <b>0</b>   | <b>0.0</b>     | <b>0</b>              | <b>0.0</b>     | <b>0.0</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| <b>Disulfide bond</b>                                                       | <b>0</b>   | <b>0.0</b>     | <b>0</b>              | <b>0.0</b>     | <b>0.0</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| <b>Total</b>                                                                | <b>440</b> | <b>100.0</b>   | <b>84</b>             | <b>19.1</b>    | <b>19.1</b>    | <b>31</b>                          | <b>7.0</b>     | <b>7.0</b>     |
| Backbone-Backbone                                                           | 29         | 6.6            | 1                     | 3.4            | 0.2            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 181        | 41.1           | 23                    | 12.7           | 5.2            | 12                                 | 6.6            | 2.7            |
| Sidechain-Sidechain                                                         | 230        | 52.3           | 60                    | 26.1           | 13.6           | 19                                 | 8.3            | 4.3            |

<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        | 7                    | 17              | 24              | 10              | 0               | 58    | 0.58     | 1.74    | 0.42                | 0.49       |
| 2        | 6                    | 14              | 19              | 9               | 0               | 48    | 0.53     | 1.56    | 0.37                | 0.44       |
| 3        | 7                    | 14              | 19              | 11              | 0               | 51    | 0.65     | 2.4     | 0.52                | 0.46       |
| 4        | 8                    | 15              | 23              | 8               | 0               | 54    | 0.62     | 1.83    | 0.44                | 0.51       |
| 5        | 8                    | 16              | 24              | 9               | 0               | 57    | 0.63     | 1.72    | 0.44                | 0.51       |
| 6        | 8                    | 18              | 21              | 10              | 0               | 57    | 0.6      | 1.86    | 0.43                | 0.5        |
| 7        | 8                    | 16              | 25              | 10              | 0               | 59    | 0.61     | 1.86    | 0.46                | 0.51       |
| 8        | 7                    | 17              | 22              | 12              | 0               | 58    | 0.62     | 1.75    | 0.43                | 0.48       |
| 9        | 7                    | 16              | 21              | 9               | 0               | 53    | 0.63     | 1.71    | 0.43                | 0.49       |
| 10       | 7                    | 17              | 17              | 8               | 0               | 49    | 0.55     | 1.48    | 0.36                | 0.45       |

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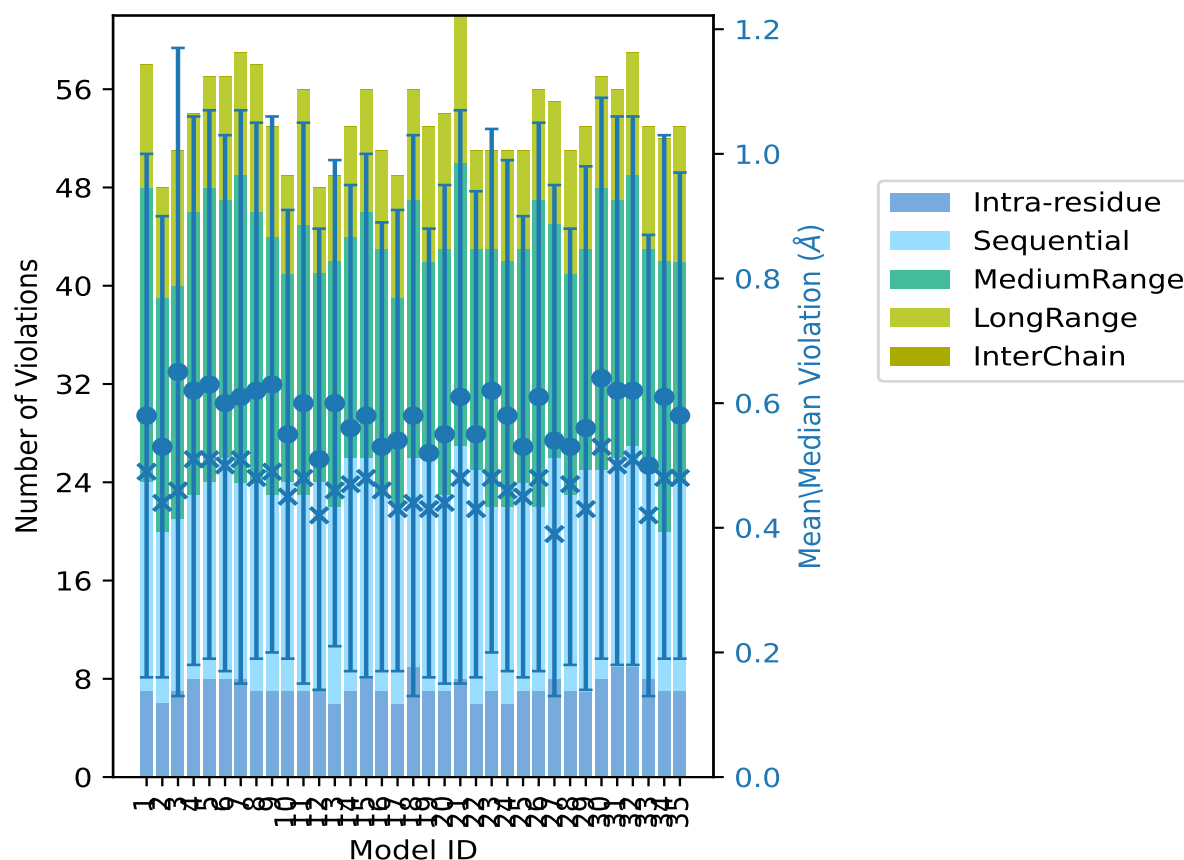
| Model ID | Number of violations |                 |                 |                 |                 |       | Mean (Å) | Max (Å) | SD <sup>6</sup> (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
|          | IR <sup>1</sup>      | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total |          |         |                     |            |
| 11       | 7                    | 16              | 22              | 11              | 0               | 56    | 0.6      | 1.82    | 0.45                | 0.48       |
| 12       | 7                    | 17              | 17              | 7               | 0               | 48    | 0.51     | 1.59    | 0.37                | 0.42       |
| 13       | 6                    | 16              | 20              | 7               | 0               | 49    | 0.6      | 1.59    | 0.39                | 0.46       |
| 14       | 7                    | 19              | 18              | 9               | 0               | 53    | 0.56     | 1.62    | 0.39                | 0.47       |
| 15       | 8                    | 18              | 20              | 10              | 0               | 56    | 0.58     | 1.67    | 0.42                | 0.48       |
| 16       | 7                    | 16              | 20              | 8               | 0               | 51    | 0.53     | 1.5     | 0.36                | 0.46       |
| 17       | 6                    | 16              | 17              | 10              | 0               | 49    | 0.54     | 1.61    | 0.37                | 0.43       |
| 18       | 9                    | 17              | 21              | 9               | 0               | 56    | 0.58     | 1.96    | 0.45                | 0.44       |
| 19       | 7                    | 19              | 16              | 11              | 0               | 53    | 0.52     | 1.56    | 0.36                | 0.43       |
| 20       | 7                    | 16              | 20              | 11              | 0               | 54    | 0.55     | 1.75    | 0.4                 | 0.44       |
| 21       | 8                    | 19              | 23              | 12              | 0               | 62    | 0.61     | 1.88    | 0.46                | 0.48       |
| 22       | 6                    | 19              | 18              | 8               | 0               | 51    | 0.55     | 1.61    | 0.39                | 0.43       |
| 23       | 7                    | 15              | 21              | 8               | 0               | 51    | 0.62     | 1.7     | 0.42                | 0.48       |
| 24       | 6                    | 16              | 20              | 9               | 0               | 51    | 0.58     | 1.7     | 0.41                | 0.46       |
| 25       | 7                    | 17              | 19              | 8               | 0               | 51    | 0.53     | 1.6     | 0.37                | 0.45       |
| 26       | 7                    | 15              | 25              | 9               | 0               | 56    | 0.61     | 1.76    | 0.44                | 0.48       |
| 27       | 8                    | 18              | 19              | 10              | 0               | 55    | 0.54     | 1.72    | 0.41                | 0.39       |
| 28       | 7                    | 16              | 18              | 10              | 0               | 51    | 0.53     | 1.62    | 0.35                | 0.47       |
| 29       | 7                    | 18              | 18              | 10              | 0               | 53    | 0.56     | 1.77    | 0.42                | 0.43       |
| 30       | 8                    | 17              | 23              | 9               | 0               | 57    | 0.64     | 1.89    | 0.45                | 0.53       |
| 31       | 9                    | 17              | 21              | 9               | 0               | 56    | 0.62     | 1.91    | 0.44                | 0.5        |
| 32       | 9                    | 18              | 22              | 10              | 0               | 59    | 0.62     | 1.89    | 0.44                | 0.51       |
| 33       | 8                    | 18              | 17              | 10              | 0               | 53    | 0.5      | 1.55    | 0.37                | 0.42       |
| 34       | 7                    | 13              | 22              | 10              | 0               | 52    | 0.61     | 1.66    | 0.42                | 0.48       |
| 35       | 7                    | 17              | 18              | 11              | 0               | 53    | 0.58     | 1.68    | 0.39                | 0.48       |

<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, 356(IR:159, SQ:85, MR:81, LR:31, 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>       | %    |
| 0                             | 3               | 1               | 3               | 0               | 7     | 1                        | 2.9  |
| 1                             | 2               | 1               | 1               | 0               | 5     | 2                        | 5.7  |
| 0                             | 1               | 0               | 0               | 0               | 1     | 3                        | 8.6  |
| 0                             | 1               | 0               | 0               | 0               | 1     | 4                        | 11.4 |
| 2                             | 0               | 0               | 2               | 0               | 4     | 5                        | 14.3 |
| 0                             | 0               | 0               | 0               | 0               | 0     | 6                        | 17.1 |

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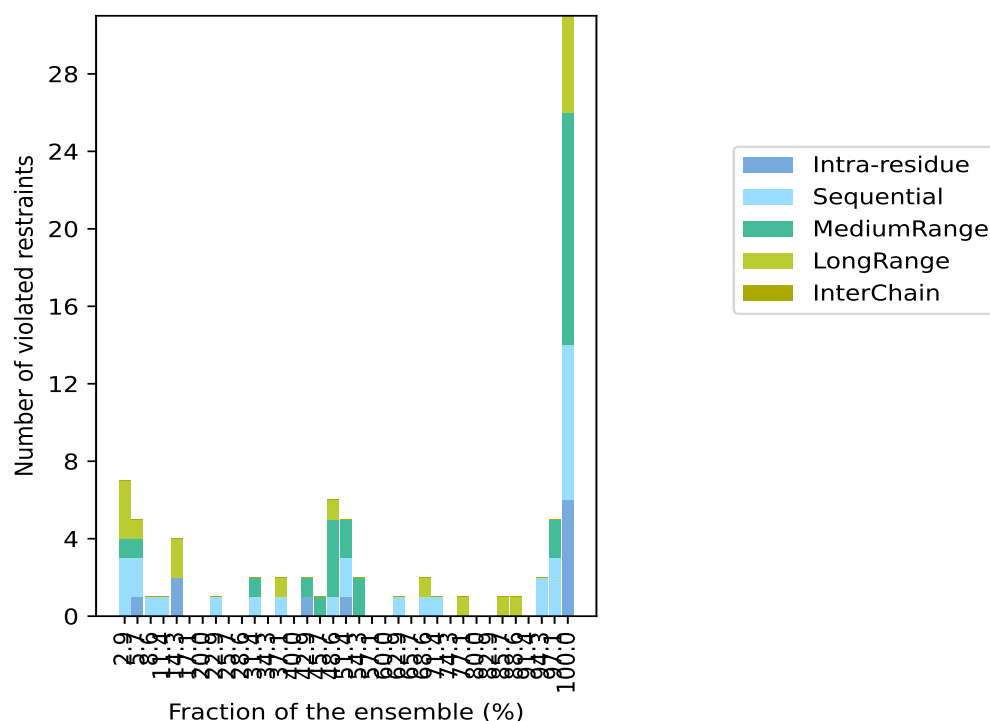
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| Number of violated restraints |                 |                 |                 |                 |       | Fraction of the ensemble |       |
|-------------------------------|-----------------|-----------------|-----------------|-----------------|-------|--------------------------|-------|
| 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>       | %     |
| 0                             | 0               | 0               | 0               | 0               | 0     | 7                        | 20.0  |
| 0                             | 1               | 0               | 0               | 0               | 1     | 8                        | 22.9  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 9                        | 25.7  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 10                       | 28.6  |
| 0                             | 1               | 1               | 0               | 0               | 2     | 11                       | 31.4  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 12                       | 34.3  |
| 0                             | 1               | 0               | 1               | 0               | 2     | 13                       | 37.1  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 14                       | 40.0  |
| 1                             | 0               | 1               | 0               | 0               | 2     | 15                       | 42.9  |
| 0                             | 0               | 1               | 0               | 0               | 1     | 16                       | 45.7  |
| 0                             | 1               | 4               | 1               | 0               | 6     | 17                       | 48.6  |
| 1                             | 2               | 2               | 0               | 0               | 5     | 18                       | 51.4  |
| 0                             | 0               | 2               | 0               | 0               | 2     | 19                       | 54.3  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 20                       | 57.1  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 21                       | 60.0  |
| 0                             | 1               | 0               | 0               | 0               | 1     | 22                       | 62.9  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 23                       | 65.7  |
| 0                             | 1               | 0               | 1               | 0               | 2     | 24                       | 68.6  |
| 0                             | 1               | 0               | 0               | 0               | 1     | 25                       | 71.4  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 26                       | 74.3  |
| 0                             | 0               | 0               | 1               | 0               | 1     | 27                       | 77.1  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 28                       | 80.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 29                       | 82.9  |
| 0                             | 0               | 0               | 1               | 0               | 1     | 30                       | 85.7  |
| 0                             | 0               | 0               | 1               | 0               | 1     | 31                       | 88.6  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 32                       | 91.4  |
| 0                             | 2               | 0               | 0               | 0               | 2     | 33                       | 94.3  |
| 0                             | 3               | 2               | 0               | 0               | 5     | 34                       | 97.1  |
| 6                             | 8               | 12              | 5               | 0               | 31    | 35                       | 100.0 |

<sup>1</sup>Intra-residue restraints, <sup>2</sup>Sequential restraints, <sup>3</sup>Medium range restraints, <sup>4</sup>Long range restraints,

<sup>5</sup>Inter-chain restraints, <sup>6</sup> Number of models with violations

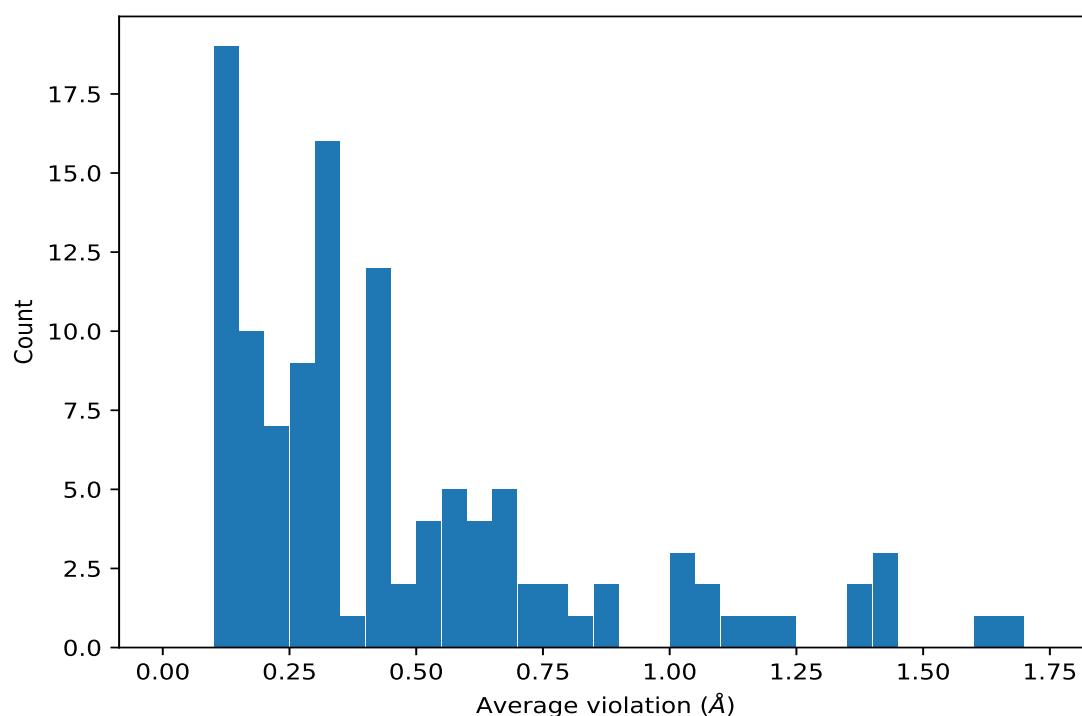
### 9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

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

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



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

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

| Key     | Atom-1         | Atom-2         | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|----------------|----------------|---------------------|----------|---------------------|------------|
| (2,225) | 1:11:A:TRP:HB2 | 1:8:A:ARG:HB3  | 35                  | 1.61     | 0.05                | 1.62       |
| (1,20)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG21 | 35                  | 1.44     | 0.07                | 1.46       |
| (1,20)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG22 | 35                  | 1.44     | 0.07                | 1.46       |
| (1,20)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG23 | 35                  | 1.44     | 0.07                | 1.46       |
| (2,136) | 1:15:A:TYR:HB2 | 1:12:A:PRO:HB3 | 35                  | 1.35     | 0.09                | 1.36       |
| (2,310) | 1:11:A:TRP:HE3 | 1:12:A:PRO:HD3 | 35                  | 1.24     | 0.05                | 1.24       |
| (3,15)  | 1:11:A:TRP:HE1 | 1:12:A:PRO:HD3 | 35                  | 1.2      | 0.02                | 1.2        |
| (2,325) | 1:5:A:HIS:HD2  | 1:5:A:HIS:HB2  | 35                  | 1.13     | 0.01                | 1.13       |
| (2,16)  | 1:11:A:TRP:HZ3 | 1:8:A:ARG:HD2  | 35                  | 1.03     | 0.74                | 1.66       |
| (2,16)  | 1:11:A:TRP:HD1 | 1:8:A:ARG:HD2  | 35                  | 1.03     | 0.74                | 1.66       |
| (2,251) | 1:5:A:HIS:HB2  | 1:4:A:HCS:HA   | 35                  | 0.89     | 0.04                | 0.88       |
| (3,12)  | 1:11:A:TRP:HE3 | 1:12:A:PRO:HG3 | 35                  | 0.81     | 0.07                | 0.82       |
| (2,161) | 1:4:A:HCS:HB3  | 1:13:A:CYS:HA  | 35                  | 0.73     | 0.05                | 0.73       |
| (3,25)  | 1:5:A:HIS:H    | 1:3:A:ILE:HG13 | 35                  | 0.7      | 0.11                | 0.73       |
| (2,41)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG11 | 35                  | 0.69     | 0.06                | 0.69       |
| (2,41)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG12 | 35                  | 0.69     | 0.06                | 0.69       |

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| Key     | Atom-1         | Atom-2         | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|----------------|----------------|---------------------|----------|---------------------|------------|
| (2,41)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG13 | 35                  | 0.69     | 0.06                | 0.69       |
| (2,146) | 1:11:A:TRP:H   | 1:11:A:TRP:HB2 | 35                  | 0.66     | 0.03                | 0.65       |
| (2,337) | 1:6:A:VAL:HA   | 1:13:A:CYS:HB3 | 35                  | 0.63     | 0.07                | 0.62       |
| (2,337) | 1:6:A:VAL:HA   | 1:13:A:CYS:HB2 | 35                  | 0.63     | 0.07                | 0.62       |
| (1,8)   | 1:11:A:TRP:HH2 | 1:15:A:TYR:HB2 | 35                  | 0.56     | 0.08                | 0.56       |
| (2,18)  | 1:11:A:TRP:HD1 | 1:12:A:PRO:HG3 | 35                  | 0.55     | 0.04                | 0.55       |
| (2,46)  | 1:11:A:TRP:HB3 | 1:15:A:TYR:HB3 | 35                  | 0.53     | 0.09                | 0.56       |
| (2,182) | 1:5:A:HIS:H    | 1:5:A:HIS:HB2  | 35                  | 0.51     | 0.03                | 0.51       |
| (1,6)   | 1:14:A:TRP:HH2 | 1:12:A:PRO:HG2 | 35                  | 0.5      | 0.02                | 0.5        |
| (2,266) | 1:9:A:PRO:HG2  | 1:9:A:PRO:HB3  | 35                  | 0.46     | 0.01                | 0.46       |
| (1,14)  | 1:15:A:TYR:HD1 | 1:11:A:TRP:HH2 | 35                  | 0.41     | 0.04                | 0.42       |
| (1,14)  | 1:15:A:TYR:HD2 | 1:11:A:TRP:HH2 | 35                  | 0.41     | 0.04                | 0.42       |
| (1,30)  | 1:15:A:TYR:HE1 | 1:12:A:PRO:HG3 | 35                  | 0.4      | 0.03                | 0.41       |
| (1,30)  | 1:15:A:TYR:HE2 | 1:12:A:PRO:HG3 | 35                  | 0.4      | 0.03                | 0.41       |
| (2,192) | 1:15:A:TYR:HB2 | 1:11:A:TRP:HA  | 35                  | 0.4      | 0.04                | 0.42       |
| (2,300) | 1:11:A:TRP:HD1 | 1:13:A:CYS:HB3 | 35                  | 0.38     | 0.07                | 0.4        |
| (2,304) | 1:9:A:PRO:HG2  | 1:8:A:ARG:HA   | 35                  | 0.32     | 0.03                | 0.33       |
| (2,264) | 1:13:A:CYS:HB3 | 1:4:A:HCS:HA   | 35                  | 0.25     | 0.04                | 0.26       |
| (2,198) | 1:8:A:ARG:H    | 1:7:A:HIS:HB2  | 35                  | 0.22     | 0.04                | 0.22       |
| (2,88)  | 1:7:A:HIS:HB3  | 1:7:A:HIS:HA   | 35                  | 0.22     | 0.0                 | 0.22       |
| (2,228) | 1:11:A:TRP:HB2 | 1:8:A:ARG:HB2  | 35                  | 0.22     | 0.03                | 0.21       |
| (2,243) | 1:15:A:TYR:H   | 1:15:A:TYR:HB2 | 35                  | 0.19     | 0.02                | 0.19       |
| (2,179) | 1:14:A:TRP:HD1 | 1:12:A:PRO:HB3 | 35                  | 0.14     | 0.01                | 0.14       |
| (2,47)  | 1:7:A:HIS:HB2  | 1:8:A:ARG:HG2  | 34                  | 0.88     | 0.27                | 0.88       |
| (3,29)  | 1:11:A:TRP:HB2 | 1:8:A:ARG:HG2  | 34                  | 0.52     | 0.06                | 0.52       |
| (2,348) | 1:11:A:TRP:HB2 | 1:8:A:ARG:HG3  | 34                  | 0.44     | 0.08                | 0.45       |
| (1,21)  | 1:4:A:HCS:HG3  | 1:3:A:ILE:HG21 | 34                  | 0.35     | 0.09                | 0.34       |
| (1,21)  | 1:4:A:HCS:HG3  | 1:3:A:ILE:HG22 | 34                  | 0.35     | 0.09                | 0.34       |
| (1,21)  | 1:4:A:HCS:HG3  | 1:3:A:ILE:HG23 | 34                  | 0.35     | 0.09                | 0.34       |
| (1,21)  | 1:4:A:HCS:HG3  | 1:6:A:VAL:HG11 | 34                  | 0.35     | 0.09                | 0.34       |
| (1,21)  | 1:4:A:HCS:HG3  | 1:6:A:VAL:HG12 | 34                  | 0.35     | 0.09                | 0.34       |
| (1,21)  | 1:4:A:HCS:HG3  | 1:6:A:VAL:HG13 | 34                  | 0.35     | 0.09                | 0.34       |
| (2,142) | 1:14:A:TRP:HD1 | 1:13:A:CYS:HB2 | 34                  | 0.29     | 0.07                | 0.3        |
| (2,142) | 1:14:A:TRP:HD1 | 1:13:A:CYS:HB3 | 34                  | 0.29     | 0.07                | 0.3        |
| (1,5)   | 1:11:A:TRP:HD1 | 1:12:A:PRO:HB2 | 33                  | 0.17     | 0.04                | 0.17       |
| (2,99)  | 1:14:A:TRP:H   | 1:13:A:CYS:HB2 | 33                  | 0.13     | 0.02                | 0.13       |
| (2,35)  | 1:5:A:HIS:HD2  | 1:13:A:CYS:HB3 | 31                  | 0.42     | 0.09                | 0.43       |
| (2,35)  | 1:5:A:HIS:HD2  | 1:13:A:CYS:HB2 | 31                  | 0.42     | 0.09                | 0.43       |
| (1,29)  | 1:11:A:TRP:HD1 | 1:1:A:PRO:HG3  | 30                  | 0.78     | 0.4                 | 0.69       |
| (1,29)  | 1:11:A:TRP:HD1 | 1:4:A:HCS:HB2  | 30                  | 0.78     | 0.4                 | 0.69       |
| (3,45)  | 1:13:A:CYS:HA  | 1:4:A:HCS:HG2  | 27                  | 0.12     | 0.01                | 0.12       |
| (1,18)  | 1:5:A:HIS:HB3  | 1:3:A:ILE:HG21 | 25                  | 0.27     | 0.09                | 0.28       |

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| Key     | Atom-1         | Atom-2         | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|----------------|----------------|---------------------|----------|---------------------|------------|
| (1,18)  | 1:5:A:HIS:HB3  | 1:3:A:ILE:HG22 | 25                  | 0.27     | 0.09                | 0.28       |
| (1,18)  | 1:5:A:HIS:HB3  | 1:3:A:ILE:HG23 | 25                  | 0.27     | 0.09                | 0.28       |
| (1,18)  | 1:5:A:HIS:HB3  | 1:6:A:VAL:HG21 | 25                  | 0.27     | 0.09                | 0.28       |
| (1,18)  | 1:5:A:HIS:HB3  | 1:6:A:VAL:HG22 | 25                  | 0.27     | 0.09                | 0.28       |
| (1,18)  | 1:5:A:HIS:HB3  | 1:6:A:VAL:HG23 | 25                  | 0.27     | 0.09                | 0.28       |
| (2,312) | 1:15:A:TYR:HD1 | 1:16:A:ARG:HG2 | 24                  | 0.6      | 0.19                | 0.59       |
| (2,312) | 1:15:A:TYR:HD2 | 1:16:A:ARG:HG2 | 24                  | 0.6      | 0.19                | 0.59       |
| (2,66)  | 1:2:A:SER:HB3  | 1:13:A:CYS:HB3 | 24                  | 0.42     | 0.1                 | 0.46       |
| (3,43)  | 1:15:A:TYR:HE1 | 1:16:A:ARG:HG2 | 22                  | 0.61     | 0.19                | 0.64       |
| (3,43)  | 1:15:A:TYR:HE2 | 1:16:A:ARG:HG2 | 22                  | 0.61     | 0.19                | 0.64       |
| (3,6)   | 1:14:A:TRP:HD1 | 1:16:A:ARG:HD3 | 19                  | 1.38     | 0.66                | 1.7        |
| (2,21)  | 1:11:A:TRP:HH2 | 1:8:A:ARG:HD2  | 19                  | 1.01     | 0.25                | 1.09       |
| (2,95)  | 1:8:A:ARG:HD2  | 1:11:A:TRP:HB2 | 18                  | 1.7      | 0.29                | 1.83       |
| (2,295) | 1:9:A:PRO:HD3  | 1:8:A:ARG:HD3  | 18                  | 1.08     | 0.03                | 1.07       |
| (2,318) | 1:9:A:PRO:HD2  | 1:8:A:ARG:HD3  | 18                  | 0.73     | 0.08                | 0.73       |
| (2,15)  | 1:11:A:TRP:HE3 | 1:8:A:ARG:HD2  | 18                  | 0.6      | 0.21                | 0.68       |
| (2,98)  | 1:8:A:ARG:HA   | 1:8:A:ARG:HD3  | 18                  | 0.48     | 0.06                | 0.49       |
| (1,7)   | 1:14:A:TRP:HH2 | 1:15:A:TYR:HB3 | 17                  | 0.4      | 0.05                | 0.41       |
| (1,7)   | 1:11:A:TRP:HH2 | 1:8:A:ARG:HD3  | 17                  | 0.4      | 0.05                | 0.41       |
| (1,2)   | 1:11:A:TRP:HZ2 | 1:8:A:ARG:HD3  | 17                  | 0.4      | 0.04                | 0.39       |
| (3,48)  | 1:11:A:TRP:HE1 | 1:8:A:ARG:HD2  | 17                  | 0.34     | 0.06                | 0.36       |
| (1,16)  | 1:7:A:HIS:HD2  | 1:8:A:ARG:HD3  | 17                  | 0.33     | 0.08                | 0.35       |
| (3,3)   | 1:11:A:TRP:HZ2 | 1:8:A:ARG:HD2  | 17                  | 0.32     | 0.04                | 0.33       |
| (1,10)  | 1:15:A:TYR:HD1 | 1:8:A:ARG:HB2  | 17                  | 0.15     | 0.03                | 0.16       |
| (1,10)  | 1:15:A:TYR:HD2 | 1:8:A:ARG:HB2  | 17                  | 0.15     | 0.03                | 0.16       |
| (2,128) | 1:14:A:TRP:HD1 | 1:12:A:PRO:HG3 | 16                  | 0.18     | 0.05                | 0.16       |
| (2,23)  | 1:14:A:TRP:HZ3 | 1:16:A:ARG:HD3 | 15                  | 1.05     | 0.17                | 1.09       |
| (2,294) | 1:10:A:ASP:H   | 1:10:A:ASP:HB2 | 15                  | 0.18     | 0.04                | 0.17       |
| (1,26)  | 1:9:A:PRO:HD3  | 1:3:A:ILE:HD11 | 13                  | 0.32     | 0.11                | 0.31       |
| (1,26)  | 1:9:A:PRO:HD3  | 1:3:A:ILE:HD12 | 13                  | 0.32     | 0.11                | 0.31       |
| (1,26)  | 1:9:A:PRO:HD3  | 1:3:A:ILE:HD13 | 13                  | 0.32     | 0.11                | 0.31       |
| (1,26)  | 1:9:A:PRO:HD3  | 1:3:A:ILE:HG21 | 13                  | 0.32     | 0.11                | 0.31       |
| (1,26)  | 1:9:A:PRO:HD3  | 1:3:A:ILE:HG22 | 13                  | 0.32     | 0.11                | 0.31       |
| (1,26)  | 1:9:A:PRO:HD3  | 1:3:A:ILE:HG23 | 13                  | 0.32     | 0.11                | 0.31       |
| (2,180) | 1:14:A:TRP:HZ3 | 1:15:A:TYR:HB3 | 13                  | 0.14     | 0.02                | 0.13       |
| (2,30)  | 1:15:A:TYR:HE1 | 1:13:A:CYS:HB2 | 11                  | 0.19     | 0.07                | 0.16       |
| (2,30)  | 1:15:A:TYR:HE2 | 1:13:A:CYS:HB2 | 11                  | 0.19     | 0.07                | 0.16       |
| (2,193) | 1:7:A:HIS:HD2  | 1:8:A:ARG:HB3  | 11                  | 0.13     | 0.02                | 0.14       |
| (2,60)  | 1:6:A:VAL:H    | 1:5:A:HIS:HA   | 8                   | 0.2      | 0.01                | 0.2        |
| (1,32)  | 1:3:A:ILE:HD11 | 1:9:A:PRO:HD3  | 5                   | 0.24     | 0.13                | 0.2        |
| (1,32)  | 1:3:A:ILE:HD12 | 1:9:A:PRO:HD3  | 5                   | 0.24     | 0.13                | 0.2        |
| (1,32)  | 1:3:A:ILE:HD13 | 1:9:A:PRO:HD3  | 5                   | 0.24     | 0.13                | 0.2        |

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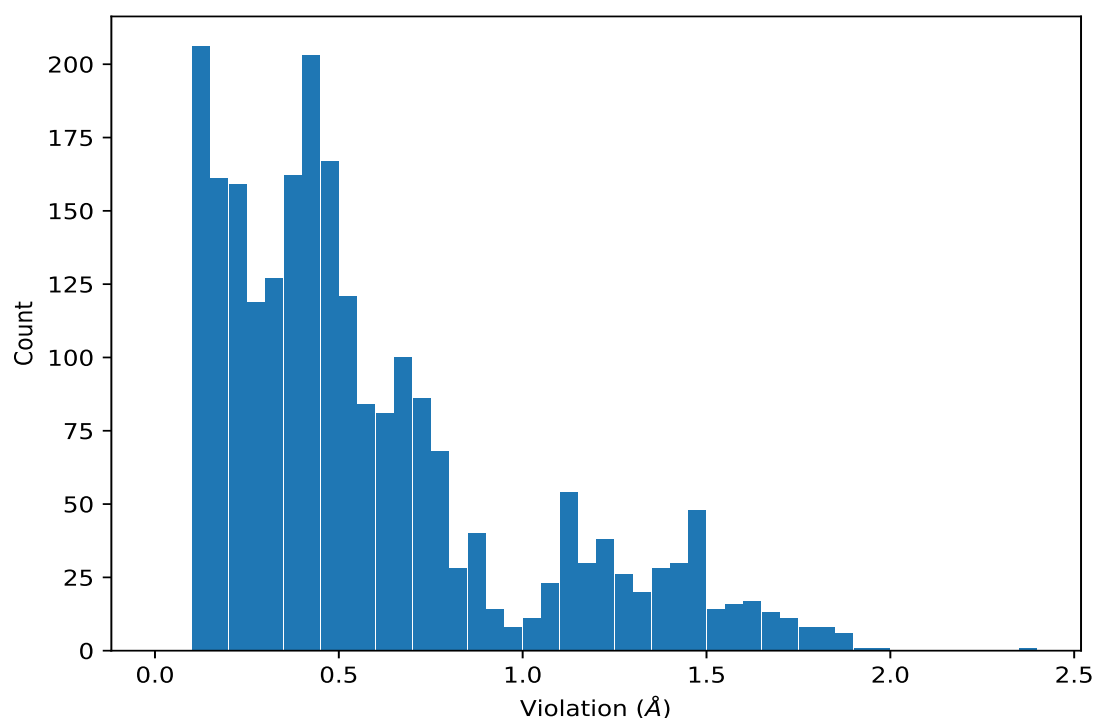
| Key     | Atom-1         | Atom-2         | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|----------------|----------------|---------------------|----------|---------------------|------------|
| (2,354) | 1:16:A:ARG:HG3 | 1:16:A:ARG:HB2 | 5                   | 0.16     | 0.04                | 0.16       |
| (2,100) | 1:8:A:ARG:H    | 1:8:A:ARG:HD3  | 5                   | 0.11     | 0.01                | 0.11       |
| (2,13)  | 1:11:A:TRP:HH2 | 1:6:A:VAL:HG11 | 5                   | 0.11     | 0.01                | 0.11       |
| (2,13)  | 1:11:A:TRP:HH2 | 1:6:A:VAL:HG12 | 5                   | 0.11     | 0.01                | 0.11       |
| (2,13)  | 1:11:A:TRP:HH2 | 1:6:A:VAL:HG13 | 5                   | 0.11     | 0.01                | 0.11       |
| (2,139) | 1:14:A:TRP:HD1 | 1:13:A:CYS:HA  | 4                   | 0.11     | 0.01                | 0.11       |
| (3,24)  | 1:14:A:TRP:HD1 | 1:15:A:TYR:HA  | 3                   | 0.11     | 0.0                 | 0.11       |
| (1,25)  | 1:9:A:PRO:HD2  | 1:3:A:ILE:HD11 | 2                   | 0.16     | 0.05                | 0.16       |
| (1,25)  | 1:9:A:PRO:HD2  | 1:3:A:ILE:HD12 | 2                   | 0.16     | 0.05                | 0.16       |
| (1,25)  | 1:9:A:PRO:HD2  | 1:3:A:ILE:HD13 | 2                   | 0.16     | 0.05                | 0.16       |
| (1,24)  | 1:6:A:VAL:HA   | 1:7:A:HIS:HB2  | 2                   | 0.12     | 0.0                 | 0.12       |
| (2,237) | 1:6:A:VAL:HA   | 1:6:A:VAL:HG21 | 2                   | 0.11     | 0.0                 | 0.11       |
| (2,237) | 1:6:A:VAL:HA   | 1:6:A:VAL:HG22 | 2                   | 0.11     | 0.0                 | 0.11       |
| (2,237) | 1:6:A:VAL:HA   | 1:6:A:VAL:HG23 | 2                   | 0.11     | 0.0                 | 0.11       |
| (2,342) | 1:4:A:HCS:H    | 1:3:A:ILE:HB   | 2                   | 0.11     | 0.0                 | 0.11       |
| (2,37)  | 1:7:A:HIS:HD2  | 1:11:A:TRP:HZ2 | 2                   | 0.11     | 0.0                 | 0.11       |

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

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

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

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



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

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

| Key    | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|--------|----------------|----------------|----------|---------------|
| (2,95) | 1:8:A:ARG:HD2  | 1:11:A:TRP:HB2 | 3        | 2.4           |
| (2,95) | 1:8:A:ARG:HD2  | 1:11:A:TRP:HB2 | 18       | 1.96          |
| (2,95) | 1:8:A:ARG:HD2  | 1:11:A:TRP:HB2 | 31       | 1.91          |
| (2,95) | 1:8:A:ARG:HD2  | 1:11:A:TRP:HB2 | 30       | 1.89          |
| (2,95) | 1:8:A:ARG:HD2  | 1:11:A:TRP:HB2 | 32       | 1.89          |
| (2,95) | 1:8:A:ARG:HD2  | 1:11:A:TRP:HB2 | 21       | 1.88          |
| (2,95) | 1:8:A:ARG:HD2  | 1:11:A:TRP:HB2 | 6        | 1.86          |
| (2,95) | 1:8:A:ARG:HD2  | 1:11:A:TRP:HB2 | 7        | 1.86          |
| (3,6)  | 1:14:A:TRP:HD1 | 1:16:A:ARG:HD3 | 21       | 1.85          |
| (2,95) | 1:8:A:ARG:HD2  | 1:11:A:TRP:HB2 | 4        | 1.83          |
| (2,95) | 1:8:A:ARG:HD2  | 1:11:A:TRP:HB2 | 11       | 1.82          |
| (2,16) | 1:11:A:TRP:HZ3 | 1:8:A:ARG:HD2  | 7        | 1.82          |
| (2,16) | 1:11:A:TRP:HZ3 | 1:8:A:ARG:HD2  | 18       | 1.82          |
| (2,16) | 1:11:A:TRP:HZ3 | 1:8:A:ARG:HD2  | 32       | 1.82          |
| (2,16) | 1:11:A:TRP:HZ3 | 1:8:A:ARG:HD2  | 30       | 1.81          |
| (2,16) | 1:11:A:TRP:HZ3 | 1:8:A:ARG:HD2  | 11       | 1.8           |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (2,16)  | 1:11:A:TRP:HZ3 | 1:8:A:ARG:HD2  | 31       | 1.8           |
| (2,16)  | 1:11:A:TRP:HZ3 | 1:8:A:ARG:HD2  | 4        | 1.79          |
| (2,16)  | 1:11:A:TRP:HZ3 | 1:8:A:ARG:HD2  | 6        | 1.78          |
| (3,6)   | 1:14:A:TRP:HD1 | 1:16:A:ARG:HD3 | 3        | 1.77          |
| (3,6)   | 1:14:A:TRP:HD1 | 1:16:A:ARG:HD3 | 29       | 1.77          |
| (3,6)   | 1:14:A:TRP:HD1 | 1:16:A:ARG:HD3 | 26       | 1.76          |
| (3,6)   | 1:14:A:TRP:HD1 | 1:16:A:ARG:HD3 | 8        | 1.75          |
| (3,6)   | 1:14:A:TRP:HD1 | 1:16:A:ARG:HD3 | 20       | 1.75          |
| (2,16)  | 1:11:A:TRP:HZ3 | 1:8:A:ARG:HD2  | 21       | 1.75          |
| (3,6)   | 1:14:A:TRP:HD1 | 1:16:A:ARG:HD3 | 7        | 1.74          |
| (2,16)  | 1:11:A:TRP:HZ3 | 1:8:A:ARG:HD2  | 1        | 1.74          |
| (2,16)  | 1:11:A:TRP:HZ3 | 1:8:A:ARG:HD2  | 3        | 1.74          |
| (2,16)  | 1:11:A:TRP:HZ3 | 1:8:A:ARG:HD2  | 26       | 1.74          |
| (3,6)   | 1:14:A:TRP:HD1 | 1:16:A:ARG:HD3 | 5        | 1.72          |
| (3,6)   | 1:14:A:TRP:HD1 | 1:16:A:ARG:HD3 | 27       | 1.72          |
| (2,16)  | 1:11:A:TRP:HZ3 | 1:8:A:ARG:HD2  | 9        | 1.71          |
| (3,6)   | 1:14:A:TRP:HD1 | 1:16:A:ARG:HD3 | 24       | 1.7           |
| (3,6)   | 1:14:A:TRP:HD1 | 1:16:A:ARG:HD3 | 30       | 1.7           |
| (2,225) | 1:11:A:TRP:HB2 | 1:8:A:ARG:HB3  | 11       | 1.7           |
| (2,16)  | 1:11:A:TRP:HZ3 | 1:8:A:ARG:HD2  | 23       | 1.7           |
| (3,6)   | 1:14:A:TRP:HD1 | 1:16:A:ARG:HD3 | 35       | 1.68          |
| (2,225) | 1:11:A:TRP:HB2 | 1:8:A:ARG:HB3  | 3        | 1.68          |
| (2,16)  | 1:11:A:TRP:HZ3 | 1:8:A:ARG:HD2  | 8        | 1.68          |
| (2,225) | 1:11:A:TRP:HB2 | 1:8:A:ARG:HB3  | 6        | 1.67          |
| (2,16)  | 1:11:A:TRP:HZ3 | 1:8:A:ARG:HD2  | 15       | 1.67          |
| (2,225) | 1:11:A:TRP:HB2 | 1:8:A:ARG:HB3  | 8        | 1.66          |
| (2,225) | 1:11:A:TRP:HB2 | 1:8:A:ARG:HB3  | 18       | 1.66          |
| (2,16)  | 1:11:A:TRP:HZ3 | 1:8:A:ARG:HD2  | 5        | 1.66          |
| (2,16)  | 1:11:A:TRP:HZ3 | 1:8:A:ARG:HD2  | 34       | 1.66          |
| (2,225) | 1:11:A:TRP:HB2 | 1:8:A:ARG:HB3  | 1        | 1.65          |
| (2,225) | 1:11:A:TRP:HB2 | 1:8:A:ARG:HB3  | 15       | 1.65          |
| (2,225) | 1:11:A:TRP:HB2 | 1:8:A:ARG:HB3  | 21       | 1.65          |
| (2,225) | 1:11:A:TRP:HB2 | 1:8:A:ARG:HB3  | 32       | 1.65          |
| (2,225) | 1:11:A:TRP:HB2 | 1:8:A:ARG:HB3  | 9        | 1.64          |
| (2,225) | 1:11:A:TRP:HB2 | 1:8:A:ARG:HB3  | 31       | 1.64          |
| (2,225) | 1:11:A:TRP:HB2 | 1:8:A:ARG:HB3  | 34       | 1.64          |
| (2,225) | 1:11:A:TRP:HB2 | 1:8:A:ARG:HB3  | 4        | 1.63          |
| (2,225) | 1:11:A:TRP:HB2 | 1:8:A:ARG:HB3  | 30       | 1.63          |
| (2,225) | 1:11:A:TRP:HB2 | 1:8:A:ARG:HB3  | 7        | 1.62          |
| (2,225) | 1:11:A:TRP:HB2 | 1:8:A:ARG:HB3  | 14       | 1.62          |
| (2,225) | 1:11:A:TRP:HB2 | 1:8:A:ARG:HB3  | 23       | 1.62          |
| (2,225) | 1:11:A:TRP:HB2 | 1:8:A:ARG:HB3  | 26       | 1.62          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (2,225) | 1:11:A:TRP:HB2 | 1:8:A:ARG:HB3  | 28       | 1.62          |
| (3,6)   | 1:14:A:TRP:HD1 | 1:16:A:ARG:HD3 | 14       | 1.61          |
| (2,225) | 1:11:A:TRP:HB2 | 1:8:A:ARG:HB3  | 17       | 1.61          |
| (2,225) | 1:11:A:TRP:HB2 | 1:8:A:ARG:HB3  | 22       | 1.61          |
| (3,6)   | 1:14:A:TRP:HD1 | 1:16:A:ARG:HD3 | 32       | 1.6           |
| (2,225) | 1:11:A:TRP:HB2 | 1:8:A:ARG:HB3  | 24       | 1.6           |
| (2,225) | 1:11:A:TRP:HB2 | 1:8:A:ARG:HB3  | 25       | 1.6           |
| (2,225) | 1:11:A:TRP:HB2 | 1:8:A:ARG:HB3  | 27       | 1.6           |
| (3,6)   | 1:14:A:TRP:HD1 | 1:16:A:ARG:HD3 | 13       | 1.59          |
| (2,225) | 1:11:A:TRP:HB2 | 1:8:A:ARG:HB3  | 5        | 1.59          |
| (2,225) | 1:11:A:TRP:HB2 | 1:8:A:ARG:HB3  | 12       | 1.59          |
| (2,225) | 1:11:A:TRP:HB2 | 1:8:A:ARG:HB3  | 20       | 1.59          |
| (1,20)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG21 | 15       | 1.59          |
| (1,20)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG22 | 15       | 1.59          |
| (1,20)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG23 | 15       | 1.59          |
| (2,225) | 1:11:A:TRP:HB2 | 1:8:A:ARG:HB3  | 35       | 1.58          |
| (2,225) | 1:11:A:TRP:HB2 | 1:8:A:ARG:HB3  | 13       | 1.57          |
| (2,225) | 1:11:A:TRP:HB2 | 1:8:A:ARG:HB3  | 2        | 1.56          |
| (2,225) | 1:11:A:TRP:HB2 | 1:8:A:ARG:HB3  | 19       | 1.56          |
| (2,136) | 1:15:A:TYR:HB2 | 1:12:A:PRO:HB3 | 19       | 1.56          |
| (2,225) | 1:11:A:TRP:HB2 | 1:8:A:ARG:HB3  | 33       | 1.55          |
| (1,20)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG21 | 34       | 1.55          |
| (1,20)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG22 | 34       | 1.55          |
| (1,20)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG23 | 34       | 1.55          |
| (2,225) | 1:11:A:TRP:HB2 | 1:8:A:ARG:HB3  | 29       | 1.52          |
| (2,136) | 1:15:A:TYR:HB2 | 1:12:A:PRO:HB3 | 9        | 1.52          |
| (1,29)  | 1:11:A:TRP:HD1 | 1:1:A:PRO:HG3  | 4        | 1.52          |
| (1,20)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG21 | 14       | 1.52          |
| (1,20)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG22 | 14       | 1.52          |
| (1,20)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG23 | 14       | 1.52          |
| (1,20)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG21 | 4        | 1.51          |
| (1,20)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG22 | 4        | 1.51          |
| (1,20)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG23 | 4        | 1.51          |
| (1,20)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG21 | 20       | 1.51          |
| (1,20)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG22 | 20       | 1.51          |
| (1,20)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG23 | 20       | 1.51          |
| (2,225) | 1:11:A:TRP:HB2 | 1:8:A:ARG:HB3  | 16       | 1.5           |
| (1,29)  | 1:11:A:TRP:HD1 | 1:1:A:PRO:HG3  | 5        | 1.5           |
| (2,136) | 1:15:A:TYR:HB2 | 1:12:A:PRO:HB3 | 23       | 1.49          |
| (1,20)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG21 | 1        | 1.49          |
| (1,20)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG22 | 1        | 1.49          |
| (1,20)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG23 | 1        | 1.49          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,20)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG21 | 16       | 1.49          |
| (1,20)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG22 | 16       | 1.49          |
| (1,20)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG23 | 16       | 1.49          |
| (1,20)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG21 | 25       | 1.49          |
| (1,20)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG22 | 25       | 1.49          |
| (1,20)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG23 | 25       | 1.49          |
| (1,20)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG21 | 26       | 1.49          |
| (1,20)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG22 | 26       | 1.49          |
| (1,20)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG23 | 26       | 1.49          |
| (2,225) | 1:11:A:TRP:HB2 | 1:8:A:ARG:HB3  | 10       | 1.48          |
| (2,136) | 1:15:A:TYR:HB2 | 1:12:A:PRO:HB3 | 17       | 1.48          |
| (2,136) | 1:15:A:TYR:HB2 | 1:12:A:PRO:HB3 | 27       | 1.48          |
| (1,29)  | 1:11:A:TRP:HD1 | 1:4:A:HCS:HB2  | 21       | 1.48          |
| (1,20)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG21 | 5        | 1.48          |
| (1,20)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG22 | 5        | 1.48          |
| (1,20)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG23 | 5        | 1.48          |
| (1,20)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG21 | 9        | 1.48          |
| (1,20)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG22 | 9        | 1.48          |
| (1,20)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG23 | 9        | 1.48          |
| (1,20)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG21 | 13       | 1.48          |
| (1,20)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG22 | 13       | 1.48          |
| (1,20)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG23 | 13       | 1.48          |
| (1,20)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG21 | 18       | 1.48          |
| (1,20)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG22 | 18       | 1.48          |
| (1,20)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG23 | 18       | 1.48          |
| (1,20)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG21 | 7        | 1.47          |
| (1,20)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG22 | 7        | 1.47          |
| (1,20)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG23 | 7        | 1.47          |
| (1,20)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG21 | 24       | 1.47          |
| (1,20)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG22 | 24       | 1.47          |
| (1,20)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG23 | 24       | 1.47          |
| (1,20)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG21 | 30       | 1.47          |
| (1,20)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG22 | 30       | 1.47          |
| (1,20)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG23 | 30       | 1.47          |
| (2,95)  | 1:8:A:ARG:HD2  | 1:11:A:TRP:HB2 | 8        | 1.46          |
| (1,20)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG21 | 17       | 1.46          |
| (1,20)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG22 | 17       | 1.46          |
| (1,20)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG23 | 17       | 1.46          |
| (1,20)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG21 | 22       | 1.46          |
| (1,20)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG22 | 22       | 1.46          |
| (1,20)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG23 | 22       | 1.46          |
| (1,20)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG21 | 28       | 1.45          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,20)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG22 | 28       | 1.45          |
| (1,20)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG23 | 28       | 1.45          |
| (1,20)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG21 | 31       | 1.44          |
| (1,20)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG22 | 31       | 1.44          |
| (1,20)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG23 | 31       | 1.44          |
| (2,95)  | 1:8:A:ARG:HD2  | 1:11:A:TRP:HB2 | 34       | 1.43          |
| (2,95)  | 1:8:A:ARG:HD2  | 1:11:A:TRP:HB2 | 9        | 1.42          |
| (1,20)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG21 | 10       | 1.42          |
| (1,20)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG22 | 10       | 1.42          |
| (1,20)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG23 | 10       | 1.42          |
| (1,20)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG21 | 32       | 1.42          |
| (1,20)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG22 | 32       | 1.42          |
| (1,20)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG23 | 32       | 1.42          |
| (1,20)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG21 | 33       | 1.42          |
| (1,20)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG22 | 33       | 1.42          |
| (1,20)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG23 | 33       | 1.42          |
| (2,136) | 1:15:A:TYR:HB2 | 1:12:A:PRO:HB3 | 8        | 1.41          |
| (2,136) | 1:15:A:TYR:HB2 | 1:12:A:PRO:HB3 | 12       | 1.41          |
| (2,95)  | 1:8:A:ARG:HD2  | 1:11:A:TRP:HB2 | 1        | 1.41          |
| (2,95)  | 1:8:A:ARG:HD2  | 1:11:A:TRP:HB2 | 26       | 1.41          |
| (1,29)  | 1:11:A:TRP:HD1 | 1:4:A:HCS:HB2  | 29       | 1.41          |
| (2,136) | 1:15:A:TYR:HB2 | 1:12:A:PRO:HB3 | 35       | 1.4           |
| (2,95)  | 1:8:A:ARG:HD2  | 1:11:A:TRP:HB2 | 23       | 1.4           |
| (1,20)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG21 | 11       | 1.4           |
| (1,20)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG22 | 11       | 1.4           |
| (1,20)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG23 | 11       | 1.4           |
| (1,20)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG21 | 23       | 1.4           |
| (1,20)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG22 | 23       | 1.4           |
| (1,20)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG23 | 23       | 1.4           |
| (1,20)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG21 | 27       | 1.4           |
| (1,20)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG22 | 27       | 1.4           |
| (1,20)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG23 | 27       | 1.4           |
| (2,136) | 1:15:A:TYR:HB2 | 1:12:A:PRO:HB3 | 13       | 1.39          |
| (2,95)  | 1:8:A:ARG:HD2  | 1:11:A:TRP:HB2 | 15       | 1.39          |
| (1,20)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG21 | 2        | 1.39          |
| (1,20)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG22 | 2        | 1.39          |
| (1,20)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG23 | 2        | 1.39          |
| (1,20)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG21 | 12       | 1.39          |
| (1,20)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG22 | 12       | 1.39          |
| (1,20)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG23 | 12       | 1.39          |
| (1,20)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG21 | 35       | 1.39          |
| (1,20)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG22 | 35       | 1.39          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,20)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG23 | 35       | 1.39          |
| (2,310) | 1:11:A:TRP:HE3 | 1:12:A:PRO:HD3 | 11       | 1.38          |
| (2,136) | 1:15:A:TYR:HB2 | 1:12:A:PRO:HB3 | 15       | 1.38          |
| (2,136) | 1:15:A:TYR:HB2 | 1:12:A:PRO:HB3 | 6        | 1.37          |
| (2,136) | 1:15:A:TYR:HB2 | 1:12:A:PRO:HB3 | 10       | 1.37          |
| (2,136) | 1:15:A:TYR:HB2 | 1:12:A:PRO:HB3 | 24       | 1.37          |
| (2,136) | 1:15:A:TYR:HB2 | 1:12:A:PRO:HB3 | 31       | 1.37          |
| (2,136) | 1:15:A:TYR:HB2 | 1:12:A:PRO:HB3 | 34       | 1.37          |
| (2,136) | 1:15:A:TYR:HB2 | 1:12:A:PRO:HB3 | 3        | 1.36          |
| (2,136) | 1:15:A:TYR:HB2 | 1:12:A:PRO:HB3 | 22       | 1.36          |
| (2,136) | 1:15:A:TYR:HB2 | 1:12:A:PRO:HB3 | 29       | 1.36          |
| (2,136) | 1:15:A:TYR:HB2 | 1:12:A:PRO:HB3 | 32       | 1.36          |
| (2,95)  | 1:8:A:ARG:HD2  | 1:11:A:TRP:HB2 | 5        | 1.36          |
| (2,136) | 1:15:A:TYR:HB2 | 1:12:A:PRO:HB3 | 1        | 1.35          |
| (2,136) | 1:15:A:TYR:HB2 | 1:12:A:PRO:HB3 | 14       | 1.35          |
| (1,20)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG21 | 3        | 1.35          |
| (1,20)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG22 | 3        | 1.35          |
| (1,20)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG23 | 3        | 1.35          |
| (2,310) | 1:11:A:TRP:HE3 | 1:12:A:PRO:HD3 | 3        | 1.34          |
| (2,136) | 1:15:A:TYR:HB2 | 1:12:A:PRO:HB3 | 21       | 1.33          |
| (2,136) | 1:15:A:TYR:HB2 | 1:12:A:PRO:HB3 | 25       | 1.33          |
| (2,136) | 1:15:A:TYR:HB2 | 1:12:A:PRO:HB3 | 30       | 1.33          |
| (2,136) | 1:15:A:TYR:HB2 | 1:12:A:PRO:HB3 | 11       | 1.32          |
| (2,47)  | 1:7:A:HIS:HB2  | 1:8:A:ARG:HG2  | 33       | 1.32          |
| (1,20)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG21 | 29       | 1.32          |
| (1,20)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG22 | 29       | 1.32          |
| (1,20)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG23 | 29       | 1.32          |
| (2,136) | 1:15:A:TYR:HB2 | 1:12:A:PRO:HB3 | 18       | 1.31          |
| (1,20)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG21 | 6        | 1.31          |
| (1,20)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG22 | 6        | 1.31          |
| (1,20)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG23 | 6        | 1.31          |
| (1,20)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG21 | 21       | 1.31          |
| (1,20)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG22 | 21       | 1.31          |
| (1,20)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG23 | 21       | 1.31          |
| (2,310) | 1:11:A:TRP:HE3 | 1:12:A:PRO:HD3 | 27       | 1.3           |
| (2,136) | 1:15:A:TYR:HB2 | 1:12:A:PRO:HB3 | 2        | 1.3           |
| (2,23)  | 1:14:A:TRP:HZ3 | 1:16:A:ARG:HD3 | 3        | 1.3           |
| (1,29)  | 1:11:A:TRP:HD1 | 1:1:A:PRO:HG3  | 22       | 1.3           |
| (2,310) | 1:11:A:TRP:HE3 | 1:12:A:PRO:HD3 | 8        | 1.29          |
| (2,310) | 1:11:A:TRP:HE3 | 1:12:A:PRO:HD3 | 34       | 1.29          |
| (2,136) | 1:15:A:TYR:HB2 | 1:12:A:PRO:HB3 | 7        | 1.29          |
| (2,47)  | 1:7:A:HIS:HB2  | 1:8:A:ARG:HG2  | 10       | 1.29          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,20)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG21 | 8        | 1.29          |
| (1,20)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG22 | 8        | 1.29          |
| (1,20)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG23 | 8        | 1.29          |
| (1,20)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG21 | 19       | 1.29          |
| (1,20)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG22 | 19       | 1.29          |
| (1,20)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG23 | 19       | 1.29          |
| (2,310) | 1:11:A:TRP:HE3 | 1:12:A:PRO:HD3 | 1        | 1.28          |
| (2,310) | 1:11:A:TRP:HE3 | 1:12:A:PRO:HD3 | 23       | 1.28          |
| (2,310) | 1:11:A:TRP:HE3 | 1:12:A:PRO:HD3 | 9        | 1.27          |
| (2,310) | 1:11:A:TRP:HE3 | 1:12:A:PRO:HD3 | 26       | 1.27          |
| (2,136) | 1:15:A:TYR:HB2 | 1:12:A:PRO:HB3 | 4        | 1.27          |
| (2,310) | 1:11:A:TRP:HE3 | 1:12:A:PRO:HD3 | 12       | 1.26          |
| (2,310) | 1:11:A:TRP:HE3 | 1:12:A:PRO:HD3 | 29       | 1.26          |
| (2,310) | 1:11:A:TRP:HE3 | 1:12:A:PRO:HD3 | 30       | 1.26          |
| (2,136) | 1:15:A:TYR:HB2 | 1:12:A:PRO:HB3 | 16       | 1.26          |
| (2,310) | 1:11:A:TRP:HE3 | 1:12:A:PRO:HD3 | 6        | 1.25          |
| (2,310) | 1:11:A:TRP:HE3 | 1:12:A:PRO:HD3 | 15       | 1.25          |
| (2,310) | 1:11:A:TRP:HE3 | 1:12:A:PRO:HD3 | 17       | 1.25          |
| (2,310) | 1:11:A:TRP:HE3 | 1:12:A:PRO:HD3 | 19       | 1.25          |
| (2,310) | 1:11:A:TRP:HE3 | 1:12:A:PRO:HD3 | 21       | 1.25          |
| (2,136) | 1:15:A:TYR:HB2 | 1:12:A:PRO:HB3 | 26       | 1.25          |
| (2,47)  | 1:7:A:HIS:HB2  | 1:8:A:ARG:HG2  | 13       | 1.25          |
| (2,310) | 1:11:A:TRP:HE3 | 1:12:A:PRO:HD3 | 13       | 1.24          |
| (2,310) | 1:11:A:TRP:HE3 | 1:12:A:PRO:HD3 | 25       | 1.24          |
| (2,310) | 1:11:A:TRP:HE3 | 1:12:A:PRO:HD3 | 31       | 1.24          |
| (2,310) | 1:11:A:TRP:HE3 | 1:12:A:PRO:HD3 | 32       | 1.24          |
| (3,15)  | 1:11:A:TRP:HE1 | 1:12:A:PRO:HD3 | 2        | 1.23          |
| (3,15)  | 1:11:A:TRP:HE1 | 1:12:A:PRO:HD3 | 25       | 1.23          |
| (3,15)  | 1:11:A:TRP:HE1 | 1:12:A:PRO:HD3 | 26       | 1.23          |
| (3,15)  | 1:11:A:TRP:HE1 | 1:12:A:PRO:HD3 | 28       | 1.23          |
| (2,310) | 1:11:A:TRP:HE3 | 1:12:A:PRO:HD3 | 7        | 1.23          |
| (2,310) | 1:11:A:TRP:HE3 | 1:12:A:PRO:HD3 | 18       | 1.23          |
| (2,136) | 1:15:A:TYR:HB2 | 1:12:A:PRO:HB3 | 28       | 1.23          |
| (2,47)  | 1:7:A:HIS:HB2  | 1:8:A:ARG:HG2  | 16       | 1.23          |
| (2,47)  | 1:7:A:HIS:HB2  | 1:8:A:ARG:HG2  | 22       | 1.23          |
| (3,15)  | 1:11:A:TRP:HE1 | 1:12:A:PRO:HD3 | 11       | 1.22          |
| (3,15)  | 1:11:A:TRP:HE1 | 1:12:A:PRO:HD3 | 17       | 1.22          |
| (3,15)  | 1:11:A:TRP:HE1 | 1:12:A:PRO:HD3 | 20       | 1.22          |
| (3,15)  | 1:11:A:TRP:HE1 | 1:12:A:PRO:HD3 | 27       | 1.22          |
| (1,29)  | 1:11:A:TRP:HD1 | 1:1:A:PRO:HG3  | 11       | 1.22          |
| (3,15)  | 1:11:A:TRP:HE1 | 1:12:A:PRO:HD3 | 8        | 1.21          |
| (3,15)  | 1:11:A:TRP:HE1 | 1:12:A:PRO:HD3 | 10       | 1.21          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (3,15)  | 1:11:A:TRP:HE1 | 1:12:A:PRO:HD3 | 13       | 1.21          |
| (3,15)  | 1:11:A:TRP:HE1 | 1:12:A:PRO:HD3 | 24       | 1.21          |
| (3,15)  | 1:11:A:TRP:HE1 | 1:12:A:PRO:HD3 | 33       | 1.21          |
| (3,15)  | 1:11:A:TRP:HE1 | 1:12:A:PRO:HD3 | 35       | 1.21          |
| (2,310) | 1:11:A:TRP:HE3 | 1:12:A:PRO:HD3 | 5        | 1.21          |
| (2,23)  | 1:14:A:TRP:HZ3 | 1:16:A:ARG:HD3 | 5        | 1.21          |
| (2,23)  | 1:14:A:TRP:HZ3 | 1:16:A:ARG:HD3 | 7        | 1.21          |
| (3,15)  | 1:11:A:TRP:HE1 | 1:12:A:PRO:HD3 | 1        | 1.2           |
| (3,15)  | 1:11:A:TRP:HE1 | 1:12:A:PRO:HD3 | 5        | 1.2           |
| (3,15)  | 1:11:A:TRP:HE1 | 1:12:A:PRO:HD3 | 12       | 1.2           |
| (3,15)  | 1:11:A:TRP:HE1 | 1:12:A:PRO:HD3 | 14       | 1.2           |
| (3,15)  | 1:11:A:TRP:HE1 | 1:12:A:PRO:HD3 | 16       | 1.2           |
| (3,15)  | 1:11:A:TRP:HE1 | 1:12:A:PRO:HD3 | 19       | 1.2           |
| (3,15)  | 1:11:A:TRP:HE1 | 1:12:A:PRO:HD3 | 29       | 1.2           |
| (3,15)  | 1:11:A:TRP:HE1 | 1:12:A:PRO:HD3 | 34       | 1.2           |
| (2,310) | 1:11:A:TRP:HE3 | 1:12:A:PRO:HD3 | 2        | 1.2           |
| (2,310) | 1:11:A:TRP:HE3 | 1:12:A:PRO:HD3 | 20       | 1.2           |
| (2,310) | 1:11:A:TRP:HE3 | 1:12:A:PRO:HD3 | 35       | 1.2           |
| (3,15)  | 1:11:A:TRP:HE1 | 1:12:A:PRO:HD3 | 3        | 1.19          |
| (3,15)  | 1:11:A:TRP:HE1 | 1:12:A:PRO:HD3 | 7        | 1.19          |
| (3,15)  | 1:11:A:TRP:HE1 | 1:12:A:PRO:HD3 | 21       | 1.19          |
| (3,15)  | 1:11:A:TRP:HE1 | 1:12:A:PRO:HD3 | 22       | 1.19          |
| (3,15)  | 1:11:A:TRP:HE1 | 1:12:A:PRO:HD3 | 23       | 1.19          |
| (3,15)  | 1:11:A:TRP:HE1 | 1:12:A:PRO:HD3 | 30       | 1.19          |
| (2,310) | 1:11:A:TRP:HE3 | 1:12:A:PRO:HD3 | 4        | 1.19          |
| (2,310) | 1:11:A:TRP:HE3 | 1:12:A:PRO:HD3 | 16       | 1.19          |
| (2,310) | 1:11:A:TRP:HE3 | 1:12:A:PRO:HD3 | 24       | 1.19          |
| (2,310) | 1:11:A:TRP:HE3 | 1:12:A:PRO:HD3 | 33       | 1.19          |
| (2,136) | 1:15:A:TYR:HB2 | 1:12:A:PRO:HB3 | 33       | 1.19          |
| (2,23)  | 1:14:A:TRP:HZ3 | 1:16:A:ARG:HD3 | 24       | 1.19          |
| (2,21)  | 1:11:A:TRP:HH2 | 1:8:A:ARG:HD2  | 1        | 1.19          |
| (3,15)  | 1:11:A:TRP:HE1 | 1:12:A:PRO:HD3 | 6        | 1.18          |
| (3,15)  | 1:11:A:TRP:HE1 | 1:12:A:PRO:HD3 | 32       | 1.18          |
| (2,310) | 1:11:A:TRP:HE3 | 1:12:A:PRO:HD3 | 28       | 1.18          |
| (3,15)  | 1:11:A:TRP:HE1 | 1:12:A:PRO:HD3 | 4        | 1.17          |
| (3,15)  | 1:11:A:TRP:HE1 | 1:12:A:PRO:HD3 | 9        | 1.17          |
| (3,15)  | 1:11:A:TRP:HE1 | 1:12:A:PRO:HD3 | 15       | 1.17          |
| (3,15)  | 1:11:A:TRP:HE1 | 1:12:A:PRO:HD3 | 18       | 1.17          |
| (3,15)  | 1:11:A:TRP:HE1 | 1:12:A:PRO:HD3 | 31       | 1.17          |
| (2,310) | 1:11:A:TRP:HE3 | 1:12:A:PRO:HD3 | 10       | 1.17          |
| (2,310) | 1:11:A:TRP:HE3 | 1:12:A:PRO:HD3 | 14       | 1.17          |
| (2,136) | 1:15:A:TYR:HB2 | 1:12:A:PRO:HB3 | 20       | 1.17          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (2,47)  | 1:7:A:HIS:HB2  | 1:8:A:ARG:HG2  | 19       | 1.17          |
| (2,47)  | 1:7:A:HIS:HB2  | 1:8:A:ARG:HG2  | 2        | 1.16          |
| (2,23)  | 1:14:A:TRP:HZ3 | 1:16:A:ARG:HD3 | 26       | 1.16          |
| (2,21)  | 1:11:A:TRP:HH2 | 1:8:A:ARG:HD2  | 23       | 1.16          |
| (2,21)  | 1:11:A:TRP:HH2 | 1:8:A:ARG:HD2  | 26       | 1.16          |
| (2,21)  | 1:11:A:TRP:HH2 | 1:8:A:ARG:HD2  | 9        | 1.15          |
| (2,325) | 1:5:A:HIS:HD2  | 1:5:A:HIS:HB2  | 33       | 1.14          |
| (2,325) | 1:5:A:HIS:HD2  | 1:5:A:HIS:HB2  | 1        | 1.13          |
| (2,325) | 1:5:A:HIS:HD2  | 1:5:A:HIS:HB2  | 2        | 1.13          |
| (2,325) | 1:5:A:HIS:HD2  | 1:5:A:HIS:HB2  | 3        | 1.13          |
| (2,325) | 1:5:A:HIS:HD2  | 1:5:A:HIS:HB2  | 4        | 1.13          |
| (2,325) | 1:5:A:HIS:HD2  | 1:5:A:HIS:HB2  | 6        | 1.13          |
| (2,325) | 1:5:A:HIS:HD2  | 1:5:A:HIS:HB2  | 7        | 1.13          |
| (2,325) | 1:5:A:HIS:HD2  | 1:5:A:HIS:HB2  | 8        | 1.13          |
| (2,325) | 1:5:A:HIS:HD2  | 1:5:A:HIS:HB2  | 9        | 1.13          |
| (2,325) | 1:5:A:HIS:HD2  | 1:5:A:HIS:HB2  | 11       | 1.13          |
| (2,325) | 1:5:A:HIS:HD2  | 1:5:A:HIS:HB2  | 12       | 1.13          |
| (2,325) | 1:5:A:HIS:HD2  | 1:5:A:HIS:HB2  | 13       | 1.13          |
| (2,325) | 1:5:A:HIS:HD2  | 1:5:A:HIS:HB2  | 15       | 1.13          |
| (2,325) | 1:5:A:HIS:HD2  | 1:5:A:HIS:HB2  | 16       | 1.13          |
| (2,325) | 1:5:A:HIS:HD2  | 1:5:A:HIS:HB2  | 18       | 1.13          |
| (2,325) | 1:5:A:HIS:HD2  | 1:5:A:HIS:HB2  | 20       | 1.13          |
| (2,325) | 1:5:A:HIS:HD2  | 1:5:A:HIS:HB2  | 21       | 1.13          |
| (2,325) | 1:5:A:HIS:HD2  | 1:5:A:HIS:HB2  | 23       | 1.13          |
| (2,325) | 1:5:A:HIS:HD2  | 1:5:A:HIS:HB2  | 24       | 1.13          |
| (2,325) | 1:5:A:HIS:HD2  | 1:5:A:HIS:HB2  | 25       | 1.13          |
| (2,325) | 1:5:A:HIS:HD2  | 1:5:A:HIS:HB2  | 26       | 1.13          |
| (2,325) | 1:5:A:HIS:HD2  | 1:5:A:HIS:HB2  | 27       | 1.13          |
| (2,325) | 1:5:A:HIS:HD2  | 1:5:A:HIS:HB2  | 29       | 1.13          |
| (2,325) | 1:5:A:HIS:HD2  | 1:5:A:HIS:HB2  | 30       | 1.13          |
| (2,325) | 1:5:A:HIS:HD2  | 1:5:A:HIS:HB2  | 34       | 1.13          |
| (2,325) | 1:5:A:HIS:HD2  | 1:5:A:HIS:HB2  | 35       | 1.13          |
| (2,310) | 1:11:A:TRP:HE3 | 1:12:A:PRO:HD3 | 22       | 1.13          |
| (2,47)  | 1:7:A:HIS:HB2  | 1:8:A:ARG:HG2  | 27       | 1.13          |
| (2,47)  | 1:7:A:HIS:HB2  | 1:8:A:ARG:HG2  | 29       | 1.13          |
| (2,325) | 1:5:A:HIS:HD2  | 1:5:A:HIS:HB2  | 5        | 1.12          |
| (2,325) | 1:5:A:HIS:HD2  | 1:5:A:HIS:HB2  | 10       | 1.12          |
| (2,325) | 1:5:A:HIS:HD2  | 1:5:A:HIS:HB2  | 17       | 1.12          |
| (2,325) | 1:5:A:HIS:HD2  | 1:5:A:HIS:HB2  | 19       | 1.12          |
| (2,325) | 1:5:A:HIS:HD2  | 1:5:A:HIS:HB2  | 31       | 1.12          |
| (2,325) | 1:5:A:HIS:HD2  | 1:5:A:HIS:HB2  | 32       | 1.12          |
| (2,295) | 1:9:A:PRO:HD3  | 1:8:A:ARG:HD3  | 15       | 1.12          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (2,295) | 1:9:A:PRO:HD3  | 1:8:A:ARG:HD3  | 23       | 1.12          |
| (2,21)  | 1:11:A:TRP:HH2 | 1:8:A:ARG:HD2  | 11       | 1.12          |
| (2,325) | 1:5:A:HIS:HD2  | 1:5:A:HIS:HB2  | 22       | 1.11          |
| (2,325) | 1:5:A:HIS:HD2  | 1:5:A:HIS:HB2  | 28       | 1.11          |
| (2,312) | 1:15:A:TYR:HD1 | 1:16:A:ARG:HG2 | 31       | 1.11          |
| (2,312) | 1:15:A:TYR:HD2 | 1:16:A:ARG:HG2 | 31       | 1.11          |
| (2,295) | 1:9:A:PRO:HD3  | 1:8:A:ARG:HD3  | 9        | 1.11          |
| (2,136) | 1:15:A:TYR:HB2 | 1:12:A:PRO:HB3 | 5        | 1.11          |
| (2,47)  | 1:7:A:HIS:HB2  | 1:8:A:ARG:HG2  | 24       | 1.11          |
| (2,23)  | 1:14:A:TRP:HZ3 | 1:16:A:ARG:HD3 | 27       | 1.11          |
| (2,23)  | 1:14:A:TRP:HZ3 | 1:16:A:ARG:HD3 | 30       | 1.11          |
| (2,21)  | 1:11:A:TRP:HH2 | 1:8:A:ARG:HD2  | 5        | 1.11          |
| (3,43)  | 1:15:A:TYR:HE1 | 1:16:A:ARG:HG2 | 31       | 1.1           |
| (3,43)  | 1:15:A:TYR:HE2 | 1:16:A:ARG:HG2 | 31       | 1.1           |
| (2,295) | 1:9:A:PRO:HD3  | 1:8:A:ARG:HD3  | 5        | 1.1           |
| (2,295) | 1:9:A:PRO:HD3  | 1:8:A:ARG:HD3  | 32       | 1.1           |
| (2,21)  | 1:11:A:TRP:HH2 | 1:8:A:ARG:HD2  | 8        | 1.1           |
| (2,21)  | 1:11:A:TRP:HH2 | 1:8:A:ARG:HD2  | 15       | 1.1           |
| (2,325) | 1:5:A:HIS:HD2  | 1:5:A:HIS:HB2  | 14       | 1.09          |
| (2,295) | 1:9:A:PRO:HD3  | 1:8:A:ARG:HD3  | 4        | 1.09          |
| (2,295) | 1:9:A:PRO:HD3  | 1:8:A:ARG:HD3  | 11       | 1.09          |
| (2,295) | 1:9:A:PRO:HD3  | 1:8:A:ARG:HD3  | 26       | 1.09          |
| (2,23)  | 1:14:A:TRP:HZ3 | 1:16:A:ARG:HD3 | 20       | 1.09          |
| (2,21)  | 1:11:A:TRP:HH2 | 1:8:A:ARG:HD2  | 4        | 1.09          |
| (2,21)  | 1:11:A:TRP:HH2 | 1:8:A:ARG:HD2  | 30       | 1.09          |
| (2,15)  | 1:11:A:TRP:HE3 | 1:8:A:ARG:HD2  | 3        | 1.09          |
| (2,23)  | 1:14:A:TRP:HZ3 | 1:16:A:ARG:HD3 | 29       | 1.08          |
| (2,295) | 1:9:A:PRO:HD3  | 1:8:A:ARG:HD3  | 7        | 1.07          |
| (2,295) | 1:9:A:PRO:HD3  | 1:8:A:ARG:HD3  | 18       | 1.07          |
| (2,295) | 1:9:A:PRO:HD3  | 1:8:A:ARG:HD3  | 31       | 1.07          |
| (2,295) | 1:9:A:PRO:HD3  | 1:8:A:ARG:HD3  | 34       | 1.07          |
| (2,21)  | 1:11:A:TRP:HH2 | 1:8:A:ARG:HD2  | 7        | 1.07          |
| (2,21)  | 1:11:A:TRP:HH2 | 1:8:A:ARG:HD2  | 32       | 1.07          |
| (2,295) | 1:9:A:PRO:HD3  | 1:8:A:ARG:HD3  | 6        | 1.06          |
| (2,295) | 1:9:A:PRO:HD3  | 1:8:A:ARG:HD3  | 21       | 1.06          |
| (2,295) | 1:9:A:PRO:HD3  | 1:8:A:ARG:HD3  | 30       | 1.06          |
| (2,47)  | 1:7:A:HIS:HB2  | 1:8:A:ARG:HG2  | 35       | 1.06          |
| (2,21)  | 1:11:A:TRP:HH2 | 1:8:A:ARG:HD2  | 6        | 1.06          |
| (2,21)  | 1:11:A:TRP:HH2 | 1:8:A:ARG:HD2  | 34       | 1.06          |
| (2,295) | 1:9:A:PRO:HD3  | 1:8:A:ARG:HD3  | 1        | 1.05          |
| (1,29)  | 1:11:A:TRP:HD1 | 1:1:A:PRO:HG3  | 23       | 1.05          |
| (2,295) | 1:9:A:PRO:HD3  | 1:8:A:ARG:HD3  | 8        | 1.04          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (2,23)  | 1:14:A:TRP:HZ3 | 1:16:A:ARG:HD3 | 8        | 1.04          |
| (2,21)  | 1:11:A:TRP:HH2 | 1:8:A:ARG:HD2  | 31       | 1.04          |
| (2,47)  | 1:7:A:HIS:HB2  | 1:8:A:ARG:HG2  | 20       | 1.03          |
| (2,47)  | 1:7:A:HIS:HB2  | 1:8:A:ARG:HG2  | 25       | 1.03          |
| (2,295) | 1:9:A:PRO:HD3  | 1:8:A:ARG:HD3  | 3        | 1.02          |
| (2,21)  | 1:11:A:TRP:HH2 | 1:8:A:ARG:HD2  | 21       | 1.02          |
| (2,251) | 1:5:A:HIS:HB2  | 1:4:A:HCS:HA   | 6        | 1.01          |
| (2,21)  | 1:11:A:TRP:HH2 | 1:8:A:ARG:HD2  | 18       | 1.01          |
| (1,29)  | 1:11:A:TRP:HD1 | 1:1:A:PRO:HG3  | 13       | 1.01          |
| (1,29)  | 1:11:A:TRP:HD1 | 1:1:A:PRO:HG3  | 35       | 1.0           |
| (2,47)  | 1:7:A:HIS:HB2  | 1:8:A:ARG:HG2  | 17       | 0.98          |
| (2,251) | 1:5:A:HIS:HB2  | 1:4:A:HCS:HA   | 3        | 0.97          |
| (2,47)  | 1:7:A:HIS:HB2  | 1:8:A:ARG:HG2  | 12       | 0.97          |
| (2,251) | 1:5:A:HIS:HB2  | 1:4:A:HCS:HA   | 8        | 0.96          |
| (2,47)  | 1:7:A:HIS:HB2  | 1:8:A:ARG:HG2  | 14       | 0.96          |
| (2,47)  | 1:7:A:HIS:HB2  | 1:8:A:ARG:HG2  | 28       | 0.96          |
| (2,23)  | 1:14:A:TRP:HZ3 | 1:16:A:ARG:HD3 | 35       | 0.96          |
| (2,251) | 1:5:A:HIS:HB2  | 1:4:A:HCS:HA   | 21       | 0.95          |
| (3,12)  | 1:11:A:TRP:HE3 | 1:12:A:PRO:HG3 | 3        | 0.94          |
| (2,251) | 1:5:A:HIS:HB2  | 1:4:A:HCS:HA   | 11       | 0.94          |
| (2,23)  | 1:14:A:TRP:HZ3 | 1:16:A:ARG:HD3 | 13       | 0.93          |
| (3,12)  | 1:11:A:TRP:HE3 | 1:12:A:PRO:HG3 | 9        | 0.92          |
| (3,12)  | 1:11:A:TRP:HE3 | 1:12:A:PRO:HG3 | 27       | 0.92          |
| (2,251) | 1:5:A:HIS:HB2  | 1:4:A:HCS:HA   | 29       | 0.92          |
| (2,251) | 1:5:A:HIS:HB2  | 1:4:A:HCS:HA   | 12       | 0.91          |
| (2,251) | 1:5:A:HIS:HB2  | 1:4:A:HCS:HA   | 14       | 0.91          |
| (2,251) | 1:5:A:HIS:HB2  | 1:4:A:HCS:HA   | 22       | 0.91          |
| (3,12)  | 1:11:A:TRP:HE3 | 1:12:A:PRO:HG3 | 11       | 0.9           |
| (2,251) | 1:5:A:HIS:HB2  | 1:4:A:HCS:HA   | 16       | 0.9           |
| (2,251) | 1:5:A:HIS:HB2  | 1:4:A:HCS:HA   | 18       | 0.9           |
| (2,251) | 1:5:A:HIS:HB2  | 1:4:A:HCS:HA   | 32       | 0.9           |
| (2,23)  | 1:14:A:TRP:HZ3 | 1:16:A:ARG:HD3 | 21       | 0.9           |
| (3,12)  | 1:11:A:TRP:HE3 | 1:12:A:PRO:HG3 | 6        | 0.89          |
| (2,318) | 1:9:A:PRO:HD2  | 1:8:A:ARG:HD3  | 1        | 0.89          |
| (2,251) | 1:5:A:HIS:HB2  | 1:4:A:HCS:HA   | 1        | 0.89          |
| (2,251) | 1:5:A:HIS:HB2  | 1:4:A:HCS:HA   | 4        | 0.89          |
| (2,251) | 1:5:A:HIS:HB2  | 1:4:A:HCS:HA   | 17       | 0.89          |
| (2,251) | 1:5:A:HIS:HB2  | 1:4:A:HCS:HA   | 24       | 0.89          |
| (2,251) | 1:5:A:HIS:HB2  | 1:4:A:HCS:HA   | 7        | 0.88          |
| (2,251) | 1:5:A:HIS:HB2  | 1:4:A:HCS:HA   | 9        | 0.88          |
| (2,251) | 1:5:A:HIS:HB2  | 1:4:A:HCS:HA   | 15       | 0.88          |
| (2,251) | 1:5:A:HIS:HB2  | 1:4:A:HCS:HA   | 19       | 0.88          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (2,251) | 1:5:A:HIS:HB2  | 1:4:A:HCS:HA   | 20       | 0.88          |
| (2,251) | 1:5:A:HIS:HB2  | 1:4:A:HCS:HA   | 25       | 0.88          |
| (2,251) | 1:5:A:HIS:HB2  | 1:4:A:HCS:HA   | 35       | 0.88          |
| (1,29)  | 1:11:A:TRP:HD1 | 1:1:A:PRO:HG3  | 9        | 0.88          |
| (2,251) | 1:5:A:HIS:HB2  | 1:4:A:HCS:HA   | 23       | 0.87          |
| (2,251) | 1:5:A:HIS:HB2  | 1:4:A:HCS:HA   | 26       | 0.87          |
| (2,251) | 1:5:A:HIS:HB2  | 1:4:A:HCS:HA   | 27       | 0.87          |
| (2,251) | 1:5:A:HIS:HB2  | 1:4:A:HCS:HA   | 28       | 0.87          |
| (2,251) | 1:5:A:HIS:HB2  | 1:4:A:HCS:HA   | 30       | 0.87          |
| (2,251) | 1:5:A:HIS:HB2  | 1:4:A:HCS:HA   | 31       | 0.87          |
| (2,251) | 1:5:A:HIS:HB2  | 1:4:A:HCS:HA   | 33       | 0.87          |
| (2,251) | 1:5:A:HIS:HB2  | 1:4:A:HCS:HA   | 34       | 0.87          |
| (2,23)  | 1:14:A:TRP:HZ3 | 1:16:A:ARG:HD3 | 14       | 0.87          |
| (3,12)  | 1:11:A:TRP:HE3 | 1:12:A:PRO:HG3 | 8        | 0.86          |
| (3,12)  | 1:11:A:TRP:HE3 | 1:12:A:PRO:HG3 | 15       | 0.86          |
| (3,12)  | 1:11:A:TRP:HE3 | 1:12:A:PRO:HG3 | 32       | 0.86          |
| (2,312) | 1:15:A:TYR:HD1 | 1:16:A:ARG:HG2 | 9        | 0.86          |
| (2,312) | 1:15:A:TYR:HD2 | 1:16:A:ARG:HG2 | 9        | 0.86          |
| (2,251) | 1:5:A:HIS:HB2  | 1:4:A:HCS:HA   | 13       | 0.86          |
| (3,43)  | 1:15:A:TYR:HE1 | 1:16:A:ARG:HG2 | 9        | 0.85          |
| (3,43)  | 1:15:A:TYR:HE2 | 1:16:A:ARG:HG2 | 9        | 0.85          |
| (3,43)  | 1:15:A:TYR:HE1 | 1:16:A:ARG:HG2 | 10       | 0.85          |
| (3,43)  | 1:15:A:TYR:HE2 | 1:16:A:ARG:HG2 | 10       | 0.85          |
| (3,12)  | 1:11:A:TRP:HE3 | 1:12:A:PRO:HG3 | 19       | 0.85          |
| (3,12)  | 1:11:A:TRP:HE3 | 1:12:A:PRO:HG3 | 23       | 0.85          |
| (3,12)  | 1:11:A:TRP:HE3 | 1:12:A:PRO:HG3 | 30       | 0.85          |
| (3,12)  | 1:11:A:TRP:HE3 | 1:12:A:PRO:HG3 | 31       | 0.85          |
| (2,251) | 1:5:A:HIS:HB2  | 1:4:A:HCS:HA   | 5        | 0.85          |
| (2,251) | 1:5:A:HIS:HB2  | 1:4:A:HCS:HA   | 10       | 0.85          |
| (1,29)  | 1:11:A:TRP:HD1 | 1:1:A:PRO:HG3  | 6        | 0.85          |
| (3,12)  | 1:11:A:TRP:HE3 | 1:12:A:PRO:HG3 | 12       | 0.84          |
| (2,312) | 1:15:A:TYR:HD1 | 1:16:A:ARG:HG2 | 14       | 0.84          |
| (2,312) | 1:15:A:TYR:HD2 | 1:16:A:ARG:HG2 | 14       | 0.84          |
| (2,251) | 1:5:A:HIS:HB2  | 1:4:A:HCS:HA   | 2        | 0.84          |
| (3,12)  | 1:11:A:TRP:HE3 | 1:12:A:PRO:HG3 | 1        | 0.83          |
| (3,12)  | 1:11:A:TRP:HE3 | 1:12:A:PRO:HG3 | 17       | 0.83          |
| (3,12)  | 1:11:A:TRP:HE3 | 1:12:A:PRO:HG3 | 21       | 0.83          |
| (2,318) | 1:9:A:PRO:HD2  | 1:8:A:ARG:HD3  | 26       | 0.83          |
| (2,318) | 1:9:A:PRO:HD2  | 1:8:A:ARG:HD3  | 34       | 0.83          |
| (1,29)  | 1:11:A:TRP:HD1 | 1:1:A:PRO:HG3  | 20       | 0.83          |
| (3,12)  | 1:11:A:TRP:HE3 | 1:12:A:PRO:HG3 | 24       | 0.82          |
| (3,12)  | 1:11:A:TRP:HE3 | 1:12:A:PRO:HG3 | 29       | 0.82          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (2,161) | 1:4:A:HCS:HB3  | 1:13:A:CYS:HA  | 15       | 0.82          |
| (2,161) | 1:4:A:HCS:HB3  | 1:13:A:CYS:HA  | 33       | 0.82          |
| (2,41)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG11 | 9        | 0.82          |
| (2,41)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG12 | 9        | 0.82          |
| (2,41)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG13 | 9        | 0.82          |
| (2,15)  | 1:11:A:TRP:HE3 | 1:8:A:ARG:HD2  | 18       | 0.82          |
| (2,161) | 1:4:A:HCS:HB3  | 1:13:A:CYS:HA  | 34       | 0.81          |
| (3,25)  | 1:5:A:HIS:H    | 1:3:A:ILE:HG13 | 34       | 0.8           |
| (3,12)  | 1:11:A:TRP:HE3 | 1:12:A:PRO:HG3 | 5        | 0.8           |
| (3,12)  | 1:11:A:TRP:HE3 | 1:12:A:PRO:HG3 | 26       | 0.8           |
| (3,12)  | 1:11:A:TRP:HE3 | 1:12:A:PRO:HG3 | 34       | 0.8           |
| (3,12)  | 1:11:A:TRP:HE3 | 1:12:A:PRO:HG3 | 35       | 0.8           |
| (2,337) | 1:6:A:VAL:HA   | 1:13:A:CYS:HB2 | 15       | 0.8           |
| (2,318) | 1:9:A:PRO:HD2  | 1:8:A:ARG:HD3  | 15       | 0.8           |
| (2,161) | 1:4:A:HCS:HB3  | 1:13:A:CYS:HA  | 18       | 0.8           |
| (2,47)  | 1:7:A:HIS:HB2  | 1:8:A:ARG:HG2  | 23       | 0.8           |
| (3,12)  | 1:11:A:TRP:HE3 | 1:12:A:PRO:HG3 | 13       | 0.79          |
| (3,12)  | 1:11:A:TRP:HE3 | 1:12:A:PRO:HG3 | 25       | 0.79          |
| (2,161) | 1:4:A:HCS:HB3  | 1:13:A:CYS:HA  | 22       | 0.79          |
| (2,161) | 1:4:A:HCS:HB3  | 1:13:A:CYS:HA  | 31       | 0.79          |
| (1,29)  | 1:11:A:TRP:HD1 | 1:1:A:PRO:HG3  | 16       | 0.79          |
| (3,43)  | 1:15:A:TYR:HE1 | 1:16:A:ARG:HG2 | 14       | 0.78          |
| (3,43)  | 1:15:A:TYR:HE2 | 1:16:A:ARG:HG2 | 14       | 0.78          |
| (3,25)  | 1:5:A:HIS:H    | 1:3:A:ILE:HG13 | 16       | 0.78          |
| (3,25)  | 1:5:A:HIS:H    | 1:3:A:ILE:HG13 | 24       | 0.78          |
| (3,12)  | 1:11:A:TRP:HE3 | 1:12:A:PRO:HG3 | 4        | 0.78          |
| (2,337) | 1:6:A:VAL:HA   | 1:13:A:CYS:HB3 | 22       | 0.78          |
| (2,318) | 1:9:A:PRO:HD2  | 1:8:A:ARG:HD3  | 4        | 0.78          |
| (2,161) | 1:4:A:HCS:HB3  | 1:13:A:CYS:HA  | 30       | 0.78          |
| (2,47)  | 1:7:A:HIS:HB2  | 1:8:A:ARG:HG2  | 1        | 0.78          |
| (2,41)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG11 | 8        | 0.78          |
| (2,41)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG12 | 8        | 0.78          |
| (2,41)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG13 | 8        | 0.78          |
| (2,41)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG11 | 25       | 0.78          |
| (2,41)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG12 | 25       | 0.78          |
| (2,41)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG13 | 25       | 0.78          |
| (2,41)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG11 | 34       | 0.78          |
| (2,41)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG12 | 34       | 0.78          |
| (2,41)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG13 | 34       | 0.78          |
| (3,25)  | 1:5:A:HIS:H    | 1:3:A:ILE:HG13 | 2        | 0.77          |
| (3,12)  | 1:11:A:TRP:HE3 | 1:12:A:PRO:HG3 | 14       | 0.77          |
| (3,12)  | 1:11:A:TRP:HE3 | 1:12:A:PRO:HG3 | 18       | 0.77          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (2,318) | 1:9:A:PRO:HD2  | 1:8:A:ARG:HD3  | 5        | 0.77          |
| (2,161) | 1:4:A:HCS:HB3  | 1:13:A:CYS:HA  | 32       | 0.77          |
| (2,47)  | 1:7:A:HIS:HB2  | 1:8:A:ARG:HG2  | 5        | 0.77          |
| (3,43)  | 1:15:A:TYR:HE1 | 1:16:A:ARG:HG2 | 6        | 0.76          |
| (3,43)  | 1:15:A:TYR:HE2 | 1:16:A:ARG:HG2 | 6        | 0.76          |
| (3,25)  | 1:5:A:HIS:H    | 1:3:A:ILE:HG13 | 1        | 0.76          |
| (3,25)  | 1:5:A:HIS:H    | 1:3:A:ILE:HG13 | 7        | 0.76          |
| (3,25)  | 1:5:A:HIS:H    | 1:3:A:ILE:HG13 | 8        | 0.76          |
| (3,25)  | 1:5:A:HIS:H    | 1:3:A:ILE:HG13 | 20       | 0.76          |
| (3,25)  | 1:5:A:HIS:H    | 1:3:A:ILE:HG13 | 23       | 0.76          |
| (3,25)  | 1:5:A:HIS:H    | 1:3:A:ILE:HG13 | 25       | 0.76          |
| (3,25)  | 1:5:A:HIS:H    | 1:3:A:ILE:HG13 | 27       | 0.76          |
| (3,25)  | 1:5:A:HIS:H    | 1:3:A:ILE:HG13 | 35       | 0.76          |
| (3,12)  | 1:11:A:TRP:HE3 | 1:12:A:PRO:HG3 | 7        | 0.76          |
| (2,312) | 1:15:A:TYR:HD1 | 1:16:A:ARG:HG2 | 10       | 0.76          |
| (2,312) | 1:15:A:TYR:HD2 | 1:16:A:ARG:HG2 | 10       | 0.76          |
| (2,312) | 1:15:A:TYR:HD1 | 1:16:A:ARG:HG2 | 32       | 0.76          |
| (2,312) | 1:15:A:TYR:HD2 | 1:16:A:ARG:HG2 | 32       | 0.76          |
| (2,161) | 1:4:A:HCS:HB3  | 1:13:A:CYS:HA  | 7        | 0.76          |
| (2,161) | 1:4:A:HCS:HB3  | 1:13:A:CYS:HA  | 21       | 0.76          |
| (2,161) | 1:4:A:HCS:HB3  | 1:13:A:CYS:HA  | 24       | 0.76          |
| (2,161) | 1:4:A:HCS:HB3  | 1:13:A:CYS:HA  | 35       | 0.76          |
| (2,41)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG11 | 3        | 0.76          |
| (2,41)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG12 | 3        | 0.76          |
| (2,41)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG13 | 3        | 0.76          |
| (2,15)  | 1:11:A:TRP:HE3 | 1:8:A:ARG:HD2  | 31       | 0.76          |
| (1,29)  | 1:11:A:TRP:HD1 | 1:1:A:PRO:HG3  | 18       | 0.76          |
| (1,8)   | 1:11:A:TRP:HH2 | 1:15:A:TYR:HB2 | 9        | 0.76          |
| (3,25)  | 1:5:A:HIS:H    | 1:3:A:ILE:HG13 | 4        | 0.75          |
| (3,25)  | 1:5:A:HIS:H    | 1:3:A:ILE:HG13 | 9        | 0.75          |
| (2,318) | 1:9:A:PRO:HD2  | 1:8:A:ARG:HD3  | 18       | 0.75          |
| (2,312) | 1:15:A:TYR:HD1 | 1:16:A:ARG:HG2 | 25       | 0.75          |
| (2,312) | 1:15:A:TYR:HD2 | 1:16:A:ARG:HG2 | 25       | 0.75          |
| (2,161) | 1:4:A:HCS:HB3  | 1:13:A:CYS:HA  | 10       | 0.75          |
| (2,161) | 1:4:A:HCS:HB3  | 1:13:A:CYS:HA  | 17       | 0.75          |
| (2,161) | 1:4:A:HCS:HB3  | 1:13:A:CYS:HA  | 20       | 0.75          |
| (2,161) | 1:4:A:HCS:HB3  | 1:13:A:CYS:HA  | 29       | 0.75          |
| (2,41)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG11 | 24       | 0.75          |
| (2,41)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG12 | 24       | 0.75          |
| (2,41)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG13 | 24       | 0.75          |
| (2,15)  | 1:11:A:TRP:HE3 | 1:8:A:ARG:HD2  | 30       | 0.75          |
| (2,15)  | 1:11:A:TRP:HE3 | 1:8:A:ARG:HD2  | 32       | 0.75          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (3,25)  | 1:5:A:HIS:H    | 1:3:A:ILE:HG13 | 22       | 0.74          |
| (3,25)  | 1:5:A:HIS:H    | 1:3:A:ILE:HG13 | 28       | 0.74          |
| (3,12)  | 1:11:A:TRP:HE3 | 1:12:A:PRO:HG3 | 2        | 0.74          |
| (3,12)  | 1:11:A:TRP:HE3 | 1:12:A:PRO:HG3 | 20       | 0.74          |
| (3,4)   | 1:14:A:TRP:HZ2 | 1:1:A:PRO:HB3  | 5        | 0.74          |
| (2,337) | 1:6:A:VAL:HA   | 1:13:A:CYS:HB2 | 24       | 0.74          |
| (2,318) | 1:9:A:PRO:HD2  | 1:8:A:ARG:HD3  | 7        | 0.74          |
| (2,312) | 1:15:A:TYR:HD1 | 1:16:A:ARG:HG2 | 6        | 0.74          |
| (2,312) | 1:15:A:TYR:HD2 | 1:16:A:ARG:HG2 | 6        | 0.74          |
| (2,161) | 1:4:A:HCS:HB3  | 1:13:A:CYS:HA  | 9        | 0.74          |
| (2,41)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG11 | 30       | 0.74          |
| (2,41)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG12 | 30       | 0.74          |
| (2,41)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG13 | 30       | 0.74          |
| (2,41)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG11 | 35       | 0.74          |
| (2,41)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG12 | 35       | 0.74          |
| (2,41)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG13 | 35       | 0.74          |
| (2,15)  | 1:11:A:TRP:HE3 | 1:8:A:ARG:HD2  | 7        | 0.74          |
| (3,43)  | 1:15:A:TYR:HE1 | 1:16:A:ARG:HG2 | 32       | 0.73          |
| (3,43)  | 1:15:A:TYR:HE2 | 1:16:A:ARG:HG2 | 32       | 0.73          |
| (3,25)  | 1:5:A:HIS:H    | 1:3:A:ILE:HG13 | 5        | 0.73          |
| (3,25)  | 1:5:A:HIS:H    | 1:3:A:ILE:HG13 | 18       | 0.73          |
| (3,25)  | 1:5:A:HIS:H    | 1:3:A:ILE:HG13 | 26       | 0.73          |
| (2,318) | 1:9:A:PRO:HD2  | 1:8:A:ARG:HD3  | 30       | 0.73          |
| (2,318) | 1:9:A:PRO:HD2  | 1:8:A:ARG:HD3  | 31       | 0.73          |
| (2,161) | 1:4:A:HCS:HB3  | 1:13:A:CYS:HA  | 1        | 0.73          |
| (2,161) | 1:4:A:HCS:HB3  | 1:13:A:CYS:HA  | 6        | 0.73          |
| (2,161) | 1:4:A:HCS:HB3  | 1:13:A:CYS:HA  | 19       | 0.73          |
| (2,161) | 1:4:A:HCS:HB3  | 1:13:A:CYS:HA  | 27       | 0.73          |
| (2,41)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG11 | 1        | 0.73          |
| (2,41)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG12 | 1        | 0.73          |
| (2,41)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG13 | 1        | 0.73          |
| (2,41)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG11 | 27       | 0.73          |
| (2,41)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG12 | 27       | 0.73          |
| (2,41)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG13 | 27       | 0.73          |
| (3,43)  | 1:15:A:TYR:HE1 | 1:16:A:ARG:HG2 | 22       | 0.72          |
| (3,43)  | 1:15:A:TYR:HE2 | 1:16:A:ARG:HG2 | 22       | 0.72          |
| (3,25)  | 1:5:A:HIS:H    | 1:3:A:ILE:HG13 | 3        | 0.72          |
| (3,25)  | 1:5:A:HIS:H    | 1:3:A:ILE:HG13 | 17       | 0.72          |
| (3,25)  | 1:5:A:HIS:H    | 1:3:A:ILE:HG13 | 32       | 0.72          |
| (3,12)  | 1:11:A:TRP:HE3 | 1:12:A:PRO:HG3 | 10       | 0.72          |
| (3,12)  | 1:11:A:TRP:HE3 | 1:12:A:PRO:HG3 | 16       | 0.72          |
| (2,337) | 1:6:A:VAL:HA   | 1:13:A:CYS:HB2 | 33       | 0.72          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (2,161) | 1:4:A:HCS:HB3  | 1:13:A:CYS:HA  | 13       | 0.72          |
| (2,161) | 1:4:A:HCS:HB3  | 1:13:A:CYS:HA  | 14       | 0.72          |
| (2,47)  | 1:7:A:HIS:HB2  | 1:8:A:ARG:HG2  | 15       | 0.72          |
| (2,41)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG11 | 2        | 0.72          |
| (2,41)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG12 | 2        | 0.72          |
| (2,41)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG13 | 2        | 0.72          |
| (2,41)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG11 | 7        | 0.72          |
| (2,41)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG12 | 7        | 0.72          |
| (2,41)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG13 | 7        | 0.72          |
| (2,41)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG11 | 13       | 0.72          |
| (2,41)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG12 | 13       | 0.72          |
| (2,41)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG13 | 13       | 0.72          |
| (2,41)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG11 | 17       | 0.72          |
| (2,41)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG12 | 17       | 0.72          |
| (2,41)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG13 | 17       | 0.72          |
| (2,41)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG11 | 23       | 0.72          |
| (2,41)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG12 | 23       | 0.72          |
| (2,41)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG13 | 23       | 0.72          |
| (3,43)  | 1:15:A:TYR:HE1 | 1:16:A:ARG:HG2 | 1        | 0.71          |
| (3,43)  | 1:15:A:TYR:HE2 | 1:16:A:ARG:HG2 | 1        | 0.71          |
| (3,25)  | 1:5:A:HIS:H    | 1:3:A:ILE:HG13 | 13       | 0.71          |
| (2,337) | 1:6:A:VAL:HA   | 1:13:A:CYS:HB3 | 1        | 0.71          |
| (2,337) | 1:6:A:VAL:HA   | 1:13:A:CYS:HB2 | 14       | 0.71          |
| (2,161) | 1:4:A:HCS:HB3  | 1:13:A:CYS:HA  | 4        | 0.71          |
| (2,161) | 1:4:A:HCS:HB3  | 1:13:A:CYS:HA  | 12       | 0.71          |
| (2,146) | 1:11:A:TRP:H   | 1:11:A:TRP:HB2 | 9        | 0.71          |
| (2,47)  | 1:7:A:HIS:HB2  | 1:8:A:ARG:HG2  | 8        | 0.71          |
| (2,46)  | 1:11:A:TRP:HB3 | 1:15:A:TYR:HB3 | 5        | 0.71          |
| (2,46)  | 1:11:A:TRP:HB3 | 1:15:A:TYR:HB3 | 20       | 0.71          |
| (3,12)  | 1:11:A:TRP:HE3 | 1:12:A:PRO:HG3 | 33       | 0.7           |
| (2,337) | 1:6:A:VAL:HA   | 1:13:A:CYS:HB2 | 18       | 0.7           |
| (2,318) | 1:9:A:PRO:HD2  | 1:8:A:ARG:HD3  | 6        | 0.7           |
| (2,318) | 1:9:A:PRO:HD2  | 1:8:A:ARG:HD3  | 9        | 0.7           |
| (2,318) | 1:9:A:PRO:HD2  | 1:8:A:ARG:HD3  | 23       | 0.7           |
| (2,318) | 1:9:A:PRO:HD2  | 1:8:A:ARG:HD3  | 32       | 0.7           |
| (2,312) | 1:15:A:TYR:HD1 | 1:16:A:ARG:HG2 | 22       | 0.7           |
| (2,312) | 1:15:A:TYR:HD2 | 1:16:A:ARG:HG2 | 22       | 0.7           |
| (2,161) | 1:4:A:HCS:HB3  | 1:13:A:CYS:HA  | 3        | 0.7           |
| (2,161) | 1:4:A:HCS:HB3  | 1:13:A:CYS:HA  | 8        | 0.7           |
| (2,146) | 1:11:A:TRP:H   | 1:11:A:TRP:HB2 | 3        | 0.7           |
| (2,146) | 1:11:A:TRP:H   | 1:11:A:TRP:HB2 | 27       | 0.7           |
| (2,41)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG11 | 21       | 0.7           |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (2,41)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG12 | 21       | 0.7           |
| (2,41)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG13 | 21       | 0.7           |
| (3,12)  | 1:11:A:TRP:HE3 | 1:12:A:PRO:HG3 | 22       | 0.69          |
| (2,161) | 1:4:A:HCS:HB3  | 1:13:A:CYS:HA  | 23       | 0.69          |
| (2,146) | 1:11:A:TRP:H   | 1:11:A:TRP:HB2 | 1        | 0.69          |
| (2,146) | 1:11:A:TRP:H   | 1:11:A:TRP:HB2 | 16       | 0.69          |
| (2,146) | 1:11:A:TRP:H   | 1:11:A:TRP:HB2 | 23       | 0.69          |
| (2,146) | 1:11:A:TRP:H   | 1:11:A:TRP:HB2 | 25       | 0.69          |
| (2,146) | 1:11:A:TRP:H   | 1:11:A:TRP:HB2 | 33       | 0.69          |
| (2,47)  | 1:7:A:HIS:HB2  | 1:8:A:ARG:HG2  | 4        | 0.69          |
| (2,41)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG11 | 29       | 0.69          |
| (2,41)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG12 | 29       | 0.69          |
| (2,41)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG13 | 29       | 0.69          |
| (2,41)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG11 | 31       | 0.69          |
| (2,41)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG12 | 31       | 0.69          |
| (2,41)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG13 | 31       | 0.69          |
| (2,15)  | 1:11:A:TRP:HE3 | 1:8:A:ARG:HD2  | 6        | 0.69          |
| (2,15)  | 1:11:A:TRP:HE3 | 1:8:A:ARG:HD2  | 21       | 0.69          |
| (1,29)  | 1:11:A:TRP:HD1 | 1:1:A:PRO:HG3  | 31       | 0.69          |
| (1,29)  | 1:11:A:TRP:HD1 | 1:1:A:PRO:HG3  | 34       | 0.69          |
| (1,8)   | 1:11:A:TRP:HH2 | 1:15:A:TYR:HB2 | 6        | 0.69          |
| (3,43)  | 1:15:A:TYR:HE1 | 1:16:A:ARG:HG2 | 28       | 0.68          |
| (3,43)  | 1:15:A:TYR:HE2 | 1:16:A:ARG:HG2 | 28       | 0.68          |
| (3,25)  | 1:5:A:HIS:H    | 1:3:A:ILE:HG13 | 29       | 0.68          |
| (3,12)  | 1:11:A:TRP:HE3 | 1:12:A:PRO:HG3 | 28       | 0.68          |
| (2,337) | 1:6:A:VAL:HA   | 1:13:A:CYS:HB2 | 10       | 0.68          |
| (2,161) | 1:4:A:HCS:HB3  | 1:13:A:CYS:HA  | 25       | 0.68          |
| (2,146) | 1:11:A:TRP:H   | 1:11:A:TRP:HB2 | 10       | 0.68          |
| (2,146) | 1:11:A:TRP:H   | 1:11:A:TRP:HB2 | 12       | 0.68          |
| (2,146) | 1:11:A:TRP:H   | 1:11:A:TRP:HB2 | 19       | 0.68          |
| (2,146) | 1:11:A:TRP:H   | 1:11:A:TRP:HB2 | 22       | 0.68          |
| (2,146) | 1:11:A:TRP:H   | 1:11:A:TRP:HB2 | 24       | 0.68          |
| (2,146) | 1:11:A:TRP:H   | 1:11:A:TRP:HB2 | 29       | 0.68          |
| (2,47)  | 1:7:A:HIS:HB2  | 1:8:A:ARG:HG2  | 26       | 0.68          |
| (2,15)  | 1:11:A:TRP:HE3 | 1:8:A:ARG:HD2  | 4        | 0.68          |
| (1,8)   | 1:11:A:TRP:HH2 | 1:15:A:TYR:HB2 | 25       | 0.68          |
| (3,43)  | 1:15:A:TYR:HE1 | 1:16:A:ARG:HG2 | 35       | 0.67          |
| (3,43)  | 1:15:A:TYR:HE2 | 1:16:A:ARG:HG2 | 35       | 0.67          |
| (3,25)  | 1:5:A:HIS:H    | 1:3:A:ILE:HG13 | 10       | 0.67          |
| (3,25)  | 1:5:A:HIS:H    | 1:3:A:ILE:HG13 | 33       | 0.67          |
| (2,337) | 1:6:A:VAL:HA   | 1:13:A:CYS:HB2 | 7        | 0.67          |
| (2,337) | 1:6:A:VAL:HA   | 1:13:A:CYS:HB3 | 30       | 0.67          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (2,337) | 1:6:A:VAL:HA   | 1:13:A:CYS:HB2 | 32       | 0.67          |
| (2,318) | 1:9:A:PRO:HD2  | 1:8:A:ARG:HD3  | 21       | 0.67          |
| (2,312) | 1:15:A:TYR:HD1 | 1:16:A:ARG:HG2 | 1        | 0.67          |
| (2,312) | 1:15:A:TYR:HD2 | 1:16:A:ARG:HG2 | 1        | 0.67          |
| (2,161) | 1:4:A:HCS:HB3  | 1:13:A:CYS:HA  | 5        | 0.67          |
| (2,161) | 1:4:A:HCS:HB3  | 1:13:A:CYS:HA  | 16       | 0.67          |
| (2,161) | 1:4:A:HCS:HB3  | 1:13:A:CYS:HA  | 26       | 0.67          |
| (2,161) | 1:4:A:HCS:HB3  | 1:13:A:CYS:HA  | 28       | 0.67          |
| (2,146) | 1:11:A:TRP:H   | 1:11:A:TRP:HB2 | 17       | 0.67          |
| (2,146) | 1:11:A:TRP:H   | 1:11:A:TRP:HB2 | 26       | 0.67          |
| (2,47)  | 1:7:A:HIS:HB2  | 1:8:A:ARG:HG2  | 9        | 0.67          |
| (2,46)  | 1:11:A:TRP:HB3 | 1:15:A:TYR:HB3 | 4        | 0.67          |
| (2,41)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG11 | 11       | 0.67          |
| (2,41)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG12 | 11       | 0.67          |
| (2,41)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG13 | 11       | 0.67          |
| (2,41)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG11 | 12       | 0.67          |
| (2,41)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG12 | 12       | 0.67          |
| (2,41)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG13 | 12       | 0.67          |
| (2,41)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG11 | 20       | 0.67          |
| (2,41)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG12 | 20       | 0.67          |
| (2,41)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG13 | 20       | 0.67          |
| (2,41)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG11 | 22       | 0.67          |
| (2,41)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG12 | 22       | 0.67          |
| (2,41)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG13 | 22       | 0.67          |
| (2,41)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG11 | 33       | 0.67          |
| (2,41)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG12 | 33       | 0.67          |
| (2,41)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG13 | 33       | 0.67          |
| (2,15)  | 1:11:A:TRP:HE3 | 1:8:A:ARG:HD2  | 11       | 0.67          |
| (1,29)  | 1:11:A:TRP:HD1 | 1:1:A:PRO:HG3  | 25       | 0.67          |
| (3,25)  | 1:5:A:HIS:H    | 1:3:A:ILE:HG13 | 14       | 0.66          |
| (3,25)  | 1:5:A:HIS:H    | 1:3:A:ILE:HG13 | 15       | 0.66          |
| (2,161) | 1:4:A:HCS:HB3  | 1:13:A:CYS:HA  | 2        | 0.66          |
| (2,146) | 1:11:A:TRP:H   | 1:11:A:TRP:HB2 | 13       | 0.66          |
| (2,41)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG11 | 28       | 0.66          |
| (2,41)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG12 | 28       | 0.66          |
| (2,41)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG13 | 28       | 0.66          |
| (1,29)  | 1:11:A:TRP:HD1 | 1:1:A:PRO:HG3  | 28       | 0.66          |
| (1,8)   | 1:11:A:TRP:HH2 | 1:15:A:TYR:HB2 | 8        | 0.66          |
| (3,25)  | 1:5:A:HIS:H    | 1:3:A:ILE:HG13 | 30       | 0.65          |
| (2,337) | 1:6:A:VAL:HA   | 1:13:A:CYS:HB2 | 4        | 0.65          |
| (2,337) | 1:6:A:VAL:HA   | 1:13:A:CYS:HB3 | 9        | 0.65          |
| (2,337) | 1:6:A:VAL:HA   | 1:13:A:CYS:HB2 | 20       | 0.65          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (2,312) | 1:15:A:TYR:HD1 | 1:16:A:ARG:HG2 | 28       | 0.65          |
| (2,312) | 1:15:A:TYR:HD2 | 1:16:A:ARG:HG2 | 28       | 0.65          |
| (2,146) | 1:11:A:TRP:H   | 1:11:A:TRP:HB2 | 2        | 0.65          |
| (2,146) | 1:11:A:TRP:H   | 1:11:A:TRP:HB2 | 5        | 0.65          |
| (2,146) | 1:11:A:TRP:H   | 1:11:A:TRP:HB2 | 11       | 0.65          |
| (2,146) | 1:11:A:TRP:H   | 1:11:A:TRP:HB2 | 14       | 0.65          |
| (2,146) | 1:11:A:TRP:H   | 1:11:A:TRP:HB2 | 15       | 0.65          |
| (2,146) | 1:11:A:TRP:H   | 1:11:A:TRP:HB2 | 18       | 0.65          |
| (2,146) | 1:11:A:TRP:H   | 1:11:A:TRP:HB2 | 35       | 0.65          |
| (2,47)  | 1:7:A:HIS:HB2  | 1:8:A:ARG:HG2  | 11       | 0.65          |
| (2,41)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG11 | 16       | 0.65          |
| (2,41)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG12 | 16       | 0.65          |
| (2,41)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG13 | 16       | 0.65          |
| (2,41)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG11 | 26       | 0.65          |
| (2,41)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG12 | 26       | 0.65          |
| (2,41)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG13 | 26       | 0.65          |
| (1,8)   | 1:11:A:TRP:HH2 | 1:15:A:TYR:HB2 | 5        | 0.65          |
| (1,8)   | 1:11:A:TRP:HH2 | 1:15:A:TYR:HB2 | 24       | 0.65          |
| (3,43)  | 1:15:A:TYR:HE1 | 1:16:A:ARG:HG2 | 21       | 0.64          |
| (3,43)  | 1:15:A:TYR:HE2 | 1:16:A:ARG:HG2 | 21       | 0.64          |
| (3,25)  | 1:5:A:HIS:H    | 1:3:A:ILE:HG13 | 11       | 0.64          |
| (3,25)  | 1:5:A:HIS:H    | 1:3:A:ILE:HG13 | 19       | 0.64          |
| (2,337) | 1:6:A:VAL:HA   | 1:13:A:CYS:HB3 | 23       | 0.64          |
| (2,337) | 1:6:A:VAL:HA   | 1:13:A:CYS:HB3 | 31       | 0.64          |
| (2,318) | 1:9:A:PRO:HD2  | 1:8:A:ARG:HD3  | 8        | 0.64          |
| (2,318) | 1:9:A:PRO:HD2  | 1:8:A:ARG:HD3  | 11       | 0.64          |
| (2,146) | 1:11:A:TRP:H   | 1:11:A:TRP:HB2 | 21       | 0.64          |
| (2,146) | 1:11:A:TRP:H   | 1:11:A:TRP:HB2 | 31       | 0.64          |
| (2,41)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG11 | 19       | 0.64          |
| (2,41)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG12 | 19       | 0.64          |
| (2,41)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG13 | 19       | 0.64          |
| (2,18)  | 1:11:A:TRP:HD1 | 1:12:A:PRO:HG3 | 28       | 0.64          |
| (1,29)  | 1:11:A:TRP:HD1 | 1:1:A:PRO:HG3  | 8        | 0.64          |
| (1,8)   | 1:11:A:TRP:HH2 | 1:15:A:TYR:HB2 | 3        | 0.64          |
| (1,8)   | 1:11:A:TRP:HH2 | 1:15:A:TYR:HB2 | 31       | 0.64          |
| (3,43)  | 1:15:A:TYR:HE1 | 1:16:A:ARG:HG2 | 19       | 0.63          |
| (3,43)  | 1:15:A:TYR:HE2 | 1:16:A:ARG:HG2 | 19       | 0.63          |
| (2,337) | 1:6:A:VAL:HA   | 1:13:A:CYS:HB2 | 34       | 0.63          |
| (2,161) | 1:4:A:HCS:HB3  | 1:13:A:CYS:HA  | 11       | 0.63          |
| (2,146) | 1:11:A:TRP:H   | 1:11:A:TRP:HB2 | 6        | 0.63          |
| (2,146) | 1:11:A:TRP:H   | 1:11:A:TRP:HB2 | 8        | 0.63          |
| (2,146) | 1:11:A:TRP:H   | 1:11:A:TRP:HB2 | 30       | 0.63          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (2,41)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG11 | 6        | 0.63          |
| (2,41)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG12 | 6        | 0.63          |
| (2,41)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG13 | 6        | 0.63          |
| (2,41)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG11 | 10       | 0.63          |
| (2,41)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG12 | 10       | 0.63          |
| (2,41)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG13 | 10       | 0.63          |
| (2,41)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG11 | 15       | 0.63          |
| (2,41)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG12 | 15       | 0.63          |
| (2,41)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG13 | 15       | 0.63          |
| (2,18)  | 1:11:A:TRP:HD1 | 1:12:A:PRO:HG3 | 2        | 0.63          |
| (3,29)  | 1:11:A:TRP:HB2 | 1:8:A:ARG:HG2  | 32       | 0.62          |
| (2,337) | 1:6:A:VAL:HA   | 1:13:A:CYS:HB2 | 13       | 0.62          |
| (2,337) | 1:6:A:VAL:HA   | 1:13:A:CYS:HB2 | 16       | 0.62          |
| (2,337) | 1:6:A:VAL:HA   | 1:13:A:CYS:HB3 | 17       | 0.62          |
| (2,337) | 1:6:A:VAL:HA   | 1:13:A:CYS:HB3 | 27       | 0.62          |
| (2,312) | 1:15:A:TYR:HD1 | 1:16:A:ARG:HG2 | 21       | 0.62          |
| (2,312) | 1:15:A:TYR:HD2 | 1:16:A:ARG:HG2 | 21       | 0.62          |
| (2,146) | 1:11:A:TRP:H   | 1:11:A:TRP:HB2 | 7        | 0.62          |
| (2,146) | 1:11:A:TRP:H   | 1:11:A:TRP:HB2 | 28       | 0.62          |
| (2,146) | 1:11:A:TRP:H   | 1:11:A:TRP:HB2 | 32       | 0.62          |
| (2,146) | 1:11:A:TRP:H   | 1:11:A:TRP:HB2 | 34       | 0.62          |
| (2,47)  | 1:7:A:HIS:HB2  | 1:8:A:ARG:HG2  | 21       | 0.62          |
| (2,46)  | 1:11:A:TRP:HB3 | 1:15:A:TYR:HB3 | 2        | 0.62          |
| (2,41)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG11 | 4        | 0.62          |
| (2,41)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG12 | 4        | 0.62          |
| (2,41)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG13 | 4        | 0.62          |
| (2,41)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG11 | 5        | 0.62          |
| (2,41)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG12 | 5        | 0.62          |
| (2,41)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG13 | 5        | 0.62          |
| (2,337) | 1:6:A:VAL:HA   | 1:13:A:CYS:HB2 | 5        | 0.61          |
| (2,337) | 1:6:A:VAL:HA   | 1:13:A:CYS:HB2 | 35       | 0.61          |
| (2,312) | 1:15:A:TYR:HD1 | 1:16:A:ARG:HG2 | 35       | 0.61          |
| (2,312) | 1:15:A:TYR:HD2 | 1:16:A:ARG:HG2 | 35       | 0.61          |
| (2,146) | 1:11:A:TRP:H   | 1:11:A:TRP:HB2 | 4        | 0.61          |
| (2,146) | 1:11:A:TRP:H   | 1:11:A:TRP:HB2 | 20       | 0.61          |
| (2,47)  | 1:7:A:HIS:HB2  | 1:8:A:ARG:HG2  | 34       | 0.61          |
| (2,46)  | 1:11:A:TRP:HB3 | 1:15:A:TYR:HB3 | 21       | 0.61          |
| (2,46)  | 1:11:A:TRP:HB3 | 1:15:A:TYR:HB3 | 28       | 0.61          |
| (2,46)  | 1:11:A:TRP:HB3 | 1:15:A:TYR:HB3 | 33       | 0.61          |
| (1,29)  | 1:11:A:TRP:HD1 | 1:1:A:PRO:HG3  | 1        | 0.61          |
| (1,29)  | 1:11:A:TRP:HD1 | 1:1:A:PRO:HG3  | 24       | 0.61          |
| (1,8)   | 1:11:A:TRP:HH2 | 1:15:A:TYR:HB2 | 13       | 0.61          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,8)   | 1:11:A:TRP:HH2 | 1:15:A:TYR:HB2 | 26       | 0.61          |
| (1,8)   | 1:11:A:TRP:HH2 | 1:15:A:TYR:HB2 | 30       | 0.61          |
| (3,29)  | 1:11:A:TRP:HB2 | 1:8:A:ARG:HG2  | 11       | 0.6           |
| (3,25)  | 1:5:A:HIS:H    | 1:3:A:ILE:HG13 | 6        | 0.6           |
| (3,25)  | 1:5:A:HIS:H    | 1:3:A:ILE:HG13 | 31       | 0.6           |
| (2,337) | 1:6:A:VAL:HA   | 1:13:A:CYS:HB3 | 2        | 0.6           |
| (2,337) | 1:6:A:VAL:HA   | 1:13:A:CYS:HB2 | 25       | 0.6           |
| (2,337) | 1:6:A:VAL:HA   | 1:13:A:CYS:HB2 | 26       | 0.6           |
| (2,47)  | 1:7:A:HIS:HB2  | 1:8:A:ARG:HG2  | 6        | 0.6           |
| (2,46)  | 1:11:A:TRP:HB3 | 1:15:A:TYR:HB3 | 14       | 0.6           |
| (2,46)  | 1:11:A:TRP:HB3 | 1:15:A:TYR:HB3 | 24       | 0.6           |
| (2,18)  | 1:11:A:TRP:HD1 | 1:12:A:PRO:HG3 | 20       | 0.6           |
| (1,29)  | 1:11:A:TRP:HD1 | 1:1:A:PRO:HG3  | 27       | 0.6           |
| (1,8)   | 1:11:A:TRP:HH2 | 1:15:A:TYR:HB2 | 15       | 0.6           |
| (1,8)   | 1:11:A:TRP:HH2 | 1:15:A:TYR:HB2 | 27       | 0.6           |
| (3,29)  | 1:11:A:TRP:HB2 | 1:8:A:ARG:HG2  | 6        | 0.59          |
| (3,29)  | 1:11:A:TRP:HB2 | 1:8:A:ARG:HG2  | 8        | 0.59          |
| (3,29)  | 1:11:A:TRP:HB2 | 1:8:A:ARG:HG2  | 31       | 0.59          |
| (2,337) | 1:6:A:VAL:HA   | 1:13:A:CYS:HB2 | 28       | 0.59          |
| (2,46)  | 1:11:A:TRP:HB3 | 1:15:A:TYR:HB3 | 6        | 0.59          |
| (2,18)  | 1:11:A:TRP:HD1 | 1:12:A:PRO:HG3 | 14       | 0.59          |
| (2,18)  | 1:11:A:TRP:HD1 | 1:12:A:PRO:HG3 | 35       | 0.59          |
| (3,43)  | 1:15:A:TYR:HE1 | 1:16:A:ARG:HG2 | 15       | 0.58          |
| (3,43)  | 1:15:A:TYR:HE2 | 1:16:A:ARG:HG2 | 15       | 0.58          |
| (3,29)  | 1:11:A:TRP:HB2 | 1:8:A:ARG:HG2  | 4        | 0.58          |
| (3,29)  | 1:11:A:TRP:HB2 | 1:8:A:ARG:HG2  | 9        | 0.58          |
| (3,29)  | 1:11:A:TRP:HB2 | 1:8:A:ARG:HG2  | 15       | 0.58          |
| (3,29)  | 1:11:A:TRP:HB2 | 1:8:A:ARG:HG2  | 30       | 0.58          |
| (2,46)  | 1:11:A:TRP:HB3 | 1:15:A:TYR:HB3 | 18       | 0.58          |
| (2,46)  | 1:11:A:TRP:HB3 | 1:15:A:TYR:HB3 | 30       | 0.58          |
| (2,46)  | 1:11:A:TRP:HB3 | 1:15:A:TYR:HB3 | 32       | 0.58          |
| (2,41)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG11 | 14       | 0.58          |
| (2,41)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG12 | 14       | 0.58          |
| (2,41)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG13 | 14       | 0.58          |
| (2,23)  | 1:14:A:TRP:HZ3 | 1:16:A:ARG:HD3 | 32       | 0.58          |
| (2,18)  | 1:11:A:TRP:HD1 | 1:12:A:PRO:HG3 | 17       | 0.58          |
| (2,18)  | 1:11:A:TRP:HD1 | 1:12:A:PRO:HG3 | 24       | 0.58          |
| (1,8)   | 1:11:A:TRP:HH2 | 1:15:A:TYR:HB2 | 4        | 0.58          |
| (1,8)   | 1:11:A:TRP:HH2 | 1:15:A:TYR:HB2 | 21       | 0.58          |
| (3,29)  | 1:11:A:TRP:HB2 | 1:8:A:ARG:HG2  | 28       | 0.57          |
| (3,29)  | 1:11:A:TRP:HB2 | 1:8:A:ARG:HG2  | 34       | 0.57          |
| (2,318) | 1:9:A:PRO:HD2  | 1:8:A:ARG:HD3  | 3        | 0.57          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (2,312) | 1:15:A:TYR:HD1 | 1:16:A:ARG:HG2 | 24       | 0.57          |
| (2,312) | 1:15:A:TYR:HD2 | 1:16:A:ARG:HG2 | 24       | 0.57          |
| (2,46)  | 1:11:A:TRP:HB3 | 1:15:A:TYR:HB3 | 3        | 0.57          |
| (2,46)  | 1:11:A:TRP:HB3 | 1:15:A:TYR:HB3 | 26       | 0.57          |
| (2,18)  | 1:11:A:TRP:HD1 | 1:12:A:PRO:HG3 | 6        | 0.57          |
| (2,18)  | 1:11:A:TRP:HD1 | 1:12:A:PRO:HG3 | 10       | 0.57          |
| (2,18)  | 1:11:A:TRP:HD1 | 1:12:A:PRO:HG3 | 21       | 0.57          |
| (1,21)  | 1:4:A:HCS:HG3  | 1:6:A:VAL:HG11 | 30       | 0.57          |
| (1,21)  | 1:4:A:HCS:HG3  | 1:6:A:VAL:HG12 | 30       | 0.57          |
| (1,21)  | 1:4:A:HCS:HG3  | 1:6:A:VAL:HG13 | 30       | 0.57          |
| (1,8)   | 1:11:A:TRP:HH2 | 1:15:A:TYR:HB2 | 20       | 0.57          |
| (1,8)   | 1:11:A:TRP:HH2 | 1:15:A:TYR:HB2 | 35       | 0.57          |
| (3,29)  | 1:11:A:TRP:HB2 | 1:8:A:ARG:HG2  | 5        | 0.56          |
| (3,29)  | 1:11:A:TRP:HB2 | 1:8:A:ARG:HG2  | 7        | 0.56          |
| (3,29)  | 1:11:A:TRP:HB2 | 1:8:A:ARG:HG2  | 21       | 0.56          |
| (2,337) | 1:6:A:VAL:HA   | 1:13:A:CYS:HB2 | 6        | 0.56          |
| (2,337) | 1:6:A:VAL:HA   | 1:13:A:CYS:HB2 | 8        | 0.56          |
| (2,312) | 1:15:A:TYR:HD1 | 1:16:A:ARG:HG2 | 30       | 0.56          |
| (2,312) | 1:15:A:TYR:HD2 | 1:16:A:ARG:HG2 | 30       | 0.56          |
| (2,47)  | 1:7:A:HIS:HB2  | 1:8:A:ARG:HG2  | 7        | 0.56          |
| (2,47)  | 1:7:A:HIS:HB2  | 1:8:A:ARG:HG2  | 32       | 0.56          |
| (2,46)  | 1:11:A:TRP:HB3 | 1:15:A:TYR:HB3 | 7        | 0.56          |
| (2,46)  | 1:11:A:TRP:HB3 | 1:15:A:TYR:HB3 | 11       | 0.56          |
| (2,46)  | 1:11:A:TRP:HB3 | 1:15:A:TYR:HB3 | 29       | 0.56          |
| (2,35)  | 1:5:A:HIS:HD2  | 1:13:A:CYS:HB2 | 35       | 0.56          |
| (2,18)  | 1:11:A:TRP:HD1 | 1:12:A:PRO:HG3 | 8        | 0.56          |
| (2,18)  | 1:11:A:TRP:HD1 | 1:12:A:PRO:HG3 | 19       | 0.56          |
| (2,18)  | 1:11:A:TRP:HD1 | 1:12:A:PRO:HG3 | 25       | 0.56          |
| (2,18)  | 1:11:A:TRP:HD1 | 1:12:A:PRO:HG3 | 26       | 0.56          |
| (2,18)  | 1:11:A:TRP:HD1 | 1:12:A:PRO:HG3 | 30       | 0.56          |
| (1,8)   | 1:11:A:TRP:HH2 | 1:15:A:TYR:HB2 | 7        | 0.56          |
| (1,8)   | 1:11:A:TRP:HH2 | 1:15:A:TYR:HB2 | 11       | 0.56          |
| (1,8)   | 1:11:A:TRP:HH2 | 1:15:A:TYR:HB2 | 17       | 0.56          |
| (3,29)  | 1:11:A:TRP:HB2 | 1:8:A:ARG:HG2  | 23       | 0.55          |
| (3,29)  | 1:11:A:TRP:HB2 | 1:8:A:ARG:HG2  | 26       | 0.55          |
| (2,312) | 1:15:A:TYR:HD1 | 1:16:A:ARG:HG2 | 15       | 0.55          |
| (2,312) | 1:15:A:TYR:HD2 | 1:16:A:ARG:HG2 | 15       | 0.55          |
| (2,182) | 1:5:A:HIS:H    | 1:5:A:HIS:HB2  | 12       | 0.55          |
| (2,182) | 1:5:A:HIS:H    | 1:5:A:HIS:HB2  | 34       | 0.55          |
| (2,46)  | 1:11:A:TRP:HB3 | 1:15:A:TYR:HB3 | 31       | 0.55          |
| (2,41)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG11 | 18       | 0.55          |
| (2,41)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG12 | 18       | 0.55          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (2,41)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG13 | 18       | 0.55          |
| (2,41)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG11 | 32       | 0.55          |
| (2,41)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG12 | 32       | 0.55          |
| (2,41)  | 1:15:A:TYR:HB2 | 1:6:A:VAL:HG13 | 32       | 0.55          |
| (2,35)  | 1:5:A:HIS:HD2  | 1:13:A:CYS:HB3 | 1        | 0.55          |
| (2,18)  | 1:11:A:TRP:HD1 | 1:12:A:PRO:HG3 | 4        | 0.55          |
| (2,18)  | 1:11:A:TRP:HD1 | 1:12:A:PRO:HG3 | 7        | 0.55          |
| (2,18)  | 1:11:A:TRP:HD1 | 1:12:A:PRO:HG3 | 12       | 0.55          |
| (2,18)  | 1:11:A:TRP:HD1 | 1:12:A:PRO:HG3 | 13       | 0.55          |
| (2,18)  | 1:11:A:TRP:HD1 | 1:12:A:PRO:HG3 | 16       | 0.55          |
| (2,18)  | 1:11:A:TRP:HD1 | 1:12:A:PRO:HG3 | 22       | 0.55          |
| (2,18)  | 1:11:A:TRP:HD1 | 1:12:A:PRO:HG3 | 29       | 0.55          |
| (1,8)   | 1:11:A:TRP:HH2 | 1:15:A:TYR:HB2 | 1        | 0.55          |
| (1,8)   | 1:11:A:TRP:HH2 | 1:15:A:TYR:HB2 | 14       | 0.55          |
| (1,8)   | 1:11:A:TRP:HH2 | 1:15:A:TYR:HB2 | 34       | 0.55          |
| (2,348) | 1:11:A:TRP:HB2 | 1:8:A:ARG:HG3  | 16       | 0.54          |
| (2,337) | 1:6:A:VAL:HA   | 1:13:A:CYS:HB2 | 11       | 0.54          |
| (2,337) | 1:6:A:VAL:HA   | 1:13:A:CYS:HB2 | 21       | 0.54          |
| (2,182) | 1:5:A:HIS:H    | 1:5:A:HIS:HB2  | 2        | 0.54          |
| (2,182) | 1:5:A:HIS:H    | 1:5:A:HIS:HB2  | 7        | 0.54          |
| (2,182) | 1:5:A:HIS:H    | 1:5:A:HIS:HB2  | 15       | 0.54          |
| (2,182) | 1:5:A:HIS:H    | 1:5:A:HIS:HB2  | 31       | 0.54          |
| (2,182) | 1:5:A:HIS:H    | 1:5:A:HIS:HB2  | 33       | 0.54          |
| (2,47)  | 1:7:A:HIS:HB2  | 1:8:A:ARG:HG2  | 30       | 0.54          |
| (2,35)  | 1:5:A:HIS:HD2  | 1:13:A:CYS:HB2 | 7        | 0.54          |
| (2,35)  | 1:5:A:HIS:HD2  | 1:13:A:CYS:HB3 | 22       | 0.54          |
| (2,21)  | 1:11:A:TRP:HH2 | 1:8:A:ARG:HD2  | 3        | 0.54          |
| (2,18)  | 1:11:A:TRP:HD1 | 1:12:A:PRO:HG3 | 5        | 0.54          |
| (2,18)  | 1:11:A:TRP:HD1 | 1:12:A:PRO:HG3 | 32       | 0.54          |
| (2,18)  | 1:11:A:TRP:HD1 | 1:12:A:PRO:HG3 | 33       | 0.54          |
| (1,29)  | 1:11:A:TRP:HD1 | 1:1:A:PRO:HG3  | 7        | 0.54          |
| (3,29)  | 1:11:A:TRP:HB2 | 1:8:A:ARG:HG2  | 1        | 0.53          |
| (2,348) | 1:11:A:TRP:HB2 | 1:8:A:ARG:HG3  | 29       | 0.53          |
| (2,348) | 1:11:A:TRP:HB2 | 1:8:A:ARG:HG3  | 33       | 0.53          |
| (2,312) | 1:15:A:TYR:HD1 | 1:16:A:ARG:HG2 | 19       | 0.53          |
| (2,312) | 1:15:A:TYR:HD2 | 1:16:A:ARG:HG2 | 19       | 0.53          |
| (2,182) | 1:5:A:HIS:H    | 1:5:A:HIS:HB2  | 19       | 0.53          |
| (2,182) | 1:5:A:HIS:H    | 1:5:A:HIS:HB2  | 30       | 0.53          |
| (2,98)  | 1:8:A:ARG:HA   | 1:8:A:ARG:HD3  | 1        | 0.53          |
| (2,98)  | 1:8:A:ARG:HA   | 1:8:A:ARG:HD3  | 4        | 0.53          |
| (2,66)  | 1:2:A:SER:HB3  | 1:13:A:CYS:HB3 | 14       | 0.53          |
| (2,66)  | 1:2:A:SER:HB3  | 1:13:A:CYS:HB3 | 20       | 0.53          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (2,18)  | 1:11:A:TRP:HD1 | 1:12:A:PRO:HG3 | 27       | 0.53          |
| (2,18)  | 1:11:A:TRP:HD1 | 1:12:A:PRO:HG3 | 31       | 0.53          |
| (2,18)  | 1:11:A:TRP:HD1 | 1:12:A:PRO:HG3 | 34       | 0.53          |
| (1,8)   | 1:11:A:TRP:HH2 | 1:15:A:TYR:HB2 | 28       | 0.53          |
| (1,8)   | 1:11:A:TRP:HH2 | 1:15:A:TYR:HB2 | 32       | 0.53          |
| (1,6)   | 1:14:A:TRP:HH2 | 1:12:A:PRO:HG2 | 3        | 0.53          |
| (1,6)   | 1:14:A:TRP:HH2 | 1:12:A:PRO:HG2 | 16       | 0.53          |
| (1,6)   | 1:14:A:TRP:HH2 | 1:12:A:PRO:HG2 | 18       | 0.53          |
| (1,6)   | 1:14:A:TRP:HH2 | 1:12:A:PRO:HG2 | 26       | 0.53          |
| (3,43)  | 1:15:A:TYR:HE1 | 1:16:A:ARG:HG2 | 8        | 0.52          |
| (3,43)  | 1:15:A:TYR:HE2 | 1:16:A:ARG:HG2 | 8        | 0.52          |
| (3,29)  | 1:11:A:TRP:HB2 | 1:8:A:ARG:HG2  | 14       | 0.52          |
| (2,348) | 1:11:A:TRP:HB2 | 1:8:A:ARG:HG3  | 2        | 0.52          |
| (2,348) | 1:11:A:TRP:HB2 | 1:8:A:ARG:HG3  | 10       | 0.52          |
| (2,348) | 1:11:A:TRP:HB2 | 1:8:A:ARG:HG3  | 19       | 0.52          |
| (2,348) | 1:11:A:TRP:HB2 | 1:8:A:ARG:HG3  | 25       | 0.52          |
| (2,348) | 1:11:A:TRP:HB2 | 1:8:A:ARG:HG3  | 28       | 0.52          |
| (2,348) | 1:11:A:TRP:HB2 | 1:8:A:ARG:HG3  | 35       | 0.52          |
| (2,337) | 1:6:A:VAL:HA   | 1:13:A:CYS:HB2 | 12       | 0.52          |
| (2,337) | 1:6:A:VAL:HA   | 1:13:A:CYS:HB2 | 19       | 0.52          |
| (2,182) | 1:5:A:HIS:H    | 1:5:A:HIS:HB2  | 29       | 0.52          |
| (2,66)  | 1:2:A:SER:HB3  | 1:13:A:CYS:HB3 | 32       | 0.52          |
| (2,66)  | 1:2:A:SER:HB3  | 1:13:A:CYS:HB3 | 33       | 0.52          |
| (2,46)  | 1:11:A:TRP:HB3 | 1:15:A:TYR:HB3 | 16       | 0.52          |
| (2,46)  | 1:11:A:TRP:HB3 | 1:15:A:TYR:HB3 | 22       | 0.52          |
| (2,35)  | 1:5:A:HIS:HD2  | 1:13:A:CYS:HB2 | 2        | 0.52          |
| (2,18)  | 1:11:A:TRP:HD1 | 1:12:A:PRO:HG3 | 11       | 0.52          |
| (1,29)  | 1:11:A:TRP:HD1 | 1:1:A:PRO:HG3  | 19       | 0.52          |
| (1,6)   | 1:14:A:TRP:HH2 | 1:12:A:PRO:HG2 | 4        | 0.52          |
| (1,6)   | 1:14:A:TRP:HH2 | 1:12:A:PRO:HG2 | 5        | 0.52          |
| (1,6)   | 1:14:A:TRP:HH2 | 1:12:A:PRO:HG2 | 11       | 0.52          |
| (1,6)   | 1:14:A:TRP:HH2 | 1:12:A:PRO:HG2 | 30       | 0.52          |
| (3,29)  | 1:11:A:TRP:HB2 | 1:8:A:ARG:HG2  | 17       | 0.51          |
| (3,29)  | 1:11:A:TRP:HB2 | 1:8:A:ARG:HG2  | 20       | 0.51          |
| (3,29)  | 1:11:A:TRP:HB2 | 1:8:A:ARG:HG2  | 29       | 0.51          |
| (3,29)  | 1:11:A:TRP:HB2 | 1:8:A:ARG:HG2  | 35       | 0.51          |
| (2,348) | 1:11:A:TRP:HB2 | 1:8:A:ARG:HG3  | 13       | 0.51          |
| (2,348) | 1:11:A:TRP:HB2 | 1:8:A:ARG:HG3  | 20       | 0.51          |
| (2,348) | 1:11:A:TRP:HB2 | 1:8:A:ARG:HG3  | 22       | 0.51          |
| (2,337) | 1:6:A:VAL:HA   | 1:13:A:CYS:HB2 | 3        | 0.51          |
| (2,337) | 1:6:A:VAL:HA   | 1:13:A:CYS:HB2 | 29       | 0.51          |
| (2,182) | 1:5:A:HIS:H    | 1:5:A:HIS:HB2  | 1        | 0.51          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (2,182) | 1:5:A:HIS:H    | 1:5:A:HIS:HB2  | 5        | 0.51          |
| (2,182) | 1:5:A:HIS:H    | 1:5:A:HIS:HB2  | 9        | 0.51          |
| (2,182) | 1:5:A:HIS:H    | 1:5:A:HIS:HB2  | 17       | 0.51          |
| (2,182) | 1:5:A:HIS:H    | 1:5:A:HIS:HB2  | 18       | 0.51          |
| (2,182) | 1:5:A:HIS:H    | 1:5:A:HIS:HB2  | 20       | 0.51          |
| (2,182) | 1:5:A:HIS:H    | 1:5:A:HIS:HB2  | 23       | 0.51          |
| (2,182) | 1:5:A:HIS:H    | 1:5:A:HIS:HB2  | 26       | 0.51          |
| (2,182) | 1:5:A:HIS:H    | 1:5:A:HIS:HB2  | 27       | 0.51          |
| (2,182) | 1:5:A:HIS:H    | 1:5:A:HIS:HB2  | 35       | 0.51          |
| (2,98)  | 1:8:A:ARG:HA   | 1:8:A:ARG:HD3  | 6        | 0.51          |
| (2,98)  | 1:8:A:ARG:HA   | 1:8:A:ARG:HD3  | 32       | 0.51          |
| (2,46)  | 1:11:A:TRP:HB3 | 1:15:A:TYR:HB3 | 1        | 0.51          |
| (2,35)  | 1:5:A:HIS:HD2  | 1:13:A:CYS:HB3 | 11       | 0.51          |
| (2,18)  | 1:11:A:TRP:HD1 | 1:12:A:PRO:HG3 | 1        | 0.51          |
| (2,18)  | 1:11:A:TRP:HD1 | 1:12:A:PRO:HG3 | 18       | 0.51          |
| (2,18)  | 1:11:A:TRP:HD1 | 1:12:A:PRO:HG3 | 23       | 0.51          |
| (1,21)  | 1:4:A:HCS:HG3  | 1:3:A:ILE:HG21 | 31       | 0.51          |
| (1,21)  | 1:4:A:HCS:HG3  | 1:3:A:ILE:HG22 | 31       | 0.51          |
| (1,21)  | 1:4:A:HCS:HG3  | 1:3:A:ILE:HG23 | 31       | 0.51          |
| (1,8)   | 1:11:A:TRP:HH2 | 1:15:A:TYR:HB2 | 23       | 0.51          |
| (1,7)   | 1:14:A:TRP:HH2 | 1:15:A:TYR:HB3 | 13       | 0.51          |
| (1,7)   | 1:14:A:TRP:HH2 | 1:15:A:TYR:HB3 | 16       | 0.51          |
| (1,6)   | 1:14:A:TRP:HH2 | 1:12:A:PRO:HG2 | 7        | 0.51          |
| (1,6)   | 1:14:A:TRP:HH2 | 1:12:A:PRO:HG2 | 13       | 0.51          |
| (1,6)   | 1:14:A:TRP:HH2 | 1:12:A:PRO:HG2 | 20       | 0.51          |
| (1,6)   | 1:14:A:TRP:HH2 | 1:12:A:PRO:HG2 | 22       | 0.51          |
| (1,6)   | 1:14:A:TRP:HH2 | 1:12:A:PRO:HG2 | 29       | 0.51          |
| (1,6)   | 1:14:A:TRP:HH2 | 1:12:A:PRO:HG2 | 34       | 0.51          |
| (3,43)  | 1:15:A:TYR:HE1 | 1:16:A:ARG:HG2 | 30       | 0.5           |
| (3,43)  | 1:15:A:TYR:HE2 | 1:16:A:ARG:HG2 | 30       | 0.5           |
| (2,348) | 1:11:A:TRP:HB2 | 1:8:A:ARG:HG3  | 17       | 0.5           |
| (2,182) | 1:5:A:HIS:H    | 1:5:A:HIS:HB2  | 4        | 0.5           |
| (2,182) | 1:5:A:HIS:H    | 1:5:A:HIS:HB2  | 21       | 0.5           |
| (2,182) | 1:5:A:HIS:H    | 1:5:A:HIS:HB2  | 22       | 0.5           |
| (2,182) | 1:5:A:HIS:H    | 1:5:A:HIS:HB2  | 24       | 0.5           |
| (2,98)  | 1:8:A:ARG:HA   | 1:8:A:ARG:HD3  | 7        | 0.5           |
| (2,98)  | 1:8:A:ARG:HA   | 1:8:A:ARG:HD3  | 30       | 0.5           |
| (2,47)  | 1:7:A:HIS:HB2  | 1:8:A:ARG:HG2  | 31       | 0.5           |
| (2,46)  | 1:11:A:TRP:HB3 | 1:15:A:TYR:HB3 | 12       | 0.5           |
| (2,46)  | 1:11:A:TRP:HB3 | 1:15:A:TYR:HB3 | 35       | 0.5           |
| (2,35)  | 1:5:A:HIS:HD2  | 1:13:A:CYS:HB2 | 9        | 0.5           |
| (2,35)  | 1:5:A:HIS:HD2  | 1:13:A:CYS:HB2 | 17       | 0.5           |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (2,35)  | 1:5:A:HIS:HD2  | 1:13:A:CYS:HB3 | 19       | 0.5           |
| (2,35)  | 1:5:A:HIS:HD2  | 1:13:A:CYS:HB2 | 30       | 0.5           |
| (2,18)  | 1:11:A:TRP:HD1 | 1:12:A:PRO:HG3 | 15       | 0.5           |
| (1,6)   | 1:14:A:TRP:HH2 | 1:12:A:PRO:HG2 | 6        | 0.5           |
| (1,6)   | 1:14:A:TRP:HH2 | 1:12:A:PRO:HG2 | 8        | 0.5           |
| (1,6)   | 1:14:A:TRP:HH2 | 1:12:A:PRO:HG2 | 15       | 0.5           |
| (1,6)   | 1:14:A:TRP:HH2 | 1:12:A:PRO:HG2 | 23       | 0.5           |
| (1,6)   | 1:14:A:TRP:HH2 | 1:12:A:PRO:HG2 | 25       | 0.5           |
| (1,6)   | 1:14:A:TRP:HH2 | 1:12:A:PRO:HG2 | 28       | 0.5           |
| (1,6)   | 1:14:A:TRP:HH2 | 1:12:A:PRO:HG2 | 31       | 0.5           |
| (3,43)  | 1:15:A:TYR:HE1 | 1:16:A:ARG:HG2 | 24       | 0.49          |
| (3,43)  | 1:15:A:TYR:HE2 | 1:16:A:ARG:HG2 | 24       | 0.49          |
| (3,43)  | 1:15:A:TYR:HE1 | 1:16:A:ARG:HG2 | 25       | 0.49          |
| (3,43)  | 1:15:A:TYR:HE2 | 1:16:A:ARG:HG2 | 25       | 0.49          |
| (3,29)  | 1:11:A:TRP:HB2 | 1:8:A:ARG:HG2  | 12       | 0.49          |
| (3,29)  | 1:11:A:TRP:HB2 | 1:8:A:ARG:HG2  | 18       | 0.49          |
| (3,29)  | 1:11:A:TRP:HB2 | 1:8:A:ARG:HG2  | 25       | 0.49          |
| (2,348) | 1:11:A:TRP:HB2 | 1:8:A:ARG:HG3  | 14       | 0.49          |
| (2,312) | 1:15:A:TYR:HD1 | 1:16:A:ARG:HG2 | 8        | 0.49          |
| (2,312) | 1:15:A:TYR:HD2 | 1:16:A:ARG:HG2 | 8        | 0.49          |
| (2,182) | 1:5:A:HIS:H    | 1:5:A:HIS:HB2  | 10       | 0.49          |
| (2,182) | 1:5:A:HIS:H    | 1:5:A:HIS:HB2  | 11       | 0.49          |
| (2,182) | 1:5:A:HIS:H    | 1:5:A:HIS:HB2  | 25       | 0.49          |
| (2,182) | 1:5:A:HIS:H    | 1:5:A:HIS:HB2  | 28       | 0.49          |
| (2,98)  | 1:8:A:ARG:HA   | 1:8:A:ARG:HD3  | 5        | 0.49          |
| (2,98)  | 1:8:A:ARG:HA   | 1:8:A:ARG:HD3  | 9        | 0.49          |
| (2,98)  | 1:8:A:ARG:HA   | 1:8:A:ARG:HD3  | 15       | 0.49          |
| (2,98)  | 1:8:A:ARG:HA   | 1:8:A:ARG:HD3  | 21       | 0.49          |
| (2,98)  | 1:8:A:ARG:HA   | 1:8:A:ARG:HD3  | 26       | 0.49          |
| (2,98)  | 1:8:A:ARG:HA   | 1:8:A:ARG:HD3  | 31       | 0.49          |
| (2,98)  | 1:8:A:ARG:HA   | 1:8:A:ARG:HD3  | 34       | 0.49          |
| (2,66)  | 1:2:A:SER:HB3  | 1:13:A:CYS:HB3 | 10       | 0.49          |
| (2,46)  | 1:11:A:TRP:HB3 | 1:15:A:TYR:HB3 | 15       | 0.49          |
| (1,14)  | 1:15:A:TYR:HD1 | 1:11:A:TRP:HH2 | 9        | 0.49          |
| (1,14)  | 1:15:A:TYR:HD2 | 1:11:A:TRP:HH2 | 9        | 0.49          |
| (1,8)   | 1:11:A:TRP:HH2 | 1:15:A:TYR:HB2 | 2        | 0.49          |
| (1,8)   | 1:11:A:TRP:HH2 | 1:15:A:TYR:HB2 | 16       | 0.49          |
| (1,8)   | 1:11:A:TRP:HH2 | 1:15:A:TYR:HB2 | 33       | 0.49          |
| (1,6)   | 1:14:A:TRP:HH2 | 1:12:A:PRO:HG2 | 2        | 0.49          |
| (1,6)   | 1:14:A:TRP:HH2 | 1:12:A:PRO:HG2 | 24       | 0.49          |
| (1,6)   | 1:14:A:TRP:HH2 | 1:12:A:PRO:HG2 | 27       | 0.49          |
| (3,29)  | 1:11:A:TRP:HB2 | 1:8:A:ARG:HG2  | 2        | 0.48          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (3,29)  | 1:11:A:TRP:HB2 | 1:8:A:ARG:HG2  | 19       | 0.48          |
| (2,348) | 1:11:A:TRP:HB2 | 1:8:A:ARG:HG3  | 12       | 0.48          |
| (2,348) | 1:11:A:TRP:HB2 | 1:8:A:ARG:HG3  | 27       | 0.48          |
| (2,300) | 1:11:A:TRP:HD1 | 1:13:A:CYS:HB3 | 34       | 0.48          |
| (2,300) | 1:11:A:TRP:HD1 | 1:13:A:CYS:HB3 | 35       | 0.48          |
| (2,266) | 1:9:A:PRO:HG2  | 1:9:A:PRO:HB3  | 8        | 0.48          |
| (2,266) | 1:9:A:PRO:HG2  | 1:9:A:PRO:HB3  | 10       | 0.48          |
| (2,266) | 1:9:A:PRO:HG2  | 1:9:A:PRO:HB3  | 20       | 0.48          |
| (2,266) | 1:9:A:PRO:HG2  | 1:9:A:PRO:HB3  | 21       | 0.48          |
| (2,266) | 1:9:A:PRO:HG2  | 1:9:A:PRO:HB3  | 28       | 0.48          |
| (2,182) | 1:5:A:HIS:H    | 1:5:A:HIS:HB2  | 13       | 0.48          |
| (2,182) | 1:5:A:HIS:H    | 1:5:A:HIS:HB2  | 16       | 0.48          |
| (2,182) | 1:5:A:HIS:H    | 1:5:A:HIS:HB2  | 32       | 0.48          |
| (2,98)  | 1:8:A:ARG:HA   | 1:8:A:ARG:HD3  | 11       | 0.48          |
| (2,98)  | 1:8:A:ARG:HA   | 1:8:A:ARG:HD3  | 18       | 0.48          |
| (2,98)  | 1:8:A:ARG:HA   | 1:8:A:ARG:HD3  | 23       | 0.48          |
| (2,66)  | 1:2:A:SER:HB3  | 1:13:A:CYS:HB3 | 35       | 0.48          |
| (2,61)  | 1:4:A:HCS:H    | 1:3:A:ILE:HG13 | 12       | 0.48          |
| (2,18)  | 1:11:A:TRP:HD1 | 1:12:A:PRO:HG3 | 9        | 0.48          |
| (1,30)  | 1:15:A:TYR:HE1 | 1:12:A:PRO:HG3 | 16       | 0.48          |
| (1,30)  | 1:15:A:TYR:HE2 | 1:12:A:PRO:HG3 | 16       | 0.48          |
| (1,21)  | 1:4:A:HCS:HG3  | 1:3:A:ILE:HG21 | 14       | 0.48          |
| (1,21)  | 1:4:A:HCS:HG3  | 1:3:A:ILE:HG22 | 14       | 0.48          |
| (1,21)  | 1:4:A:HCS:HG3  | 1:3:A:ILE:HG23 | 14       | 0.48          |
| (1,21)  | 1:4:A:HCS:HG3  | 1:3:A:ILE:HG21 | 33       | 0.48          |
| (1,21)  | 1:4:A:HCS:HG3  | 1:3:A:ILE:HG22 | 33       | 0.48          |
| (1,21)  | 1:4:A:HCS:HG3  | 1:3:A:ILE:HG23 | 33       | 0.48          |
| (1,16)  | 1:7:A:HIS:HD2  | 1:8:A:ARG:HD3  | 33       | 0.48          |
| (1,6)   | 1:14:A:TRP:HH2 | 1:12:A:PRO:HG2 | 10       | 0.48          |
| (1,6)   | 1:14:A:TRP:HH2 | 1:12:A:PRO:HG2 | 12       | 0.48          |
| (1,6)   | 1:14:A:TRP:HH2 | 1:12:A:PRO:HG2 | 33       | 0.48          |
| (2,348) | 1:11:A:TRP:HB2 | 1:8:A:ARG:HG3  | 24       | 0.47          |
| (2,266) | 1:9:A:PRO:HG2  | 1:9:A:PRO:HB3  | 4        | 0.47          |
| (2,266) | 1:9:A:PRO:HG2  | 1:9:A:PRO:HB3  | 11       | 0.47          |
| (2,266) | 1:9:A:PRO:HG2  | 1:9:A:PRO:HB3  | 12       | 0.47          |
| (2,266) | 1:9:A:PRO:HG2  | 1:9:A:PRO:HB3  | 14       | 0.47          |
| (2,266) | 1:9:A:PRO:HG2  | 1:9:A:PRO:HB3  | 16       | 0.47          |
| (2,266) | 1:9:A:PRO:HG2  | 1:9:A:PRO:HB3  | 19       | 0.47          |
| (2,266) | 1:9:A:PRO:HG2  | 1:9:A:PRO:HB3  | 27       | 0.47          |
| (2,266) | 1:9:A:PRO:HG2  | 1:9:A:PRO:HB3  | 29       | 0.47          |
| (2,266) | 1:9:A:PRO:HG2  | 1:9:A:PRO:HB3  | 32       | 0.47          |
| (2,266) | 1:9:A:PRO:HG2  | 1:9:A:PRO:HB3  | 35       | 0.47          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (2,182) | 1:5:A:HIS:H    | 1:5:A:HIS:HB2  | 3        | 0.47          |
| (2,98)  | 1:8:A:ARG:HA   | 1:8:A:ARG:HD3  | 8        | 0.47          |
| (2,66)  | 1:2:A:SER:HB3  | 1:13:A:CYS:HB3 | 2        | 0.47          |
| (2,66)  | 1:2:A:SER:HB3  | 1:13:A:CYS:HB3 | 16       | 0.47          |
| (2,66)  | 1:2:A:SER:HB3  | 1:13:A:CYS:HB3 | 28       | 0.47          |
| (2,66)  | 1:2:A:SER:HB3  | 1:13:A:CYS:HB3 | 30       | 0.47          |
| (1,26)  | 1:9:A:PRO:HD3  | 1:3:A:ILE:HD11 | 15       | 0.47          |
| (1,26)  | 1:9:A:PRO:HD3  | 1:3:A:ILE:HD12 | 15       | 0.47          |
| (1,26)  | 1:9:A:PRO:HD3  | 1:3:A:ILE:HD13 | 15       | 0.47          |
| (1,18)  | 1:5:A:HIS:HB3  | 1:6:A:VAL:HG21 | 32       | 0.47          |
| (1,18)  | 1:5:A:HIS:HB3  | 1:6:A:VAL:HG22 | 32       | 0.47          |
| (1,18)  | 1:5:A:HIS:HB3  | 1:6:A:VAL:HG23 | 32       | 0.47          |
| (1,16)  | 1:7:A:HIS:HD2  | 1:8:A:ARG:HD3  | 10       | 0.47          |
| (1,8)   | 1:11:A:TRP:HH2 | 1:15:A:TYR:HB2 | 10       | 0.47          |
| (1,6)   | 1:14:A:TRP:HH2 | 1:12:A:PRO:HG2 | 1        | 0.47          |
| (1,6)   | 1:14:A:TRP:HH2 | 1:12:A:PRO:HG2 | 9        | 0.47          |
| (1,6)   | 1:14:A:TRP:HH2 | 1:12:A:PRO:HG2 | 14       | 0.47          |
| (1,6)   | 1:14:A:TRP:HH2 | 1:12:A:PRO:HG2 | 19       | 0.47          |
| (1,6)   | 1:14:A:TRP:HH2 | 1:12:A:PRO:HG2 | 21       | 0.47          |
| (1,6)   | 1:14:A:TRP:HH2 | 1:12:A:PRO:HG2 | 32       | 0.47          |
| (1,6)   | 1:14:A:TRP:HH2 | 1:12:A:PRO:HG2 | 35       | 0.47          |
| (3,43)  | 1:15:A:TYR:HE1 | 1:16:A:ARG:HG2 | 17       | 0.46          |
| (3,43)  | 1:15:A:TYR:HE2 | 1:16:A:ARG:HG2 | 17       | 0.46          |
| (3,29)  | 1:11:A:TRP:HB2 | 1:8:A:ARG:HG2  | 16       | 0.46          |
| (2,266) | 1:9:A:PRO:HG2  | 1:9:A:PRO:HB3  | 2        | 0.46          |
| (2,266) | 1:9:A:PRO:HG2  | 1:9:A:PRO:HB3  | 3        | 0.46          |
| (2,266) | 1:9:A:PRO:HG2  | 1:9:A:PRO:HB3  | 5        | 0.46          |
| (2,266) | 1:9:A:PRO:HG2  | 1:9:A:PRO:HB3  | 6        | 0.46          |
| (2,266) | 1:9:A:PRO:HG2  | 1:9:A:PRO:HB3  | 7        | 0.46          |
| (2,266) | 1:9:A:PRO:HG2  | 1:9:A:PRO:HB3  | 13       | 0.46          |
| (2,266) | 1:9:A:PRO:HG2  | 1:9:A:PRO:HB3  | 17       | 0.46          |
| (2,266) | 1:9:A:PRO:HG2  | 1:9:A:PRO:HB3  | 18       | 0.46          |
| (2,266) | 1:9:A:PRO:HG2  | 1:9:A:PRO:HB3  | 23       | 0.46          |
| (2,266) | 1:9:A:PRO:HG2  | 1:9:A:PRO:HB3  | 24       | 0.46          |
| (2,266) | 1:9:A:PRO:HG2  | 1:9:A:PRO:HB3  | 30       | 0.46          |
| (2,266) | 1:9:A:PRO:HG2  | 1:9:A:PRO:HB3  | 31       | 0.46          |
| (2,266) | 1:9:A:PRO:HG2  | 1:9:A:PRO:HB3  | 33       | 0.46          |
| (2,192) | 1:15:A:TYR:HB2 | 1:11:A:TRP:HA  | 13       | 0.46          |
| (2,182) | 1:5:A:HIS:H    | 1:5:A:HIS:HB2  | 14       | 0.46          |
| (2,66)  | 1:2:A:SER:HB3  | 1:13:A:CYS:HB3 | 23       | 0.46          |
| (2,66)  | 1:2:A:SER:HB3  | 1:13:A:CYS:HB3 | 24       | 0.46          |
| (2,66)  | 1:2:A:SER:HB3  | 1:13:A:CYS:HB3 | 34       | 0.46          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (2,46)  | 1:11:A:TRP:HB3 | 1:15:A:TYR:HB3 | 8        | 0.46          |
| (1,30)  | 1:15:A:TYR:HE1 | 1:12:A:PRO:HG3 | 4        | 0.46          |
| (1,30)  | 1:15:A:TYR:HE2 | 1:12:A:PRO:HG3 | 4        | 0.46          |
| (1,26)  | 1:9:A:PRO:HD3  | 1:3:A:ILE:HD11 | 34       | 0.46          |
| (1,26)  | 1:9:A:PRO:HD3  | 1:3:A:ILE:HD12 | 34       | 0.46          |
| (1,26)  | 1:9:A:PRO:HD3  | 1:3:A:ILE:HD13 | 34       | 0.46          |
| (1,21)  | 1:4:A:HCS:HG3  | 1:3:A:ILE:HG21 | 15       | 0.46          |
| (1,21)  | 1:4:A:HCS:HG3  | 1:3:A:ILE:HG22 | 15       | 0.46          |
| (1,21)  | 1:4:A:HCS:HG3  | 1:3:A:ILE:HG23 | 15       | 0.46          |
| (1,14)  | 1:15:A:TYR:HD1 | 1:11:A:TRP:HH2 | 25       | 0.46          |
| (1,14)  | 1:15:A:TYR:HD2 | 1:11:A:TRP:HH2 | 25       | 0.46          |
| (1,14)  | 1:15:A:TYR:HD1 | 1:11:A:TRP:HH2 | 26       | 0.46          |
| (1,14)  | 1:15:A:TYR:HD2 | 1:11:A:TRP:HH2 | 26       | 0.46          |
| (1,14)  | 1:15:A:TYR:HD1 | 1:11:A:TRP:HH2 | 31       | 0.46          |
| (1,14)  | 1:15:A:TYR:HD2 | 1:11:A:TRP:HH2 | 31       | 0.46          |
| (1,6)   | 1:14:A:TRP:HH2 | 1:12:A:PRO:HG2 | 17       | 0.46          |
| (1,2)   | 1:11:A:TRP:HZ2 | 1:8:A:ARG:HD3  | 29       | 0.46          |
| (3,29)  | 1:11:A:TRP:HB2 | 1:8:A:ARG:HG2  | 24       | 0.45          |
| (3,29)  | 1:11:A:TRP:HB2 | 1:8:A:ARG:HG2  | 27       | 0.45          |
| (2,266) | 1:9:A:PRO:HG2  | 1:9:A:PRO:HB3  | 15       | 0.45          |
| (2,266) | 1:9:A:PRO:HG2  | 1:9:A:PRO:HB3  | 22       | 0.45          |
| (2,266) | 1:9:A:PRO:HG2  | 1:9:A:PRO:HB3  | 25       | 0.45          |
| (2,266) | 1:9:A:PRO:HG2  | 1:9:A:PRO:HB3  | 34       | 0.45          |
| (2,192) | 1:15:A:TYR:HB2 | 1:11:A:TRP:HA  | 16       | 0.45          |
| (2,192) | 1:15:A:TYR:HB2 | 1:11:A:TRP:HA  | 20       | 0.45          |
| (2,192) | 1:15:A:TYR:HB2 | 1:11:A:TRP:HA  | 22       | 0.45          |
| (2,182) | 1:5:A:HIS:H    | 1:5:A:HIS:HB2  | 8        | 0.45          |
| (2,66)  | 1:2:A:SER:HB3  | 1:13:A:CYS:HB3 | 7        | 0.45          |
| (2,66)  | 1:2:A:SER:HB3  | 1:13:A:CYS:HB3 | 13       | 0.45          |
| (2,66)  | 1:2:A:SER:HB3  | 1:13:A:CYS:HB3 | 25       | 0.45          |
| (2,46)  | 1:11:A:TRP:HB3 | 1:15:A:TYR:HB3 | 10       | 0.45          |
| (2,35)  | 1:5:A:HIS:HD2  | 1:13:A:CYS:HB3 | 21       | 0.45          |
| (2,35)  | 1:5:A:HIS:HD2  | 1:13:A:CYS:HB3 | 29       | 0.45          |
| (2,18)  | 1:11:A:TRP:HD1 | 1:12:A:PRO:HG3 | 3        | 0.45          |
| (1,26)  | 1:9:A:PRO:HD3  | 1:3:A:ILE:HG21 | 8        | 0.45          |
| (1,26)  | 1:9:A:PRO:HD3  | 1:3:A:ILE:HG22 | 8        | 0.45          |
| (1,26)  | 1:9:A:PRO:HD3  | 1:3:A:ILE:HG23 | 8        | 0.45          |
| (1,21)  | 1:4:A:HCS:HG3  | 1:3:A:ILE:HG21 | 5        | 0.45          |
| (1,21)  | 1:4:A:HCS:HG3  | 1:3:A:ILE:HG22 | 5        | 0.45          |
| (1,21)  | 1:4:A:HCS:HG3  | 1:3:A:ILE:HG23 | 5        | 0.45          |
| (1,21)  | 1:4:A:HCS:HG3  | 1:3:A:ILE:HG21 | 10       | 0.45          |
| (1,21)  | 1:4:A:HCS:HG3  | 1:3:A:ILE:HG22 | 10       | 0.45          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,21)  | 1:4:A:HCS:HG3  | 1:3:A:ILE:HG23 | 10       | 0.45          |
| (1,21)  | 1:4:A:HCS:HG3  | 1:3:A:ILE:HG21 | 17       | 0.45          |
| (1,21)  | 1:4:A:HCS:HG3  | 1:3:A:ILE:HG22 | 17       | 0.45          |
| (1,21)  | 1:4:A:HCS:HG3  | 1:3:A:ILE:HG23 | 17       | 0.45          |
| (1,14)  | 1:15:A:TYR:HD1 | 1:11:A:TRP:HH2 | 6        | 0.45          |
| (1,14)  | 1:15:A:TYR:HD2 | 1:11:A:TRP:HH2 | 6        | 0.45          |
| (1,8)   | 1:11:A:TRP:HH2 | 1:15:A:TYR:HB2 | 12       | 0.45          |
| (1,2)   | 1:11:A:TRP:HZ2 | 1:8:A:ARG:HD3  | 10       | 0.45          |
| (1,2)   | 1:11:A:TRP:HZ2 | 1:8:A:ARG:HD3  | 16       | 0.45          |
| (3,29)  | 1:11:A:TRP:HB2 | 1:8:A:ARG:HG2  | 33       | 0.44          |
| (2,348) | 1:11:A:TRP:HB2 | 1:8:A:ARG:HG3  | 15       | 0.44          |
| (2,300) | 1:11:A:TRP:HD1 | 1:13:A:CYS:HB3 | 6        | 0.44          |
| (2,300) | 1:11:A:TRP:HD1 | 1:13:A:CYS:HB3 | 15       | 0.44          |
| (2,300) | 1:11:A:TRP:HD1 | 1:13:A:CYS:HB3 | 24       | 0.44          |
| (2,266) | 1:9:A:PRO:HG2  | 1:9:A:PRO:HB3  | 9        | 0.44          |
| (2,266) | 1:9:A:PRO:HG2  | 1:9:A:PRO:HB3  | 26       | 0.44          |
| (2,192) | 1:15:A:TYR:HB2 | 1:11:A:TRP:HA  | 4        | 0.44          |
| (2,192) | 1:15:A:TYR:HB2 | 1:11:A:TRP:HA  | 5        | 0.44          |
| (2,182) | 1:5:A:HIS:H    | 1:5:A:HIS:HB2  | 6        | 0.44          |
| (2,142) | 1:14:A:TRP:HD1 | 1:13:A:CYS:HB3 | 19       | 0.44          |
| (2,66)  | 1:2:A:SER:HB3  | 1:13:A:CYS:HB3 | 18       | 0.44          |
| (2,46)  | 1:11:A:TRP:HB3 | 1:15:A:TYR:HB3 | 25       | 0.44          |
| (2,46)  | 1:11:A:TRP:HB3 | 1:15:A:TYR:HB3 | 34       | 0.44          |
| (2,35)  | 1:5:A:HIS:HD2  | 1:13:A:CYS:HB3 | 12       | 0.44          |
| (2,35)  | 1:5:A:HIS:HD2  | 1:13:A:CYS:HB2 | 34       | 0.44          |
| (1,30)  | 1:15:A:TYR:HE1 | 1:12:A:PRO:HG3 | 13       | 0.44          |
| (1,30)  | 1:15:A:TYR:HE2 | 1:12:A:PRO:HG3 | 13       | 0.44          |
| (1,30)  | 1:15:A:TYR:HE1 | 1:12:A:PRO:HG3 | 20       | 0.44          |
| (1,30)  | 1:15:A:TYR:HE2 | 1:12:A:PRO:HG3 | 20       | 0.44          |
| (1,26)  | 1:9:A:PRO:HD3  | 1:3:A:ILE:HG21 | 6        | 0.44          |
| (1,26)  | 1:9:A:PRO:HD3  | 1:3:A:ILE:HG22 | 6        | 0.44          |
| (1,26)  | 1:9:A:PRO:HD3  | 1:3:A:ILE:HG23 | 6        | 0.44          |
| (1,14)  | 1:15:A:TYR:HD1 | 1:11:A:TRP:HH2 | 3        | 0.44          |
| (1,14)  | 1:15:A:TYR:HD2 | 1:11:A:TRP:HH2 | 3        | 0.44          |
| (1,14)  | 1:15:A:TYR:HD1 | 1:11:A:TRP:HH2 | 32       | 0.44          |
| (1,14)  | 1:15:A:TYR:HD2 | 1:11:A:TRP:HH2 | 32       | 0.44          |
| (3,48)  | 1:11:A:TRP:HE1 | 1:8:A:ARG:HD2  | 30       | 0.43          |
| (3,25)  | 1:5:A:HIS:H    | 1:3:A:ILE:HG13 | 21       | 0.43          |
| (2,312) | 1:15:A:TYR:HD1 | 1:16:A:ARG:HG2 | 17       | 0.43          |
| (2,312) | 1:15:A:TYR:HD2 | 1:16:A:ARG:HG2 | 17       | 0.43          |
| (2,312) | 1:15:A:TYR:HD1 | 1:16:A:ARG:HG2 | 20       | 0.43          |
| (2,312) | 1:15:A:TYR:HD2 | 1:16:A:ARG:HG2 | 20       | 0.43          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (2,300) | 1:11:A:TRP:HD1 | 1:13:A:CYS:HB3 | 18       | 0.43          |
| (2,300) | 1:11:A:TRP:HD1 | 1:13:A:CYS:HB3 | 20       | 0.43          |
| (2,300) | 1:11:A:TRP:HD1 | 1:13:A:CYS:HB3 | 33       | 0.43          |
| (2,192) | 1:15:A:TYR:HB2 | 1:11:A:TRP:HA  | 15       | 0.43          |
| (2,192) | 1:15:A:TYR:HB2 | 1:11:A:TRP:HA  | 19       | 0.43          |
| (2,142) | 1:14:A:TRP:HD1 | 1:13:A:CYS:HB3 | 29       | 0.43          |
| (2,46)  | 1:11:A:TRP:HB3 | 1:15:A:TYR:HB3 | 17       | 0.43          |
| (2,35)  | 1:5:A:HIS:HD2  | 1:13:A:CYS:HB2 | 24       | 0.43          |
| (2,35)  | 1:5:A:HIS:HD2  | 1:13:A:CYS:HB2 | 25       | 0.43          |
| (2,35)  | 1:5:A:HIS:HD2  | 1:13:A:CYS:HB2 | 31       | 0.43          |
| (2,15)  | 1:11:A:TRP:HE3 | 1:8:A:ARG:HD2  | 26       | 0.43          |
| (1,32)  | 1:3:A:ILE:HD11 | 1:9:A:PRO:HD3  | 29       | 0.43          |
| (1,32)  | 1:3:A:ILE:HD12 | 1:9:A:PRO:HD3  | 29       | 0.43          |
| (1,32)  | 1:3:A:ILE:HD13 | 1:9:A:PRO:HD3  | 29       | 0.43          |
| (1,30)  | 1:15:A:TYR:HE1 | 1:12:A:PRO:HG3 | 7        | 0.43          |
| (1,30)  | 1:15:A:TYR:HE2 | 1:12:A:PRO:HG3 | 7        | 0.43          |
| (1,30)  | 1:15:A:TYR:HE1 | 1:12:A:PRO:HG3 | 22       | 0.43          |
| (1,30)  | 1:15:A:TYR:HE2 | 1:12:A:PRO:HG3 | 22       | 0.43          |
| (1,14)  | 1:15:A:TYR:HD1 | 1:11:A:TRP:HH2 | 4        | 0.43          |
| (1,14)  | 1:15:A:TYR:HD2 | 1:11:A:TRP:HH2 | 4        | 0.43          |
| (1,14)  | 1:15:A:TYR:HD1 | 1:11:A:TRP:HH2 | 10       | 0.43          |
| (1,14)  | 1:15:A:TYR:HD2 | 1:11:A:TRP:HH2 | 10       | 0.43          |
| (1,14)  | 1:15:A:TYR:HD1 | 1:11:A:TRP:HH2 | 11       | 0.43          |
| (1,14)  | 1:15:A:TYR:HD2 | 1:11:A:TRP:HH2 | 11       | 0.43          |
| (1,14)  | 1:15:A:TYR:HD1 | 1:11:A:TRP:HH2 | 23       | 0.43          |
| (1,14)  | 1:15:A:TYR:HD2 | 1:11:A:TRP:HH2 | 23       | 0.43          |
| (1,14)  | 1:15:A:TYR:HD1 | 1:11:A:TRP:HH2 | 35       | 0.43          |
| (1,14)  | 1:15:A:TYR:HD2 | 1:11:A:TRP:HH2 | 35       | 0.43          |
| (1,8)   | 1:11:A:TRP:HH2 | 1:15:A:TYR:HB2 | 22       | 0.43          |
| (1,7)   | 1:14:A:TRP:HH2 | 1:15:A:TYR:HB3 | 19       | 0.43          |
| (1,7)   | 1:14:A:TRP:HH2 | 1:15:A:TYR:HB3 | 25       | 0.43          |
| (1,7)   | 1:14:A:TRP:HH2 | 1:15:A:TYR:HB3 | 27       | 0.43          |
| (1,2)   | 1:11:A:TRP:HZ2 | 1:8:A:ARG:HD3  | 2        | 0.43          |
| (3,48)  | 1:11:A:TRP:HE1 | 1:8:A:ARG:HD2  | 6        | 0.42          |
| (3,48)  | 1:11:A:TRP:HE1 | 1:8:A:ARG:HD2  | 21       | 0.42          |
| (3,43)  | 1:15:A:TYR:HE1 | 1:16:A:ARG:HG2 | 27       | 0.42          |
| (3,43)  | 1:15:A:TYR:HE2 | 1:16:A:ARG:HG2 | 27       | 0.42          |
| (3,29)  | 1:11:A:TRP:HB2 | 1:8:A:ARG:HG2  | 10       | 0.42          |
| (3,29)  | 1:11:A:TRP:HB2 | 1:8:A:ARG:HG2  | 13       | 0.42          |
| (2,348) | 1:11:A:TRP:HB2 | 1:8:A:ARG:HG3  | 5        | 0.42          |
| (2,348) | 1:11:A:TRP:HB2 | 1:8:A:ARG:HG3  | 8        | 0.42          |
| (2,348) | 1:11:A:TRP:HB2 | 1:8:A:ARG:HG3  | 9        | 0.42          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (2,300) | 1:11:A:TRP:HD1 | 1:13:A:CYS:HB3 | 2        | 0.42          |
| (2,300) | 1:11:A:TRP:HD1 | 1:13:A:CYS:HB3 | 13       | 0.42          |
| (2,192) | 1:15:A:TYR:HB2 | 1:11:A:TRP:HA  | 3        | 0.42          |
| (2,192) | 1:15:A:TYR:HB2 | 1:11:A:TRP:HA  | 12       | 0.42          |
| (2,192) | 1:15:A:TYR:HB2 | 1:11:A:TRP:HA  | 14       | 0.42          |
| (2,192) | 1:15:A:TYR:HB2 | 1:11:A:TRP:HA  | 17       | 0.42          |
| (2,192) | 1:15:A:TYR:HB2 | 1:11:A:TRP:HA  | 18       | 0.42          |
| (2,192) | 1:15:A:TYR:HB2 | 1:11:A:TRP:HA  | 21       | 0.42          |
| (2,192) | 1:15:A:TYR:HB2 | 1:11:A:TRP:HA  | 24       | 0.42          |
| (2,192) | 1:15:A:TYR:HB2 | 1:11:A:TRP:HA  | 28       | 0.42          |
| (2,192) | 1:15:A:TYR:HB2 | 1:11:A:TRP:HA  | 29       | 0.42          |
| (2,192) | 1:15:A:TYR:HB2 | 1:11:A:TRP:HA  | 33       | 0.42          |
| (2,66)  | 1:2:A:SER:HB3  | 1:13:A:CYS:HB3 | 11       | 0.42          |
| (2,35)  | 1:5:A:HIS:HD2  | 1:13:A:CYS:HB2 | 4        | 0.42          |
| (1,30)  | 1:15:A:TYR:HE1 | 1:12:A:PRO:HG3 | 5        | 0.42          |
| (1,30)  | 1:15:A:TYR:HE2 | 1:12:A:PRO:HG3 | 5        | 0.42          |
| (1,30)  | 1:15:A:TYR:HE1 | 1:12:A:PRO:HG3 | 12       | 0.42          |
| (1,30)  | 1:15:A:TYR:HE2 | 1:12:A:PRO:HG3 | 12       | 0.42          |
| (1,30)  | 1:15:A:TYR:HE1 | 1:12:A:PRO:HG3 | 23       | 0.42          |
| (1,30)  | 1:15:A:TYR:HE2 | 1:12:A:PRO:HG3 | 23       | 0.42          |
| (1,30)  | 1:15:A:TYR:HE1 | 1:12:A:PRO:HG3 | 28       | 0.42          |
| (1,30)  | 1:15:A:TYR:HE2 | 1:12:A:PRO:HG3 | 28       | 0.42          |
| (1,30)  | 1:15:A:TYR:HE1 | 1:12:A:PRO:HG3 | 29       | 0.42          |
| (1,30)  | 1:15:A:TYR:HE2 | 1:12:A:PRO:HG3 | 29       | 0.42          |
| (1,30)  | 1:15:A:TYR:HE1 | 1:12:A:PRO:HG3 | 34       | 0.42          |
| (1,30)  | 1:15:A:TYR:HE2 | 1:12:A:PRO:HG3 | 34       | 0.42          |
| (1,16)  | 1:7:A:HIS:HD2  | 1:8:A:ARG:HD3  | 13       | 0.42          |
| (1,14)  | 1:15:A:TYR:HD1 | 1:11:A:TRP:HH2 | 5        | 0.42          |
| (1,14)  | 1:15:A:TYR:HD2 | 1:11:A:TRP:HH2 | 5        | 0.42          |
| (1,14)  | 1:15:A:TYR:HD1 | 1:11:A:TRP:HH2 | 8        | 0.42          |
| (1,14)  | 1:15:A:TYR:HD2 | 1:11:A:TRP:HH2 | 8        | 0.42          |
| (1,14)  | 1:15:A:TYR:HD1 | 1:11:A:TRP:HH2 | 14       | 0.42          |
| (1,14)  | 1:15:A:TYR:HD2 | 1:11:A:TRP:HH2 | 14       | 0.42          |
| (1,14)  | 1:15:A:TYR:HD1 | 1:11:A:TRP:HH2 | 27       | 0.42          |
| (1,14)  | 1:15:A:TYR:HD2 | 1:11:A:TRP:HH2 | 27       | 0.42          |
| (1,14)  | 1:15:A:TYR:HD1 | 1:11:A:TRP:HH2 | 30       | 0.42          |
| (1,14)  | 1:15:A:TYR:HD2 | 1:11:A:TRP:HH2 | 30       | 0.42          |
| (1,14)  | 1:15:A:TYR:HD1 | 1:11:A:TRP:HH2 | 34       | 0.42          |
| (1,14)  | 1:15:A:TYR:HD2 | 1:11:A:TRP:HH2 | 34       | 0.42          |
| (1,7)   | 1:11:A:TRP:HH2 | 1:8:A:ARG:HD3  | 12       | 0.42          |
| (1,7)   | 1:14:A:TRP:HH2 | 1:15:A:TYR:HB3 | 29       | 0.42          |
| (1,2)   | 1:11:A:TRP:HZ2 | 1:8:A:ARG:HD3  | 33       | 0.42          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,2)   | 1:11:A:TRP:HZ2 | 1:8:A:ARG:HD3  | 35       | 0.42          |
| (3,48)  | 1:11:A:TRP:HE1 | 1:8:A:ARG:HD2  | 4        | 0.41          |
| (3,48)  | 1:11:A:TRP:HE1 | 1:8:A:ARG:HD2  | 11       | 0.41          |
| (2,348) | 1:11:A:TRP:HB2 | 1:8:A:ARG:HG3  | 32       | 0.41          |
| (2,348) | 1:11:A:TRP:HB2 | 1:8:A:ARG:HG3  | 34       | 0.41          |
| (2,300) | 1:11:A:TRP:HD1 | 1:13:A:CYS:HB3 | 7        | 0.41          |
| (2,300) | 1:11:A:TRP:HD1 | 1:13:A:CYS:HB3 | 9        | 0.41          |
| (2,300) | 1:11:A:TRP:HD1 | 1:13:A:CYS:HB3 | 14       | 0.41          |
| (2,300) | 1:11:A:TRP:HD1 | 1:13:A:CYS:HB3 | 22       | 0.41          |
| (2,300) | 1:11:A:TRP:HD1 | 1:13:A:CYS:HB3 | 28       | 0.41          |
| (2,192) | 1:15:A:TYR:HB2 | 1:11:A:TRP:HA  | 2        | 0.41          |
| (2,192) | 1:15:A:TYR:HB2 | 1:11:A:TRP:HA  | 10       | 0.41          |
| (2,192) | 1:15:A:TYR:HB2 | 1:11:A:TRP:HA  | 11       | 0.41          |
| (2,46)  | 1:11:A:TRP:HB3 | 1:15:A:TYR:HB3 | 13       | 0.41          |
| (2,15)  | 1:11:A:TRP:HE3 | 1:8:A:ARG:HD2  | 1        | 0.41          |
| (1,30)  | 1:15:A:TYR:HE1 | 1:12:A:PRO:HG3 | 2        | 0.41          |
| (1,30)  | 1:15:A:TYR:HE2 | 1:12:A:PRO:HG3 | 2        | 0.41          |
| (1,30)  | 1:15:A:TYR:HE1 | 1:12:A:PRO:HG3 | 6        | 0.41          |
| (1,30)  | 1:15:A:TYR:HE2 | 1:12:A:PRO:HG3 | 6        | 0.41          |
| (1,30)  | 1:15:A:TYR:HE1 | 1:12:A:PRO:HG3 | 15       | 0.41          |
| (1,30)  | 1:15:A:TYR:HE2 | 1:12:A:PRO:HG3 | 15       | 0.41          |
| (1,30)  | 1:15:A:TYR:HE1 | 1:12:A:PRO:HG3 | 17       | 0.41          |
| (1,30)  | 1:15:A:TYR:HE2 | 1:12:A:PRO:HG3 | 17       | 0.41          |
| (1,30)  | 1:15:A:TYR:HE1 | 1:12:A:PRO:HG3 | 24       | 0.41          |
| (1,30)  | 1:15:A:TYR:HE2 | 1:12:A:PRO:HG3 | 24       | 0.41          |
| (1,30)  | 1:15:A:TYR:HE1 | 1:12:A:PRO:HG3 | 26       | 0.41          |
| (1,30)  | 1:15:A:TYR:HE2 | 1:12:A:PRO:HG3 | 26       | 0.41          |
| (1,26)  | 1:9:A:PRO:HD3  | 1:3:A:ILE:HG21 | 21       | 0.41          |
| (1,26)  | 1:9:A:PRO:HD3  | 1:3:A:ILE:HG22 | 21       | 0.41          |
| (1,26)  | 1:9:A:PRO:HD3  | 1:3:A:ILE:HG23 | 21       | 0.41          |
| (1,14)  | 1:15:A:TYR:HD1 | 1:11:A:TRP:HH2 | 1        | 0.41          |
| (1,14)  | 1:15:A:TYR:HD2 | 1:11:A:TRP:HH2 | 1        | 0.41          |
| (1,14)  | 1:15:A:TYR:HD1 | 1:11:A:TRP:HH2 | 13       | 0.41          |
| (1,14)  | 1:15:A:TYR:HD2 | 1:11:A:TRP:HH2 | 13       | 0.41          |
| (1,14)  | 1:15:A:TYR:HD1 | 1:11:A:TRP:HH2 | 15       | 0.41          |
| (1,14)  | 1:15:A:TYR:HD2 | 1:11:A:TRP:HH2 | 15       | 0.41          |
| (1,14)  | 1:15:A:TYR:HD1 | 1:11:A:TRP:HH2 | 17       | 0.41          |
| (1,14)  | 1:15:A:TYR:HD2 | 1:11:A:TRP:HH2 | 17       | 0.41          |
| (1,14)  | 1:15:A:TYR:HD1 | 1:11:A:TRP:HH2 | 24       | 0.41          |
| (1,14)  | 1:15:A:TYR:HD2 | 1:11:A:TRP:HH2 | 24       | 0.41          |
| (1,8)   | 1:11:A:TRP:HH2 | 1:15:A:TYR:HB2 | 18       | 0.41          |
| (1,7)   | 1:14:A:TRP:HH2 | 1:15:A:TYR:HB3 | 2        | 0.41          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,7)   | 1:14:A:TRP:HH2 | 1:15:A:TYR:HB3 | 10       | 0.41          |
| (3,3)   | 1:11:A:TRP:HZ2 | 1:8:A:ARG:HD2  | 1        | 0.4           |
| (2,348) | 1:11:A:TRP:HB2 | 1:8:A:ARG:HG3  | 23       | 0.4           |
| (2,312) | 1:15:A:TYR:HD1 | 1:16:A:ARG:HG2 | 13       | 0.4           |
| (2,312) | 1:15:A:TYR:HD2 | 1:16:A:ARG:HG2 | 13       | 0.4           |
| (2,300) | 1:11:A:TRP:HD1 | 1:13:A:CYS:HB3 | 1        | 0.4           |
| (2,300) | 1:11:A:TRP:HD1 | 1:13:A:CYS:HB3 | 10       | 0.4           |
| (2,300) | 1:11:A:TRP:HD1 | 1:13:A:CYS:HB3 | 17       | 0.4           |
| (2,266) | 1:9:A:PRO:HG2  | 1:9:A:PRO:HB3  | 1        | 0.4           |
| (2,192) | 1:15:A:TYR:HB2 | 1:11:A:TRP:HA  | 6        | 0.4           |
| (2,192) | 1:15:A:TYR:HB2 | 1:11:A:TRP:HA  | 8        | 0.4           |
| (2,192) | 1:15:A:TYR:HB2 | 1:11:A:TRP:HA  | 32       | 0.4           |
| (2,46)  | 1:11:A:TRP:HB3 | 1:15:A:TYR:HB3 | 9        | 0.4           |
| (2,46)  | 1:11:A:TRP:HB3 | 1:15:A:TYR:HB3 | 19       | 0.4           |
| (2,15)  | 1:11:A:TRP:HE3 | 1:8:A:ARG:HD2  | 8        | 0.4           |
| (2,15)  | 1:11:A:TRP:HE3 | 1:8:A:ARG:HD2  | 34       | 0.4           |
| (1,30)  | 1:15:A:TYR:HE1 | 1:12:A:PRO:HG3 | 10       | 0.4           |
| (1,30)  | 1:15:A:TYR:HE2 | 1:12:A:PRO:HG3 | 10       | 0.4           |
| (1,30)  | 1:15:A:TYR:HE1 | 1:12:A:PRO:HG3 | 18       | 0.4           |
| (1,30)  | 1:15:A:TYR:HE2 | 1:12:A:PRO:HG3 | 18       | 0.4           |
| (1,30)  | 1:15:A:TYR:HE1 | 1:12:A:PRO:HG3 | 30       | 0.4           |
| (1,30)  | 1:15:A:TYR:HE2 | 1:12:A:PRO:HG3 | 30       | 0.4           |
| (1,30)  | 1:15:A:TYR:HE1 | 1:12:A:PRO:HG3 | 32       | 0.4           |
| (1,30)  | 1:15:A:TYR:HE2 | 1:12:A:PRO:HG3 | 32       | 0.4           |
| (1,29)  | 1:11:A:TRP:HD1 | 1:1:A:PRO:HG3  | 3        | 0.4           |
| (1,21)  | 1:4:A:HCS:HG3  | 1:3:A:ILE:HG21 | 32       | 0.4           |
| (1,21)  | 1:4:A:HCS:HG3  | 1:3:A:ILE:HG22 | 32       | 0.4           |
| (1,21)  | 1:4:A:HCS:HG3  | 1:3:A:ILE:HG23 | 32       | 0.4           |
| (1,16)  | 1:7:A:HIS:HD2  | 1:8:A:ARG:HD3  | 22       | 0.4           |
| (1,14)  | 1:15:A:TYR:HD1 | 1:11:A:TRP:HH2 | 2        | 0.4           |
| (1,14)  | 1:15:A:TYR:HD2 | 1:11:A:TRP:HH2 | 2        | 0.4           |
| (1,14)  | 1:15:A:TYR:HD1 | 1:11:A:TRP:HH2 | 7        | 0.4           |
| (1,14)  | 1:15:A:TYR:HD2 | 1:11:A:TRP:HH2 | 7        | 0.4           |
| (1,14)  | 1:15:A:TYR:HD1 | 1:11:A:TRP:HH2 | 18       | 0.4           |
| (1,14)  | 1:15:A:TYR:HD2 | 1:11:A:TRP:HH2 | 18       | 0.4           |
| (1,14)  | 1:15:A:TYR:HD1 | 1:11:A:TRP:HH2 | 28       | 0.4           |
| (1,14)  | 1:15:A:TYR:HD2 | 1:11:A:TRP:HH2 | 28       | 0.4           |
| (1,8)   | 1:11:A:TRP:HH2 | 1:15:A:TYR:HB2 | 19       | 0.4           |
| (1,8)   | 1:11:A:TRP:HH2 | 1:15:A:TYR:HB2 | 29       | 0.4           |
| (1,7)   | 1:14:A:TRP:HH2 | 1:15:A:TYR:HB3 | 17       | 0.4           |
| (1,7)   | 1:14:A:TRP:HH2 | 1:15:A:TYR:HB3 | 28       | 0.4           |
| (1,7)   | 1:14:A:TRP:HH2 | 1:15:A:TYR:HB3 | 35       | 0.4           |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,2)   | 1:11:A:TRP:HZ2 | 1:8:A:ARG:HD3  | 19       | 0.4           |
| (1,2)   | 1:11:A:TRP:HZ2 | 1:8:A:ARG:HD3  | 28       | 0.4           |
| (3,29)  | 1:11:A:TRP:HB2 | 1:8:A:ARG:HG2  | 22       | 0.39          |
| (3,3)   | 1:11:A:TRP:HZ2 | 1:8:A:ARG:HD2  | 23       | 0.39          |
| (2,348) | 1:11:A:TRP:HB2 | 1:8:A:ARG:HG3  | 26       | 0.39          |
| (2,300) | 1:11:A:TRP:HD1 | 1:13:A:CYS:HB3 | 4        | 0.39          |
| (2,300) | 1:11:A:TRP:HD1 | 1:13:A:CYS:HB3 | 25       | 0.39          |
| (2,192) | 1:15:A:TYR:HB2 | 1:11:A:TRP:HA  | 7        | 0.39          |
| (2,192) | 1:15:A:TYR:HB2 | 1:11:A:TRP:HA  | 26       | 0.39          |
| (2,66)  | 1:2:A:SER:HB3  | 1:13:A:CYS:HB3 | 3        | 0.39          |
| (2,35)  | 1:5:A:HIS:HD2  | 1:13:A:CYS:HB2 | 14       | 0.39          |
| (2,35)  | 1:5:A:HIS:HD2  | 1:13:A:CYS:HB2 | 23       | 0.39          |
| (2,15)  | 1:11:A:TRP:HE3 | 1:8:A:ARG:HD2  | 9        | 0.39          |
| (1,30)  | 1:15:A:TYR:HE1 | 1:12:A:PRO:HG3 | 1        | 0.39          |
| (1,30)  | 1:15:A:TYR:HE2 | 1:12:A:PRO:HG3 | 1        | 0.39          |
| (1,30)  | 1:15:A:TYR:HE1 | 1:12:A:PRO:HG3 | 3        | 0.39          |
| (1,30)  | 1:15:A:TYR:HE2 | 1:12:A:PRO:HG3 | 3        | 0.39          |
| (1,30)  | 1:15:A:TYR:HE1 | 1:12:A:PRO:HG3 | 25       | 0.39          |
| (1,30)  | 1:15:A:TYR:HE2 | 1:12:A:PRO:HG3 | 25       | 0.39          |
| (1,30)  | 1:15:A:TYR:HE1 | 1:12:A:PRO:HG3 | 27       | 0.39          |
| (1,30)  | 1:15:A:TYR:HE2 | 1:12:A:PRO:HG3 | 27       | 0.39          |
| (1,30)  | 1:15:A:TYR:HE1 | 1:12:A:PRO:HG3 | 31       | 0.39          |
| (1,30)  | 1:15:A:TYR:HE2 | 1:12:A:PRO:HG3 | 31       | 0.39          |
| (1,21)  | 1:4:A:HCS:HG3  | 1:3:A:ILE:HG21 | 29       | 0.39          |
| (1,21)  | 1:4:A:HCS:HG3  | 1:3:A:ILE:HG22 | 29       | 0.39          |
| (1,21)  | 1:4:A:HCS:HG3  | 1:3:A:ILE:HG23 | 29       | 0.39          |
| (1,18)  | 1:5:A:HIS:HB3  | 1:6:A:VAL:HG21 | 14       | 0.39          |
| (1,18)  | 1:5:A:HIS:HB3  | 1:6:A:VAL:HG22 | 14       | 0.39          |
| (1,18)  | 1:5:A:HIS:HB3  | 1:6:A:VAL:HG23 | 14       | 0.39          |
| (1,14)  | 1:15:A:TYR:HD1 | 1:11:A:TRP:HH2 | 21       | 0.39          |
| (1,14)  | 1:15:A:TYR:HD2 | 1:11:A:TRP:HH2 | 21       | 0.39          |
| (1,2)   | 1:11:A:TRP:HZ2 | 1:8:A:ARG:HD3  | 13       | 0.39          |
| (3,48)  | 1:11:A:TRP:HE1 | 1:8:A:ARG:HD2  | 7        | 0.38          |
| (3,48)  | 1:11:A:TRP:HE1 | 1:8:A:ARG:HD2  | 31       | 0.38          |
| (2,300) | 1:11:A:TRP:HD1 | 1:13:A:CYS:HB3 | 12       | 0.38          |
| (2,300) | 1:11:A:TRP:HD1 | 1:13:A:CYS:HB3 | 21       | 0.38          |
| (2,300) | 1:11:A:TRP:HD1 | 1:13:A:CYS:HB3 | 27       | 0.38          |
| (2,300) | 1:11:A:TRP:HD1 | 1:13:A:CYS:HB3 | 30       | 0.38          |
| (2,300) | 1:11:A:TRP:HD1 | 1:13:A:CYS:HB3 | 31       | 0.38          |
| (2,192) | 1:15:A:TYR:HB2 | 1:11:A:TRP:HA  | 25       | 0.38          |
| (2,35)  | 1:5:A:HIS:HD2  | 1:13:A:CYS:HB2 | 26       | 0.38          |
| (1,30)  | 1:15:A:TYR:HE1 | 1:12:A:PRO:HG3 | 8        | 0.38          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,30)  | 1:15:A:TYR:HE2 | 1:12:A:PRO:HG3 | 8        | 0.38          |
| (1,30)  | 1:15:A:TYR:HE1 | 1:12:A:PRO:HG3 | 14       | 0.38          |
| (1,30)  | 1:15:A:TYR:HE2 | 1:12:A:PRO:HG3 | 14       | 0.38          |
| (1,21)  | 1:4:A:HCS:HG3  | 1:3:A:ILE:HG21 | 28       | 0.38          |
| (1,21)  | 1:4:A:HCS:HG3  | 1:3:A:ILE:HG22 | 28       | 0.38          |
| (1,21)  | 1:4:A:HCS:HG3  | 1:3:A:ILE:HG23 | 28       | 0.38          |
| (1,21)  | 1:4:A:HCS:HG3  | 1:3:A:ILE:HG21 | 35       | 0.38          |
| (1,21)  | 1:4:A:HCS:HG3  | 1:3:A:ILE:HG22 | 35       | 0.38          |
| (1,21)  | 1:4:A:HCS:HG3  | 1:3:A:ILE:HG23 | 35       | 0.38          |
| (1,18)  | 1:5:A:HIS:HB3  | 1:3:A:ILE:HG21 | 17       | 0.38          |
| (1,18)  | 1:5:A:HIS:HB3  | 1:3:A:ILE:HG22 | 17       | 0.38          |
| (1,18)  | 1:5:A:HIS:HB3  | 1:3:A:ILE:HG23 | 17       | 0.38          |
| (1,18)  | 1:5:A:HIS:HB3  | 1:6:A:VAL:HG21 | 30       | 0.38          |
| (1,18)  | 1:5:A:HIS:HB3  | 1:6:A:VAL:HG22 | 30       | 0.38          |
| (1,18)  | 1:5:A:HIS:HB3  | 1:6:A:VAL:HG23 | 30       | 0.38          |
| (1,16)  | 1:7:A:HIS:HD2  | 1:8:A:ARG:HD3  | 19       | 0.38          |
| (1,2)   | 1:11:A:TRP:HZ2 | 1:8:A:ARG:HD3  | 14       | 0.38          |
| (1,2)   | 1:11:A:TRP:HZ2 | 1:8:A:ARG:HD3  | 17       | 0.38          |
| (1,2)   | 1:11:A:TRP:HZ2 | 1:8:A:ARG:HD3  | 20       | 0.38          |
| (1,2)   | 1:11:A:TRP:HZ2 | 1:8:A:ARG:HD3  | 22       | 0.38          |
| (3,43)  | 1:15:A:TYR:HE1 | 1:16:A:ARG:HG2 | 20       | 0.37          |
| (3,43)  | 1:15:A:TYR:HE2 | 1:16:A:ARG:HG2 | 20       | 0.37          |
| (2,348) | 1:11:A:TRP:HB2 | 1:8:A:ARG:HG3  | 4        | 0.37          |
| (2,348) | 1:11:A:TRP:HB2 | 1:8:A:ARG:HG3  | 11       | 0.37          |
| (2,312) | 1:15:A:TYR:HD1 | 1:16:A:ARG:HG2 | 16       | 0.37          |
| (2,312) | 1:15:A:TYR:HD2 | 1:16:A:ARG:HG2 | 16       | 0.37          |
| (2,312) | 1:15:A:TYR:HD1 | 1:16:A:ARG:HG2 | 27       | 0.37          |
| (2,312) | 1:15:A:TYR:HD2 | 1:16:A:ARG:HG2 | 27       | 0.37          |
| (2,312) | 1:15:A:TYR:HD1 | 1:16:A:ARG:HG2 | 33       | 0.37          |
| (2,312) | 1:15:A:TYR:HD2 | 1:16:A:ARG:HG2 | 33       | 0.37          |
| (2,304) | 1:9:A:PRO:HG2  | 1:8:A:ARG:HA   | 4        | 0.37          |
| (2,300) | 1:11:A:TRP:HD1 | 1:13:A:CYS:HB3 | 8        | 0.37          |
| (2,192) | 1:15:A:TYR:HB2 | 1:11:A:TRP:HA  | 30       | 0.37          |
| (2,192) | 1:15:A:TYR:HB2 | 1:11:A:TRP:HA  | 31       | 0.37          |
| (2,142) | 1:14:A:TRP:HD1 | 1:13:A:CYS:HB3 | 21       | 0.37          |
| (2,142) | 1:14:A:TRP:HD1 | 1:13:A:CYS:HB3 | 32       | 0.37          |
| (2,35)  | 1:5:A:HIS:HD2  | 1:13:A:CYS:HB3 | 8        | 0.37          |
| (2,35)  | 1:5:A:HIS:HD2  | 1:13:A:CYS:HB2 | 20       | 0.37          |
| (2,35)  | 1:5:A:HIS:HD2  | 1:13:A:CYS:HB2 | 28       | 0.37          |
| (2,15)  | 1:11:A:TRP:HE3 | 1:8:A:ARG:HD2  | 15       | 0.37          |
| (2,15)  | 1:11:A:TRP:HE3 | 1:8:A:ARG:HD2  | 23       | 0.37          |
| (1,30)  | 1:15:A:TYR:HE1 | 1:12:A:PRO:HG3 | 11       | 0.37          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,30)  | 1:15:A:TYR:HE2 | 1:12:A:PRO:HG3 | 11       | 0.37          |
| (1,30)  | 1:15:A:TYR:HE1 | 1:12:A:PRO:HG3 | 19       | 0.37          |
| (1,30)  | 1:15:A:TYR:HE2 | 1:12:A:PRO:HG3 | 19       | 0.37          |
| (1,21)  | 1:4:A:HCS:HG3  | 1:3:A:ILE:HG21 | 18       | 0.37          |
| (1,21)  | 1:4:A:HCS:HG3  | 1:3:A:ILE:HG22 | 18       | 0.37          |
| (1,21)  | 1:4:A:HCS:HG3  | 1:3:A:ILE:HG23 | 18       | 0.37          |
| (1,16)  | 1:7:A:HIS:HD2  | 1:8:A:ARG:HD3  | 2        | 0.37          |
| (1,16)  | 1:7:A:HIS:HD2  | 1:8:A:ARG:HD3  | 16       | 0.37          |
| (1,14)  | 1:15:A:TYR:HD1 | 1:11:A:TRP:HH2 | 20       | 0.37          |
| (1,14)  | 1:15:A:TYR:HD2 | 1:11:A:TRP:HH2 | 20       | 0.37          |
| (3,48)  | 1:11:A:TRP:HE1 | 1:8:A:ARG:HD2  | 18       | 0.36          |
| (3,48)  | 1:11:A:TRP:HE1 | 1:8:A:ARG:HD2  | 32       | 0.36          |
| (3,3)   | 1:11:A:TRP:HZ2 | 1:8:A:ARG:HD2  | 9        | 0.36          |
| (3,3)   | 1:11:A:TRP:HZ2 | 1:8:A:ARG:HD2  | 11       | 0.36          |
| (3,3)   | 1:11:A:TRP:HZ2 | 1:8:A:ARG:HD2  | 26       | 0.36          |
| (2,348) | 1:11:A:TRP:HB2 | 1:8:A:ARG:HG3  | 1        | 0.36          |
| (2,348) | 1:11:A:TRP:HB2 | 1:8:A:ARG:HG3  | 6        | 0.36          |
| (2,348) | 1:11:A:TRP:HB2 | 1:8:A:ARG:HG3  | 30       | 0.36          |
| (2,348) | 1:11:A:TRP:HB2 | 1:8:A:ARG:HG3  | 31       | 0.36          |
| (2,312) | 1:15:A:TYR:HD1 | 1:16:A:ARG:HG2 | 5        | 0.36          |
| (2,312) | 1:15:A:TYR:HD2 | 1:16:A:ARG:HG2 | 5        | 0.36          |
| (2,304) | 1:9:A:PRO:HG2  | 1:8:A:ARG:HA   | 2        | 0.36          |
| (2,304) | 1:9:A:PRO:HG2  | 1:8:A:ARG:HA   | 18       | 0.36          |
| (2,304) | 1:9:A:PRO:HG2  | 1:8:A:ARG:HA   | 31       | 0.36          |
| (2,300) | 1:11:A:TRP:HD1 | 1:13:A:CYS:HB3 | 23       | 0.36          |
| (2,192) | 1:15:A:TYR:HB2 | 1:11:A:TRP:HA  | 34       | 0.36          |
| (2,16)  | 1:11:A:TRP:HZ3 | 1:8:A:ARG:HD2  | 27       | 0.36          |
| (1,30)  | 1:15:A:TYR:HE1 | 1:12:A:PRO:HG3 | 9        | 0.36          |
| (1,30)  | 1:15:A:TYR:HE2 | 1:12:A:PRO:HG3 | 9        | 0.36          |
| (1,30)  | 1:15:A:TYR:HE1 | 1:12:A:PRO:HG3 | 21       | 0.36          |
| (1,30)  | 1:15:A:TYR:HE2 | 1:12:A:PRO:HG3 | 21       | 0.36          |
| (1,30)  | 1:15:A:TYR:HE1 | 1:12:A:PRO:HG3 | 33       | 0.36          |
| (1,30)  | 1:15:A:TYR:HE2 | 1:12:A:PRO:HG3 | 33       | 0.36          |
| (1,30)  | 1:15:A:TYR:HE1 | 1:12:A:PRO:HG3 | 35       | 0.36          |
| (1,30)  | 1:15:A:TYR:HE2 | 1:12:A:PRO:HG3 | 35       | 0.36          |
| (1,26)  | 1:9:A:PRO:HD3  | 1:3:A:ILE:HG21 | 19       | 0.36          |
| (1,26)  | 1:9:A:PRO:HD3  | 1:3:A:ILE:HG22 | 19       | 0.36          |
| (1,26)  | 1:9:A:PRO:HD3  | 1:3:A:ILE:HG23 | 19       | 0.36          |
| (1,21)  | 1:4:A:HCS:HG3  | 1:3:A:ILE:HG21 | 4        | 0.36          |
| (1,21)  | 1:4:A:HCS:HG3  | 1:3:A:ILE:HG22 | 4        | 0.36          |
| (1,21)  | 1:4:A:HCS:HG3  | 1:3:A:ILE:HG23 | 4        | 0.36          |
| (1,21)  | 1:4:A:HCS:HG3  | 1:3:A:ILE:HG21 | 25       | 0.36          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,21)  | 1:4:A:HCS:HG3  | 1:3:A:ILE:HG22 | 25       | 0.36          |
| (1,21)  | 1:4:A:HCS:HG3  | 1:3:A:ILE:HG23 | 25       | 0.36          |
| (1,18)  | 1:5:A:HIS:HB3  | 1:6:A:VAL:HG21 | 13       | 0.36          |
| (1,18)  | 1:5:A:HIS:HB3  | 1:6:A:VAL:HG22 | 13       | 0.36          |
| (1,18)  | 1:5:A:HIS:HB3  | 1:6:A:VAL:HG23 | 13       | 0.36          |
| (1,18)  | 1:5:A:HIS:HB3  | 1:3:A:ILE:HG21 | 31       | 0.36          |
| (1,18)  | 1:5:A:HIS:HB3  | 1:3:A:ILE:HG22 | 31       | 0.36          |
| (1,18)  | 1:5:A:HIS:HB3  | 1:3:A:ILE:HG23 | 31       | 0.36          |
| (1,16)  | 1:7:A:HIS:HD2  | 1:8:A:ARG:HD3  | 27       | 0.36          |
| (1,14)  | 1:15:A:TYR:HD1 | 1:11:A:TRP:HH2 | 12       | 0.36          |
| (1,14)  | 1:15:A:TYR:HD2 | 1:11:A:TRP:HH2 | 12       | 0.36          |
| (1,14)  | 1:15:A:TYR:HD1 | 1:11:A:TRP:HH2 | 16       | 0.36          |
| (1,14)  | 1:15:A:TYR:HD2 | 1:11:A:TRP:HH2 | 16       | 0.36          |
| (1,14)  | 1:15:A:TYR:HD1 | 1:11:A:TRP:HH2 | 29       | 0.36          |
| (1,14)  | 1:15:A:TYR:HD2 | 1:11:A:TRP:HH2 | 29       | 0.36          |
| (1,14)  | 1:15:A:TYR:HD1 | 1:11:A:TRP:HH2 | 33       | 0.36          |
| (1,14)  | 1:15:A:TYR:HD2 | 1:11:A:TRP:HH2 | 33       | 0.36          |
| (1,7)   | 1:14:A:TRP:HH2 | 1:15:A:TYR:HB3 | 22       | 0.36          |
| (1,2)   | 1:11:A:TRP:HZ2 | 1:8:A:ARG:HD3  | 24       | 0.36          |
| (1,2)   | 1:11:A:TRP:HZ2 | 1:8:A:ARG:HD3  | 25       | 0.36          |
| (1,2)   | 1:11:A:TRP:HZ2 | 1:8:A:ARG:HD3  | 27       | 0.36          |
| (2,304) | 1:9:A:PRO:HG2  | 1:8:A:ARG:HA   | 10       | 0.35          |
| (2,304) | 1:9:A:PRO:HG2  | 1:8:A:ARG:HA   | 33       | 0.35          |
| (2,192) | 1:15:A:TYR:HB2 | 1:11:A:TRP:HA  | 23       | 0.35          |
| (2,142) | 1:14:A:TRP:HD1 | 1:13:A:CYS:HB2 | 17       | 0.35          |
| (2,142) | 1:14:A:TRP:HD1 | 1:13:A:CYS:HB3 | 31       | 0.35          |
| (2,47)  | 1:7:A:HIS:HB2  | 1:8:A:ARG:HG2  | 18       | 0.35          |
| (2,46)  | 1:11:A:TRP:HB3 | 1:15:A:TYR:HB3 | 27       | 0.35          |
| (2,35)  | 1:5:A:HIS:HD2  | 1:13:A:CYS:HB2 | 32       | 0.35          |
| (1,21)  | 1:4:A:HCS:HG3  | 1:3:A:ILE:HG21 | 19       | 0.35          |
| (1,21)  | 1:4:A:HCS:HG3  | 1:3:A:ILE:HG22 | 19       | 0.35          |
| (1,21)  | 1:4:A:HCS:HG3  | 1:3:A:ILE:HG23 | 19       | 0.35          |
| (1,18)  | 1:5:A:HIS:HB3  | 1:6:A:VAL:HG21 | 35       | 0.35          |
| (1,18)  | 1:5:A:HIS:HB3  | 1:6:A:VAL:HG22 | 35       | 0.35          |
| (1,18)  | 1:5:A:HIS:HB3  | 1:6:A:VAL:HG23 | 35       | 0.35          |
| (1,16)  | 1:7:A:HIS:HD2  | 1:8:A:ARG:HD3  | 29       | 0.35          |
| (1,7)   | 1:14:A:TRP:HH2 | 1:15:A:TYR:HB3 | 14       | 0.35          |
| (1,7)   | 1:14:A:TRP:HH2 | 1:15:A:TYR:HB3 | 20       | 0.35          |
| (3,3)   | 1:11:A:TRP:HZ2 | 1:8:A:ARG:HD2  | 5        | 0.34          |
| (3,3)   | 1:11:A:TRP:HZ2 | 1:8:A:ARG:HD2  | 30       | 0.34          |
| (2,304) | 1:9:A:PRO:HG2  | 1:8:A:ARG:HA   | 7        | 0.34          |
| (2,304) | 1:9:A:PRO:HG2  | 1:8:A:ARG:HA   | 19       | 0.34          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (2,304) | 1:9:A:PRO:HG2  | 1:8:A:ARG:HA   | 32       | 0.34          |
| (2,300) | 1:11:A:TRP:HD1 | 1:13:A:CYS:HB3 | 19       | 0.34          |
| (2,300) | 1:11:A:TRP:HD1 | 1:13:A:CYS:HB3 | 32       | 0.34          |
| (2,192) | 1:15:A:TYR:HB2 | 1:11:A:TRP:HA  | 1        | 0.34          |
| (2,192) | 1:15:A:TYR:HB2 | 1:11:A:TRP:HA  | 9        | 0.34          |
| (2,192) | 1:15:A:TYR:HB2 | 1:11:A:TRP:HA  | 35       | 0.34          |
| (2,142) | 1:14:A:TRP:HD1 | 1:13:A:CYS:HB2 | 11       | 0.34          |
| (2,142) | 1:14:A:TRP:HD1 | 1:13:A:CYS:HB3 | 28       | 0.34          |
| (2,35)  | 1:5:A:HIS:HD2  | 1:13:A:CYS:HB2 | 18       | 0.34          |
| (2,15)  | 1:11:A:TRP:HE3 | 1:8:A:ARG:HD2  | 5        | 0.34          |
| (1,29)  | 1:11:A:TRP:HD1 | 1:1:A:PRO:HG3  | 10       | 0.34          |
| (1,21)  | 1:4:A:HCS:HG3  | 1:3:A:ILE:HG21 | 26       | 0.34          |
| (1,21)  | 1:4:A:HCS:HG3  | 1:3:A:ILE:HG22 | 26       | 0.34          |
| (1,21)  | 1:4:A:HCS:HG3  | 1:3:A:ILE:HG23 | 26       | 0.34          |
| (1,18)  | 1:5:A:HIS:HB3  | 1:6:A:VAL:HG21 | 27       | 0.34          |
| (1,18)  | 1:5:A:HIS:HB3  | 1:6:A:VAL:HG22 | 27       | 0.34          |
| (1,18)  | 1:5:A:HIS:HB3  | 1:6:A:VAL:HG23 | 27       | 0.34          |
| (1,14)  | 1:15:A:TYR:HD1 | 1:11:A:TRP:HH2 | 22       | 0.34          |
| (1,14)  | 1:15:A:TYR:HD2 | 1:11:A:TRP:HH2 | 22       | 0.34          |
| (3,3)   | 1:11:A:TRP:HZ2 | 1:8:A:ARG:HD2  | 4        | 0.33          |
| (3,3)   | 1:11:A:TRP:HZ2 | 1:8:A:ARG:HD2  | 8        | 0.33          |
| (2,304) | 1:9:A:PRO:HG2  | 1:8:A:ARG:HA   | 5        | 0.33          |
| (2,304) | 1:9:A:PRO:HG2  | 1:8:A:ARG:HA   | 6        | 0.33          |
| (2,304) | 1:9:A:PRO:HG2  | 1:8:A:ARG:HA   | 8        | 0.33          |
| (2,304) | 1:9:A:PRO:HG2  | 1:8:A:ARG:HA   | 12       | 0.33          |
| (2,304) | 1:9:A:PRO:HG2  | 1:8:A:ARG:HA   | 13       | 0.33          |
| (2,304) | 1:9:A:PRO:HG2  | 1:8:A:ARG:HA   | 16       | 0.33          |
| (2,304) | 1:9:A:PRO:HG2  | 1:8:A:ARG:HA   | 20       | 0.33          |
| (2,304) | 1:9:A:PRO:HG2  | 1:8:A:ARG:HA   | 21       | 0.33          |
| (2,304) | 1:9:A:PRO:HG2  | 1:8:A:ARG:HA   | 30       | 0.33          |
| (2,142) | 1:14:A:TRP:HD1 | 1:13:A:CYS:HB3 | 8        | 0.33          |
| (2,142) | 1:14:A:TRP:HD1 | 1:13:A:CYS:HB3 | 10       | 0.33          |
| (2,142) | 1:14:A:TRP:HD1 | 1:13:A:CYS:HB3 | 23       | 0.33          |
| (2,46)  | 1:11:A:TRP:HB3 | 1:15:A:TYR:HB3 | 23       | 0.33          |
| (2,35)  | 1:5:A:HIS:HD2  | 1:13:A:CYS:HB2 | 27       | 0.33          |
| (1,32)  | 1:3:A:ILE:HD11 | 1:9:A:PRO:HD3  | 19       | 0.33          |
| (1,32)  | 1:3:A:ILE:HD12 | 1:9:A:PRO:HD3  | 19       | 0.33          |
| (1,32)  | 1:3:A:ILE:HD13 | 1:9:A:PRO:HD3  | 19       | 0.33          |
| (1,29)  | 1:11:A:TRP:HD1 | 1:1:A:PRO:HG3  | 26       | 0.33          |
| (1,21)  | 1:4:A:HCS:HG3  | 1:3:A:ILE:HG21 | 1        | 0.33          |
| (1,21)  | 1:4:A:HCS:HG3  | 1:3:A:ILE:HG22 | 1        | 0.33          |
| (1,21)  | 1:4:A:HCS:HG3  | 1:3:A:ILE:HG23 | 1        | 0.33          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,21)  | 1:4:A:HCS:HG3  | 1:3:A:ILE:HG21 | 9        | 0.33          |
| (1,21)  | 1:4:A:HCS:HG3  | 1:3:A:ILE:HG22 | 9        | 0.33          |
| (1,21)  | 1:4:A:HCS:HG3  | 1:3:A:ILE:HG23 | 9        | 0.33          |
| (1,21)  | 1:4:A:HCS:HG3  | 1:3:A:ILE:HG21 | 13       | 0.33          |
| (1,21)  | 1:4:A:HCS:HG3  | 1:3:A:ILE:HG22 | 13       | 0.33          |
| (1,21)  | 1:4:A:HCS:HG3  | 1:3:A:ILE:HG23 | 13       | 0.33          |
| (1,7)   | 1:14:A:TRP:HH2 | 1:15:A:TYR:HB3 | 33       | 0.33          |
| (1,2)   | 1:11:A:TRP:HZ2 | 1:8:A:ARG:HD3  | 12       | 0.33          |
| (3,48)  | 1:11:A:TRP:HE1 | 1:8:A:ARG:HD2  | 1        | 0.32          |
| (3,3)   | 1:11:A:TRP:HZ2 | 1:8:A:ARG:HD2  | 6        | 0.32          |
| (3,3)   | 1:11:A:TRP:HZ2 | 1:8:A:ARG:HD2  | 15       | 0.32          |
| (2,348) | 1:11:A:TRP:HB2 | 1:8:A:ARG:HG3  | 7        | 0.32          |
| (2,348) | 1:11:A:TRP:HB2 | 1:8:A:ARG:HG3  | 21       | 0.32          |
| (2,304) | 1:9:A:PRO:HG2  | 1:8:A:ARG:HA   | 14       | 0.32          |
| (2,304) | 1:9:A:PRO:HG2  | 1:8:A:ARG:HA   | 17       | 0.32          |
| (2,304) | 1:9:A:PRO:HG2  | 1:8:A:ARG:HA   | 24       | 0.32          |
| (2,304) | 1:9:A:PRO:HG2  | 1:8:A:ARG:HA   | 25       | 0.32          |
| (2,304) | 1:9:A:PRO:HG2  | 1:8:A:ARG:HA   | 28       | 0.32          |
| (2,304) | 1:9:A:PRO:HG2  | 1:8:A:ARG:HA   | 29       | 0.32          |
| (2,304) | 1:9:A:PRO:HG2  | 1:8:A:ARG:HA   | 34       | 0.32          |
| (2,142) | 1:14:A:TRP:HD1 | 1:13:A:CYS:HB2 | 5        | 0.32          |
| (2,64)  | 1:2:A:SER:HB2  | 1:13:A:CYS:HB3 | 17       | 0.32          |
| (1,21)  | 1:4:A:HCS:HG3  | 1:3:A:ILE:HG21 | 6        | 0.32          |
| (1,21)  | 1:4:A:HCS:HG3  | 1:3:A:ILE:HG22 | 6        | 0.32          |
| (1,21)  | 1:4:A:HCS:HG3  | 1:3:A:ILE:HG23 | 6        | 0.32          |
| (1,18)  | 1:5:A:HIS:HB3  | 1:6:A:VAL:HG21 | 10       | 0.32          |
| (1,18)  | 1:5:A:HIS:HB3  | 1:6:A:VAL:HG22 | 10       | 0.32          |
| (1,18)  | 1:5:A:HIS:HB3  | 1:6:A:VAL:HG23 | 10       | 0.32          |
| (1,14)  | 1:15:A:TYR:HD1 | 1:11:A:TRP:HH2 | 19       | 0.32          |
| (1,14)  | 1:15:A:TYR:HD2 | 1:11:A:TRP:HH2 | 19       | 0.32          |
| (1,7)   | 1:14:A:TRP:HH2 | 1:15:A:TYR:HB3 | 24       | 0.32          |
| (3,48)  | 1:11:A:TRP:HE1 | 1:8:A:ARG:HD2  | 23       | 0.31          |
| (2,304) | 1:9:A:PRO:HG2  | 1:8:A:ARG:HA   | 26       | 0.31          |
| (2,304) | 1:9:A:PRO:HG2  | 1:8:A:ARG:HA   | 27       | 0.31          |
| (2,304) | 1:9:A:PRO:HG2  | 1:8:A:ARG:HA   | 35       | 0.31          |
| (2,264) | 1:13:A:CYS:HB3 | 1:4:A:HCS:HA   | 12       | 0.31          |
| (2,264) | 1:13:A:CYS:HB3 | 1:4:A:HCS:HA   | 29       | 0.31          |
| (2,192) | 1:15:A:TYR:HB2 | 1:11:A:TRP:HA  | 27       | 0.31          |
| (2,142) | 1:14:A:TRP:HD1 | 1:13:A:CYS:HB3 | 14       | 0.31          |
| (2,142) | 1:14:A:TRP:HD1 | 1:13:A:CYS:HB2 | 16       | 0.31          |
| (2,142) | 1:14:A:TRP:HD1 | 1:13:A:CYS:HB2 | 30       | 0.31          |
| (2,30)  | 1:15:A:TYR:HE1 | 1:13:A:CYS:HB2 | 16       | 0.31          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (2,30)  | 1:15:A:TYR:HE2 | 1:13:A:CYS:HB2 | 16       | 0.31          |
| (2,30)  | 1:15:A:TYR:HE1 | 1:13:A:CYS:HB2 | 20       | 0.31          |
| (2,30)  | 1:15:A:TYR:HE2 | 1:13:A:CYS:HB2 | 20       | 0.31          |
| (2,16)  | 1:11:A:TRP:HZ3 | 1:8:A:ARG:HD2  | 13       | 0.31          |
| (1,26)  | 1:9:A:PRO:HD3  | 1:3:A:ILE:HD11 | 11       | 0.31          |
| (1,26)  | 1:9:A:PRO:HD3  | 1:3:A:ILE:HD12 | 11       | 0.31          |
| (1,26)  | 1:9:A:PRO:HD3  | 1:3:A:ILE:HD13 | 11       | 0.31          |
| (1,21)  | 1:4:A:HCS:HG3  | 1:3:A:ILE:HG21 | 11       | 0.31          |
| (1,21)  | 1:4:A:HCS:HG3  | 1:3:A:ILE:HG22 | 11       | 0.31          |
| (1,21)  | 1:4:A:HCS:HG3  | 1:3:A:ILE:HG23 | 11       | 0.31          |
| (1,21)  | 1:4:A:HCS:HG3  | 1:3:A:ILE:HG21 | 16       | 0.31          |
| (1,21)  | 1:4:A:HCS:HG3  | 1:3:A:ILE:HG22 | 16       | 0.31          |
| (1,21)  | 1:4:A:HCS:HG3  | 1:3:A:ILE:HG23 | 16       | 0.31          |
| (3,43)  | 1:15:A:TYR:HE1 | 1:16:A:ARG:HG2 | 33       | 0.3           |
| (3,43)  | 1:15:A:TYR:HE2 | 1:16:A:ARG:HG2 | 33       | 0.3           |
| (3,3)   | 1:11:A:TRP:HZ2 | 1:8:A:ARG:HD2  | 7        | 0.3           |
| (3,3)   | 1:11:A:TRP:HZ2 | 1:8:A:ARG:HD2  | 21       | 0.3           |
| (2,304) | 1:9:A:PRO:HG2  | 1:8:A:ARG:HA   | 1        | 0.3           |
| (2,304) | 1:9:A:PRO:HG2  | 1:8:A:ARG:HA   | 22       | 0.3           |
| (2,300) | 1:11:A:TRP:HD1 | 1:13:A:CYS:HB3 | 26       | 0.3           |
| (2,300) | 1:11:A:TRP:HD1 | 1:13:A:CYS:HB3 | 29       | 0.3           |
| (2,228) | 1:11:A:TRP:HB2 | 1:8:A:ARG:HB2  | 22       | 0.3           |
| (2,198) | 1:8:A:ARG:H    | 1:7:A:HIS:HB2  | 18       | 0.3           |
| (2,142) | 1:14:A:TRP:HD1 | 1:13:A:CYS:HB2 | 3        | 0.3           |
| (2,142) | 1:14:A:TRP:HD1 | 1:13:A:CYS:HB3 | 4        | 0.3           |
| (2,142) | 1:14:A:TRP:HD1 | 1:13:A:CYS:HB2 | 12       | 0.3           |
| (2,142) | 1:14:A:TRP:HD1 | 1:13:A:CYS:HB2 | 22       | 0.3           |
| (2,142) | 1:14:A:TRP:HD1 | 1:13:A:CYS:HB2 | 26       | 0.3           |
| (2,142) | 1:14:A:TRP:HD1 | 1:13:A:CYS:HB2 | 27       | 0.3           |
| (2,66)  | 1:2:A:SER:HB3  | 1:13:A:CYS:HB3 | 27       | 0.3           |
| (2,35)  | 1:5:A:HIS:HD2  | 1:13:A:CYS:HB3 | 3        | 0.3           |
| (2,35)  | 1:5:A:HIS:HD2  | 1:13:A:CYS:HB2 | 16       | 0.3           |
| (1,21)  | 1:4:A:HCS:HG3  | 1:3:A:ILE:HG21 | 22       | 0.3           |
| (1,21)  | 1:4:A:HCS:HG3  | 1:3:A:ILE:HG22 | 22       | 0.3           |
| (1,21)  | 1:4:A:HCS:HG3  | 1:3:A:ILE:HG23 | 22       | 0.3           |
| (1,18)  | 1:5:A:HIS:HB3  | 1:3:A:ILE:HG21 | 9        | 0.3           |
| (1,18)  | 1:5:A:HIS:HB3  | 1:3:A:ILE:HG22 | 9        | 0.3           |
| (1,18)  | 1:5:A:HIS:HB3  | 1:3:A:ILE:HG23 | 9        | 0.3           |
| (1,16)  | 1:7:A:HIS:HD2  | 1:8:A:ARG:HD3  | 24       | 0.3           |
| (3,48)  | 1:11:A:TRP:HE1 | 1:8:A:ARG:HD2  | 9        | 0.29          |
| (2,304) | 1:9:A:PRO:HG2  | 1:8:A:ARG:HA   | 15       | 0.29          |
| (2,304) | 1:9:A:PRO:HG2  | 1:8:A:ARG:HA   | 23       | 0.29          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (2,300) | 1:11:A:TRP:HD1 | 1:13:A:CYS:HB3 | 11       | 0.29          |
| (2,300) | 1:11:A:TRP:HD1 | 1:13:A:CYS:HB3 | 16       | 0.29          |
| (2,264) | 1:13:A:CYS:HB3 | 1:4:A:HCS:HA   | 1        | 0.29          |
| (2,264) | 1:13:A:CYS:HB3 | 1:4:A:HCS:HA   | 5        | 0.29          |
| (2,264) | 1:13:A:CYS:HB3 | 1:4:A:HCS:HA   | 28       | 0.29          |
| (2,142) | 1:14:A:TRP:HD1 | 1:13:A:CYS:HB2 | 13       | 0.29          |
| (2,128) | 1:14:A:TRP:HD1 | 1:12:A:PRO:HG3 | 5        | 0.29          |
| (2,66)  | 1:2:A:SER:HB3  | 1:13:A:CYS:HB3 | 26       | 0.29          |
| (1,26)  | 1:9:A:PRO:HD3  | 1:3:A:ILE:HD11 | 7        | 0.29          |
| (1,26)  | 1:9:A:PRO:HD3  | 1:3:A:ILE:HD12 | 7        | 0.29          |
| (1,26)  | 1:9:A:PRO:HD3  | 1:3:A:ILE:HD13 | 7        | 0.29          |
| (1,21)  | 1:4:A:HCS:HG3  | 1:3:A:ILE:HG21 | 23       | 0.29          |
| (1,21)  | 1:4:A:HCS:HG3  | 1:3:A:ILE:HG22 | 23       | 0.29          |
| (1,21)  | 1:4:A:HCS:HG3  | 1:3:A:ILE:HG23 | 23       | 0.29          |
| (1,16)  | 1:7:A:HIS:HD2  | 1:8:A:ARG:HD3  | 25       | 0.29          |
| (1,5)   | 1:11:A:TRP:HD1 | 1:12:A:PRO:HB2 | 28       | 0.29          |
| (3,48)  | 1:11:A:TRP:HE1 | 1:8:A:ARG:HD2  | 8        | 0.28          |
| (3,48)  | 1:11:A:TRP:HE1 | 1:8:A:ARG:HD2  | 26       | 0.28          |
| (3,3)   | 1:11:A:TRP:HZ2 | 1:8:A:ARG:HD2  | 32       | 0.28          |
| (2,304) | 1:9:A:PRO:HG2  | 1:8:A:ARG:HA   | 3        | 0.28          |
| (2,304) | 1:9:A:PRO:HG2  | 1:8:A:ARG:HA   | 11       | 0.28          |
| (2,294) | 1:10:A:ASP:H   | 1:10:A:ASP:HB2 | 21       | 0.28          |
| (2,264) | 1:13:A:CYS:HB3 | 1:4:A:HCS:HA   | 2        | 0.28          |
| (2,264) | 1:13:A:CYS:HB3 | 1:4:A:HCS:HA   | 4        | 0.28          |
| (2,264) | 1:13:A:CYS:HB3 | 1:4:A:HCS:HA   | 11       | 0.28          |
| (2,264) | 1:13:A:CYS:HB3 | 1:4:A:HCS:HA   | 30       | 0.28          |
| (2,198) | 1:8:A:ARG:H    | 1:7:A:HIS:HB2  | 28       | 0.28          |
| (2,142) | 1:14:A:TRP:HD1 | 1:13:A:CYS:HB2 | 2        | 0.28          |
| (2,30)  | 1:15:A:TYR:HE1 | 1:13:A:CYS:HB2 | 4        | 0.28          |
| (2,30)  | 1:15:A:TYR:HE2 | 1:13:A:CYS:HB2 | 4        | 0.28          |
| (2,16)  | 1:11:A:TRP:HZ3 | 1:8:A:ARG:HD2  | 10       | 0.28          |
| (2,16)  | 1:11:A:TRP:HZ3 | 1:8:A:ARG:HD2  | 14       | 0.28          |
| (2,16)  | 1:11:A:TRP:HZ3 | 1:8:A:ARG:HD2  | 19       | 0.28          |
| (2,16)  | 1:11:A:TRP:HZ3 | 1:8:A:ARG:HD2  | 28       | 0.28          |
| (1,26)  | 1:9:A:PRO:HD3  | 1:3:A:ILE:HG21 | 3        | 0.28          |
| (1,26)  | 1:9:A:PRO:HD3  | 1:3:A:ILE:HG22 | 3        | 0.28          |
| (1,26)  | 1:9:A:PRO:HD3  | 1:3:A:ILE:HG23 | 3        | 0.28          |
| (1,18)  | 1:5:A:HIS:HB3  | 1:3:A:ILE:HG21 | 4        | 0.28          |
| (1,18)  | 1:5:A:HIS:HB3  | 1:3:A:ILE:HG22 | 4        | 0.28          |
| (1,18)  | 1:5:A:HIS:HB3  | 1:3:A:ILE:HG23 | 4        | 0.28          |
| (1,18)  | 1:5:A:HIS:HB3  | 1:3:A:ILE:HG21 | 5        | 0.28          |
| (1,18)  | 1:5:A:HIS:HB3  | 1:3:A:ILE:HG22 | 5        | 0.28          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,18)  | 1:5:A:HIS:HB3  | 1:3:A:ILE:HG23 | 5        | 0.28          |
| (1,18)  | 1:5:A:HIS:HB3  | 1:3:A:ILE:HG21 | 23       | 0.28          |
| (1,18)  | 1:5:A:HIS:HB3  | 1:3:A:ILE:HG22 | 23       | 0.28          |
| (1,18)  | 1:5:A:HIS:HB3  | 1:3:A:ILE:HG23 | 23       | 0.28          |
| (3,43)  | 1:15:A:TYR:HE1 | 1:16:A:ARG:HG2 | 5        | 0.27          |
| (3,43)  | 1:15:A:TYR:HE2 | 1:16:A:ARG:HG2 | 5        | 0.27          |
| (3,3)   | 1:11:A:TRP:HZ2 | 1:8:A:ARG:HD2  | 31       | 0.27          |
| (3,3)   | 1:11:A:TRP:HZ2 | 1:8:A:ARG:HD2  | 34       | 0.27          |
| (2,264) | 1:13:A:CYS:HB3 | 1:4:A:HCS:HA   | 7        | 0.27          |
| (2,264) | 1:13:A:CYS:HB3 | 1:4:A:HCS:HA   | 8        | 0.27          |
| (2,264) | 1:13:A:CYS:HB3 | 1:4:A:HCS:HA   | 21       | 0.27          |
| (2,264) | 1:13:A:CYS:HB3 | 1:4:A:HCS:HA   | 26       | 0.27          |
| (2,228) | 1:11:A:TRP:HB2 | 1:8:A:ARG:HB2  | 3        | 0.27          |
| (2,228) | 1:11:A:TRP:HB2 | 1:8:A:ARG:HB2  | 11       | 0.27          |
| (2,198) | 1:8:A:ARG:H    | 1:7:A:HIS:HB2  | 8        | 0.27          |
| (2,198) | 1:8:A:ARG:H    | 1:7:A:HIS:HB2  | 16       | 0.27          |
| (2,198) | 1:8:A:ARG:H    | 1:7:A:HIS:HB2  | 29       | 0.27          |
| (2,142) | 1:14:A:TRP:HD1 | 1:13:A:CYS:HB3 | 6        | 0.27          |
| (2,16)  | 1:11:A:TRP:HZ3 | 1:8:A:ARG:HD2  | 16       | 0.27          |
| (2,16)  | 1:11:A:TRP:HZ3 | 1:8:A:ARG:HD2  | 17       | 0.27          |
| (2,16)  | 1:11:A:TRP:HZ3 | 1:8:A:ARG:HD2  | 20       | 0.27          |
| (2,16)  | 1:11:A:TRP:HZ3 | 1:8:A:ARG:HD2  | 24       | 0.27          |
| (1,21)  | 1:4:A:HCS:HG3  | 1:3:A:ILE:HG21 | 2        | 0.27          |
| (1,21)  | 1:4:A:HCS:HG3  | 1:3:A:ILE:HG22 | 2        | 0.27          |
| (1,21)  | 1:4:A:HCS:HG3  | 1:3:A:ILE:HG23 | 2        | 0.27          |
| (1,21)  | 1:4:A:HCS:HG3  | 1:3:A:ILE:HG21 | 8        | 0.27          |
| (1,21)  | 1:4:A:HCS:HG3  | 1:3:A:ILE:HG22 | 8        | 0.27          |
| (1,21)  | 1:4:A:HCS:HG3  | 1:3:A:ILE:HG23 | 8        | 0.27          |
| (3,48)  | 1:11:A:TRP:HE1 | 1:8:A:ARG:HD2  | 5        | 0.26          |
| (2,264) | 1:13:A:CYS:HB3 | 1:4:A:HCS:HA   | 16       | 0.26          |
| (2,264) | 1:13:A:CYS:HB3 | 1:4:A:HCS:HA   | 19       | 0.26          |
| (2,264) | 1:13:A:CYS:HB3 | 1:4:A:HCS:HA   | 20       | 0.26          |
| (2,264) | 1:13:A:CYS:HB3 | 1:4:A:HCS:HA   | 23       | 0.26          |
| (2,264) | 1:13:A:CYS:HB3 | 1:4:A:HCS:HA   | 25       | 0.26          |
| (2,243) | 1:15:A:TYR:H   | 1:15:A:TYR:HB2 | 13       | 0.26          |
| (2,228) | 1:11:A:TRP:HB2 | 1:8:A:ARG:HB2  | 27       | 0.26          |
| (2,198) | 1:8:A:ARG:H    | 1:7:A:HIS:HB2  | 3        | 0.26          |
| (2,198) | 1:8:A:ARG:H    | 1:7:A:HIS:HB2  | 19       | 0.26          |
| (2,198) | 1:8:A:ARG:H    | 1:7:A:HIS:HB2  | 32       | 0.26          |
| (2,16)  | 1:11:A:TRP:HZ3 | 1:8:A:ARG:HD2  | 12       | 0.26          |
| (2,16)  | 1:11:A:TRP:HZ3 | 1:8:A:ARG:HD2  | 29       | 0.26          |
| (2,16)  | 1:11:A:TRP:HZ3 | 1:8:A:ARG:HD2  | 33       | 0.26          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,21)  | 1:4:A:HCS:HG3  | 1:3:A:ILE:HG21 | 7        | 0.26          |
| (1,21)  | 1:4:A:HCS:HG3  | 1:3:A:ILE:HG22 | 7        | 0.26          |
| (1,21)  | 1:4:A:HCS:HG3  | 1:3:A:ILE:HG23 | 7        | 0.26          |
| (1,16)  | 1:7:A:HIS:HD2  | 1:8:A:ARG:HD3  | 35       | 0.26          |
| (1,5)   | 1:11:A:TRP:HD1 | 1:12:A:PRO:HB2 | 2        | 0.26          |
| (3,48)  | 1:11:A:TRP:HE1 | 1:8:A:ARG:HD2  | 15       | 0.25          |
| (2,304) | 1:9:A:PRO:HG2  | 1:8:A:ARG:HA   | 9        | 0.25          |
| (2,264) | 1:13:A:CYS:HB3 | 1:4:A:HCS:HA   | 3        | 0.25          |
| (2,264) | 1:13:A:CYS:HB3 | 1:4:A:HCS:HA   | 17       | 0.25          |
| (2,264) | 1:13:A:CYS:HB3 | 1:4:A:HCS:HA   | 31       | 0.25          |
| (2,243) | 1:15:A:TYR:H   | 1:15:A:TYR:HB2 | 16       | 0.25          |
| (2,228) | 1:11:A:TRP:HB2 | 1:8:A:ARG:HB2  | 19       | 0.25          |
| (2,198) | 1:8:A:ARG:H    | 1:7:A:HIS:HB2  | 4        | 0.25          |
| (2,198) | 1:8:A:ARG:H    | 1:7:A:HIS:HB2  | 15       | 0.25          |
| (2,198) | 1:8:A:ARG:H    | 1:7:A:HIS:HB2  | 33       | 0.25          |
| (2,142) | 1:14:A:TRP:HD1 | 1:13:A:CYS:HB3 | 25       | 0.25          |
| (2,128) | 1:14:A:TRP:HD1 | 1:12:A:PRO:HG3 | 20       | 0.25          |
| (1,21)  | 1:4:A:HCS:HG3  | 1:3:A:ILE:HG21 | 12       | 0.25          |
| (1,21)  | 1:4:A:HCS:HG3  | 1:3:A:ILE:HG22 | 12       | 0.25          |
| (1,21)  | 1:4:A:HCS:HG3  | 1:3:A:ILE:HG23 | 12       | 0.25          |
| (1,21)  | 1:4:A:HCS:HG3  | 1:3:A:ILE:HG21 | 27       | 0.25          |
| (1,21)  | 1:4:A:HCS:HG3  | 1:3:A:ILE:HG22 | 27       | 0.25          |
| (1,21)  | 1:4:A:HCS:HG3  | 1:3:A:ILE:HG23 | 27       | 0.25          |
| (1,18)  | 1:5:A:HIS:HB3  | 1:6:A:VAL:HG21 | 15       | 0.25          |
| (1,18)  | 1:5:A:HIS:HB3  | 1:6:A:VAL:HG22 | 15       | 0.25          |
| (1,18)  | 1:5:A:HIS:HB3  | 1:6:A:VAL:HG23 | 15       | 0.25          |
| (1,18)  | 1:5:A:HIS:HB3  | 1:6:A:VAL:HG21 | 22       | 0.25          |
| (1,18)  | 1:5:A:HIS:HB3  | 1:6:A:VAL:HG22 | 22       | 0.25          |
| (1,18)  | 1:5:A:HIS:HB3  | 1:6:A:VAL:HG23 | 22       | 0.25          |
| (1,16)  | 1:7:A:HIS:HD2  | 1:8:A:ARG:HD3  | 20       | 0.25          |
| (1,10)  | 1:15:A:TYR:HD1 | 1:8:A:ARG:HB2  | 6        | 0.25          |
| (1,10)  | 1:15:A:TYR:HD2 | 1:8:A:ARG:HB2  | 6        | 0.25          |
| (3,48)  | 1:11:A:TRP:HE1 | 1:8:A:ARG:HD2  | 34       | 0.24          |
| (2,294) | 1:10:A:ASP:H   | 1:10:A:ASP:HB2 | 6        | 0.24          |
| (2,264) | 1:13:A:CYS:HB3 | 1:4:A:HCS:HA   | 13       | 0.24          |
| (2,243) | 1:15:A:TYR:H   | 1:15:A:TYR:HB2 | 25       | 0.24          |
| (2,228) | 1:11:A:TRP:HB2 | 1:8:A:ARG:HB2  | 8        | 0.24          |
| (2,228) | 1:11:A:TRP:HB2 | 1:8:A:ARG:HB2  | 13       | 0.24          |
| (2,228) | 1:11:A:TRP:HB2 | 1:8:A:ARG:HB2  | 33       | 0.24          |
| (2,198) | 1:8:A:ARG:H    | 1:7:A:HIS:HB2  | 14       | 0.24          |
| (2,198) | 1:8:A:ARG:H    | 1:7:A:HIS:HB2  | 22       | 0.24          |
| (2,142) | 1:14:A:TRP:HD1 | 1:13:A:CYS:HB3 | 15       | 0.24          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (2,128) | 1:14:A:TRP:HD1 | 1:12:A:PRO:HG3 | 33       | 0.24          |
| (2,98)  | 1:8:A:ARG:HA   | 1:8:A:ARG:HD3  | 3        | 0.24          |
| (2,66)  | 1:2:A:SER:HB3  | 1:13:A:CYS:HB3 | 1        | 0.24          |
| (2,35)  | 1:5:A:HIS:HD2  | 1:13:A:CYS:HB2 | 33       | 0.24          |
| (2,30)  | 1:15:A:TYR:HE1 | 1:13:A:CYS:HB2 | 13       | 0.24          |
| (2,30)  | 1:15:A:TYR:HE2 | 1:13:A:CYS:HB2 | 13       | 0.24          |
| (1,18)  | 1:5:A:HIS:HB3  | 1:6:A:VAL:HG21 | 33       | 0.24          |
| (1,18)  | 1:5:A:HIS:HB3  | 1:6:A:VAL:HG22 | 33       | 0.24          |
| (1,18)  | 1:5:A:HIS:HB3  | 1:6:A:VAL:HG23 | 33       | 0.24          |
| (1,16)  | 1:7:A:HIS:HD2  | 1:8:A:ARG:HD3  | 17       | 0.24          |
| (1,5)   | 1:11:A:TRP:HD1 | 1:12:A:PRO:HB2 | 14       | 0.24          |
| (3,3)   | 1:11:A:TRP:HZ2 | 1:8:A:ARG:HD2  | 18       | 0.23          |
| (2,354) | 1:16:A:ARG:HG3 | 1:16:A:ARG:HB2 | 25       | 0.23          |
| (2,264) | 1:13:A:CYS:HB3 | 1:4:A:HCS:HA   | 24       | 0.23          |
| (2,264) | 1:13:A:CYS:HB3 | 1:4:A:HCS:HA   | 27       | 0.23          |
| (2,264) | 1:13:A:CYS:HB3 | 1:4:A:HCS:HA   | 34       | 0.23          |
| (2,228) | 1:11:A:TRP:HB2 | 1:8:A:ARG:HB2  | 15       | 0.23          |
| (2,228) | 1:11:A:TRP:HB2 | 1:8:A:ARG:HB2  | 21       | 0.23          |
| (2,16)  | 1:11:A:TRP:HZ3 | 1:8:A:ARG:HD2  | 2        | 0.23          |
| (2,16)  | 1:11:A:TRP:HD1 | 1:8:A:ARG:HD2  | 22       | 0.23          |
| (2,16)  | 1:11:A:TRP:HZ3 | 1:8:A:ARG:HD2  | 25       | 0.23          |
| (2,16)  | 1:11:A:TRP:HZ3 | 1:8:A:ARG:HD2  | 35       | 0.23          |
| (1,26)  | 1:9:A:PRO:HD3  | 1:3:A:ILE:HD11 | 33       | 0.23          |
| (1,26)  | 1:9:A:PRO:HD3  | 1:3:A:ILE:HD12 | 33       | 0.23          |
| (1,26)  | 1:9:A:PRO:HD3  | 1:3:A:ILE:HD13 | 33       | 0.23          |
| (1,26)  | 1:9:A:PRO:HD3  | 1:3:A:ILE:HD11 | 35       | 0.23          |
| (1,26)  | 1:9:A:PRO:HD3  | 1:3:A:ILE:HD12 | 35       | 0.23          |
| (1,26)  | 1:9:A:PRO:HD3  | 1:3:A:ILE:HD13 | 35       | 0.23          |
| (1,21)  | 1:4:A:HCS:HG3  | 1:3:A:ILE:HG21 | 21       | 0.23          |
| (1,21)  | 1:4:A:HCS:HG3  | 1:3:A:ILE:HG22 | 21       | 0.23          |
| (1,21)  | 1:4:A:HCS:HG3  | 1:3:A:ILE:HG23 | 21       | 0.23          |
| (1,18)  | 1:5:A:HIS:HB3  | 1:3:A:ILE:HG21 | 1        | 0.23          |
| (1,18)  | 1:5:A:HIS:HB3  | 1:3:A:ILE:HG22 | 1        | 0.23          |
| (1,18)  | 1:5:A:HIS:HB3  | 1:3:A:ILE:HG23 | 1        | 0.23          |
| (1,16)  | 1:7:A:HIS:HD2  | 1:8:A:ARG:HD3  | 12       | 0.23          |
| (2,264) | 1:13:A:CYS:HB3 | 1:4:A:HCS:HA   | 10       | 0.22          |
| (2,264) | 1:13:A:CYS:HB3 | 1:4:A:HCS:HA   | 14       | 0.22          |
| (2,264) | 1:13:A:CYS:HB3 | 1:4:A:HCS:HA   | 18       | 0.22          |
| (2,264) | 1:13:A:CYS:HB3 | 1:4:A:HCS:HA   | 22       | 0.22          |
| (2,228) | 1:11:A:TRP:HB2 | 1:8:A:ARG:HB2  | 6        | 0.22          |
| (2,228) | 1:11:A:TRP:HB2 | 1:8:A:ARG:HB2  | 12       | 0.22          |
| (2,228) | 1:11:A:TRP:HB2 | 1:8:A:ARG:HB2  | 29       | 0.22          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (2,228) | 1:11:A:TRP:HB2 | 1:8:A:ARG:HB2  | 32       | 0.22          |
| (2,198) | 1:8:A:ARG:H    | 1:7:A:HIS:HB2  | 7        | 0.22          |
| (2,198) | 1:8:A:ARG:H    | 1:7:A:HIS:HB2  | 26       | 0.22          |
| (2,198) | 1:8:A:ARG:H    | 1:7:A:HIS:HB2  | 27       | 0.22          |
| (2,198) | 1:8:A:ARG:H    | 1:7:A:HIS:HB2  | 31       | 0.22          |
| (2,198) | 1:8:A:ARG:H    | 1:7:A:HIS:HB2  | 34       | 0.22          |
| (2,198) | 1:8:A:ARG:H    | 1:7:A:HIS:HB2  | 35       | 0.22          |
| (2,128) | 1:14:A:TRP:HD1 | 1:12:A:PRO:HG3 | 26       | 0.22          |
| (2,88)  | 1:7:A:HIS:HB3  | 1:7:A:HIS:HA   | 1        | 0.22          |
| (2,88)  | 1:7:A:HIS:HB3  | 1:7:A:HIS:HA   | 2        | 0.22          |
| (2,88)  | 1:7:A:HIS:HB3  | 1:7:A:HIS:HA   | 3        | 0.22          |
| (2,88)  | 1:7:A:HIS:HB3  | 1:7:A:HIS:HA   | 5        | 0.22          |
| (2,88)  | 1:7:A:HIS:HB3  | 1:7:A:HIS:HA   | 6        | 0.22          |
| (2,88)  | 1:7:A:HIS:HB3  | 1:7:A:HIS:HA   | 7        | 0.22          |
| (2,88)  | 1:7:A:HIS:HB3  | 1:7:A:HIS:HA   | 8        | 0.22          |
| (2,88)  | 1:7:A:HIS:HB3  | 1:7:A:HIS:HA   | 9        | 0.22          |
| (2,88)  | 1:7:A:HIS:HB3  | 1:7:A:HIS:HA   | 10       | 0.22          |
| (2,88)  | 1:7:A:HIS:HB3  | 1:7:A:HIS:HA   | 11       | 0.22          |
| (2,88)  | 1:7:A:HIS:HB3  | 1:7:A:HIS:HA   | 12       | 0.22          |
| (2,88)  | 1:7:A:HIS:HB3  | 1:7:A:HIS:HA   | 13       | 0.22          |
| (2,88)  | 1:7:A:HIS:HB3  | 1:7:A:HIS:HA   | 15       | 0.22          |
| (2,88)  | 1:7:A:HIS:HB3  | 1:7:A:HIS:HA   | 17       | 0.22          |
| (2,88)  | 1:7:A:HIS:HB3  | 1:7:A:HIS:HA   | 19       | 0.22          |
| (2,88)  | 1:7:A:HIS:HB3  | 1:7:A:HIS:HA   | 20       | 0.22          |
| (2,88)  | 1:7:A:HIS:HB3  | 1:7:A:HIS:HA   | 21       | 0.22          |
| (2,88)  | 1:7:A:HIS:HB3  | 1:7:A:HIS:HA   | 22       | 0.22          |
| (2,88)  | 1:7:A:HIS:HB3  | 1:7:A:HIS:HA   | 23       | 0.22          |
| (2,88)  | 1:7:A:HIS:HB3  | 1:7:A:HIS:HA   | 25       | 0.22          |
| (2,88)  | 1:7:A:HIS:HB3  | 1:7:A:HIS:HA   | 26       | 0.22          |
| (2,88)  | 1:7:A:HIS:HB3  | 1:7:A:HIS:HA   | 27       | 0.22          |
| (2,88)  | 1:7:A:HIS:HB3  | 1:7:A:HIS:HA   | 30       | 0.22          |
| (2,88)  | 1:7:A:HIS:HB3  | 1:7:A:HIS:HA   | 31       | 0.22          |
| (2,88)  | 1:7:A:HIS:HB3  | 1:7:A:HIS:HA   | 32       | 0.22          |
| (2,88)  | 1:7:A:HIS:HB3  | 1:7:A:HIS:HA   | 34       | 0.22          |
| (2,88)  | 1:7:A:HIS:HB3  | 1:7:A:HIS:HA   | 35       | 0.22          |
| (2,35)  | 1:5:A:HIS:HD2  | 1:13:A:CYS:HB2 | 5        | 0.22          |
| (2,264) | 1:13:A:CYS:HB3 | 1:4:A:HCS:HA   | 32       | 0.21          |
| (2,228) | 1:11:A:TRP:HB2 | 1:8:A:ARG:HB2  | 4        | 0.21          |
| (2,228) | 1:11:A:TRP:HB2 | 1:8:A:ARG:HB2  | 16       | 0.21          |
| (2,228) | 1:11:A:TRP:HB2 | 1:8:A:ARG:HB2  | 17       | 0.21          |
| (2,228) | 1:11:A:TRP:HB2 | 1:8:A:ARG:HB2  | 18       | 0.21          |
| (2,228) | 1:11:A:TRP:HB2 | 1:8:A:ARG:HB2  | 20       | 0.21          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (2,228) | 1:11:A:TRP:HB2 | 1:8:A:ARG:HB2  | 25       | 0.21          |
| (2,228) | 1:11:A:TRP:HB2 | 1:8:A:ARG:HB2  | 28       | 0.21          |
| (2,228) | 1:11:A:TRP:HB2 | 1:8:A:ARG:HB2  | 31       | 0.21          |
| (2,228) | 1:11:A:TRP:HB2 | 1:8:A:ARG:HB2  | 34       | 0.21          |
| (2,198) | 1:8:A:ARG:H    | 1:7:A:HIS:HB2  | 2        | 0.21          |
| (2,198) | 1:8:A:ARG:H    | 1:7:A:HIS:HB2  | 10       | 0.21          |
| (2,198) | 1:8:A:ARG:H    | 1:7:A:HIS:HB2  | 21       | 0.21          |
| (2,142) | 1:14:A:TRP:HD1 | 1:13:A:CYS:HB3 | 7        | 0.21          |
| (2,128) | 1:14:A:TRP:HD1 | 1:12:A:PRO:HG3 | 16       | 0.21          |
| (2,128) | 1:14:A:TRP:HD1 | 1:12:A:PRO:HG3 | 28       | 0.21          |
| (2,88)  | 1:7:A:HIS:HB3  | 1:7:A:HIS:HA   | 4        | 0.21          |
| (2,88)  | 1:7:A:HIS:HB3  | 1:7:A:HIS:HA   | 14       | 0.21          |
| (2,88)  | 1:7:A:HIS:HB3  | 1:7:A:HIS:HA   | 16       | 0.21          |
| (2,88)  | 1:7:A:HIS:HB3  | 1:7:A:HIS:HA   | 18       | 0.21          |
| (2,88)  | 1:7:A:HIS:HB3  | 1:7:A:HIS:HA   | 24       | 0.21          |
| (2,88)  | 1:7:A:HIS:HB3  | 1:7:A:HIS:HA   | 28       | 0.21          |
| (2,88)  | 1:7:A:HIS:HB3  | 1:7:A:HIS:HA   | 29       | 0.21          |
| (2,88)  | 1:7:A:HIS:HB3  | 1:7:A:HIS:HA   | 33       | 0.21          |
| (2,60)  | 1:6:A:VAL:H    | 1:5:A:HIS:HA   | 8        | 0.21          |
| (2,60)  | 1:6:A:VAL:H    | 1:5:A:HIS:HA   | 21       | 0.21          |
| (1,25)  | 1:9:A:PRO:HD2  | 1:3:A:ILE:HD11 | 19       | 0.21          |
| (1,25)  | 1:9:A:PRO:HD2  | 1:3:A:ILE:HD12 | 19       | 0.21          |
| (1,25)  | 1:9:A:PRO:HD2  | 1:3:A:ILE:HD13 | 19       | 0.21          |
| (1,18)  | 1:5:A:HIS:HB3  | 1:3:A:ILE:HG21 | 24       | 0.21          |
| (1,18)  | 1:5:A:HIS:HB3  | 1:3:A:ILE:HG22 | 24       | 0.21          |
| (1,18)  | 1:5:A:HIS:HB3  | 1:3:A:ILE:HG23 | 24       | 0.21          |
| (1,16)  | 1:7:A:HIS:HD2  | 1:8:A:ARG:HD3  | 14       | 0.21          |
| (1,16)  | 1:7:A:HIS:HD2  | 1:8:A:ARG:HD3  | 28       | 0.21          |
| (1,5)   | 1:11:A:TRP:HD1 | 1:12:A:PRO:HB2 | 4        | 0.21          |
| (1,5)   | 1:11:A:TRP:HD1 | 1:12:A:PRO:HB2 | 20       | 0.21          |
| (2,348) | 1:11:A:TRP:HB2 | 1:8:A:ARG:HG3  | 18       | 0.2           |
| (2,264) | 1:13:A:CYS:HB3 | 1:4:A:HCS:HA   | 6        | 0.2           |
| (2,264) | 1:13:A:CYS:HB3 | 1:4:A:HCS:HA   | 33       | 0.2           |
| (2,243) | 1:15:A:TYR:H   | 1:15:A:TYR:HB2 | 3        | 0.2           |
| (2,243) | 1:15:A:TYR:H   | 1:15:A:TYR:HB2 | 12       | 0.2           |
| (2,243) | 1:15:A:TYR:H   | 1:15:A:TYR:HB2 | 17       | 0.2           |
| (2,228) | 1:11:A:TRP:HB2 | 1:8:A:ARG:HB2  | 5        | 0.2           |
| (2,228) | 1:11:A:TRP:HB2 | 1:8:A:ARG:HB2  | 7        | 0.2           |
| (2,228) | 1:11:A:TRP:HB2 | 1:8:A:ARG:HB2  | 9        | 0.2           |
| (2,228) | 1:11:A:TRP:HB2 | 1:8:A:ARG:HB2  | 10       | 0.2           |
| (2,228) | 1:11:A:TRP:HB2 | 1:8:A:ARG:HB2  | 24       | 0.2           |
| (2,228) | 1:11:A:TRP:HB2 | 1:8:A:ARG:HB2  | 30       | 0.2           |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (2,198) | 1:8:A:ARG:H    | 1:7:A:HIS:HB2  | 1        | 0.2           |
| (2,142) | 1:14:A:TRP:HD1 | 1:13:A:CYS:HB2 | 1        | 0.2           |
| (2,66)  | 1:2:A:SER:HB3  | 1:13:A:CYS:HB3 | 8        | 0.2           |
| (2,60)  | 1:6:A:VAL:H    | 1:5:A:HIS:HA   | 3        | 0.2           |
| (2,60)  | 1:6:A:VAL:H    | 1:5:A:HIS:HA   | 11       | 0.2           |
| (2,60)  | 1:6:A:VAL:H    | 1:5:A:HIS:HA   | 12       | 0.2           |
| (2,60)  | 1:6:A:VAL:H    | 1:5:A:HIS:HA   | 19       | 0.2           |
| (2,60)  | 1:6:A:VAL:H    | 1:5:A:HIS:HA   | 29       | 0.2           |
| (1,32)  | 1:3:A:ILE:HD11 | 1:9:A:PRO:HD3  | 8        | 0.2           |
| (1,32)  | 1:3:A:ILE:HD12 | 1:9:A:PRO:HD3  | 8        | 0.2           |
| (1,32)  | 1:3:A:ILE:HD13 | 1:9:A:PRO:HD3  | 8        | 0.2           |
| (1,21)  | 1:4:A:HCS:HG3  | 1:3:A:ILE:HG21 | 3        | 0.2           |
| (1,21)  | 1:4:A:HCS:HG3  | 1:3:A:ILE:HG22 | 3        | 0.2           |
| (1,21)  | 1:4:A:HCS:HG3  | 1:3:A:ILE:HG23 | 3        | 0.2           |
| (1,18)  | 1:5:A:HIS:HB3  | 1:3:A:ILE:HG21 | 2        | 0.2           |
| (1,18)  | 1:5:A:HIS:HB3  | 1:3:A:ILE:HG22 | 2        | 0.2           |
| (1,18)  | 1:5:A:HIS:HB3  | 1:3:A:ILE:HG23 | 2        | 0.2           |
| (1,10)  | 1:15:A:TYR:HD1 | 1:8:A:ARG:HB2  | 21       | 0.2           |
| (1,10)  | 1:15:A:TYR:HD2 | 1:8:A:ARG:HB2  | 21       | 0.2           |
| (1,5)   | 1:11:A:TRP:HD1 | 1:12:A:PRO:HB2 | 6        | 0.2           |
| (1,5)   | 1:11:A:TRP:HD1 | 1:12:A:PRO:HB2 | 10       | 0.2           |
| (1,5)   | 1:11:A:TRP:HD1 | 1:12:A:PRO:HB2 | 17       | 0.2           |
| (1,5)   | 1:11:A:TRP:HD1 | 1:12:A:PRO:HB2 | 35       | 0.2           |
| (3,25)  | 1:5:A:HIS:H    | 1:3:A:ILE:HG13 | 12       | 0.19          |
| (2,300) | 1:11:A:TRP:HD1 | 1:13:A:CYS:HB3 | 5        | 0.19          |
| (2,294) | 1:10:A:ASP:H   | 1:10:A:ASP:HB2 | 4        | 0.19          |
| (2,294) | 1:10:A:ASP:H   | 1:10:A:ASP:HB2 | 5        | 0.19          |
| (2,294) | 1:10:A:ASP:H   | 1:10:A:ASP:HB2 | 30       | 0.19          |
| (2,264) | 1:13:A:CYS:HB3 | 1:4:A:HCS:HA   | 35       | 0.19          |
| (2,243) | 1:15:A:TYR:H   | 1:15:A:TYR:HB2 | 1        | 0.19          |
| (2,243) | 1:15:A:TYR:H   | 1:15:A:TYR:HB2 | 7        | 0.19          |
| (2,243) | 1:15:A:TYR:H   | 1:15:A:TYR:HB2 | 9        | 0.19          |
| (2,243) | 1:15:A:TYR:H   | 1:15:A:TYR:HB2 | 11       | 0.19          |
| (2,243) | 1:15:A:TYR:H   | 1:15:A:TYR:HB2 | 18       | 0.19          |
| (2,243) | 1:15:A:TYR:H   | 1:15:A:TYR:HB2 | 19       | 0.19          |
| (2,243) | 1:15:A:TYR:H   | 1:15:A:TYR:HB2 | 23       | 0.19          |
| (2,243) | 1:15:A:TYR:H   | 1:15:A:TYR:HB2 | 26       | 0.19          |
| (2,243) | 1:15:A:TYR:H   | 1:15:A:TYR:HB2 | 27       | 0.19          |
| (2,243) | 1:15:A:TYR:H   | 1:15:A:TYR:HB2 | 28       | 0.19          |
| (2,243) | 1:15:A:TYR:H   | 1:15:A:TYR:HB2 | 29       | 0.19          |
| (2,243) | 1:15:A:TYR:H   | 1:15:A:TYR:HB2 | 34       | 0.19          |
| (2,228) | 1:11:A:TRP:HB2 | 1:8:A:ARG:HB2  | 1        | 0.19          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (2,228) | 1:11:A:TRP:HB2 | 1:8:A:ARG:HB2  | 14       | 0.19          |
| (2,198) | 1:8:A:ARG:H    | 1:7:A:HIS:HB2  | 5        | 0.19          |
| (2,198) | 1:8:A:ARG:H    | 1:7:A:HIS:HB2  | 9        | 0.19          |
| (2,198) | 1:8:A:ARG:H    | 1:7:A:HIS:HB2  | 13       | 0.19          |
| (2,198) | 1:8:A:ARG:H    | 1:7:A:HIS:HB2  | 20       | 0.19          |
| (2,142) | 1:14:A:TRP:HD1 | 1:13:A:CYS:HB3 | 9        | 0.19          |
| (2,142) | 1:14:A:TRP:HD1 | 1:13:A:CYS:HB3 | 18       | 0.19          |
| (2,60)  | 1:6:A:VAL:H    | 1:5:A:HIS:HA   | 6        | 0.19          |
| (1,18)  | 1:5:A:HIS:HB3  | 1:3:A:ILE:HG21 | 18       | 0.19          |
| (1,18)  | 1:5:A:HIS:HB3  | 1:3:A:ILE:HG22 | 18       | 0.19          |
| (1,18)  | 1:5:A:HIS:HB3  | 1:3:A:ILE:HG23 | 18       | 0.19          |
| (1,5)   | 1:11:A:TRP:HD1 | 1:12:A:PRO:HB2 | 21       | 0.19          |
| (1,5)   | 1:11:A:TRP:HD1 | 1:12:A:PRO:HB2 | 24       | 0.19          |
| (1,5)   | 1:11:A:TRP:HD1 | 1:12:A:PRO:HB2 | 30       | 0.19          |
| (2,354) | 1:16:A:ARG:HG3 | 1:16:A:ARG:HB2 | 31       | 0.18          |
| (2,300) | 1:11:A:TRP:HD1 | 1:13:A:CYS:HB3 | 3        | 0.18          |
| (2,294) | 1:10:A:ASP:H   | 1:10:A:ASP:HB2 | 7        | 0.18          |
| (2,294) | 1:10:A:ASP:H   | 1:10:A:ASP:HB2 | 33       | 0.18          |
| (2,264) | 1:13:A:CYS:HB3 | 1:4:A:HCS:HA   | 9        | 0.18          |
| (2,243) | 1:15:A:TYR:H   | 1:15:A:TYR:HB2 | 4        | 0.18          |
| (2,243) | 1:15:A:TYR:H   | 1:15:A:TYR:HB2 | 5        | 0.18          |
| (2,243) | 1:15:A:TYR:H   | 1:15:A:TYR:HB2 | 8        | 0.18          |
| (2,243) | 1:15:A:TYR:H   | 1:15:A:TYR:HB2 | 15       | 0.18          |
| (2,243) | 1:15:A:TYR:H   | 1:15:A:TYR:HB2 | 20       | 0.18          |
| (2,243) | 1:15:A:TYR:H   | 1:15:A:TYR:HB2 | 30       | 0.18          |
| (2,243) | 1:15:A:TYR:H   | 1:15:A:TYR:HB2 | 31       | 0.18          |
| (2,243) | 1:15:A:TYR:H   | 1:15:A:TYR:HB2 | 35       | 0.18          |
| (2,228) | 1:11:A:TRP:HB2 | 1:8:A:ARG:HB2  | 2        | 0.18          |
| (2,228) | 1:11:A:TRP:HB2 | 1:8:A:ARG:HB2  | 23       | 0.18          |
| (2,228) | 1:11:A:TRP:HB2 | 1:8:A:ARG:HB2  | 26       | 0.18          |
| (2,198) | 1:8:A:ARG:H    | 1:7:A:HIS:HB2  | 6        | 0.18          |
| (2,198) | 1:8:A:ARG:H    | 1:7:A:HIS:HB2  | 17       | 0.18          |
| (2,198) | 1:8:A:ARG:H    | 1:7:A:HIS:HB2  | 23       | 0.18          |
| (2,193) | 1:7:A:HIS:HD2  | 1:8:A:ARG:HB3  | 18       | 0.18          |
| (2,180) | 1:14:A:TRP:HZ3 | 1:15:A:TYR:HB3 | 16       | 0.18          |
| (2,142) | 1:14:A:TRP:HD1 | 1:13:A:CYS:HB3 | 35       | 0.18          |
| (1,21)  | 1:4:A:HCS:HG3  | 1:3:A:ILE:HG21 | 20       | 0.18          |
| (1,21)  | 1:4:A:HCS:HG3  | 1:3:A:ILE:HG22 | 20       | 0.18          |
| (1,21)  | 1:4:A:HCS:HG3  | 1:3:A:ILE:HG23 | 20       | 0.18          |
| (1,18)  | 1:5:A:HIS:HB3  | 1:3:A:ILE:HG21 | 28       | 0.18          |
| (1,18)  | 1:5:A:HIS:HB3  | 1:3:A:ILE:HG22 | 28       | 0.18          |
| (1,18)  | 1:5:A:HIS:HB3  | 1:3:A:ILE:HG23 | 28       | 0.18          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,10)  | 1:15:A:TYR:HD1 | 1:8:A:ARG:HB2  | 14       | 0.18          |
| (1,10)  | 1:15:A:TYR:HD2 | 1:8:A:ARG:HB2  | 14       | 0.18          |
| (1,5)   | 1:11:A:TRP:HD1 | 1:12:A:PRO:HB2 | 22       | 0.18          |
| (1,5)   | 1:11:A:TRP:HD1 | 1:12:A:PRO:HB2 | 32       | 0.18          |
| (2,294) | 1:10:A:ASP:H   | 1:10:A:ASP:HB2 | 12       | 0.17          |
| (2,294) | 1:10:A:ASP:H   | 1:10:A:ASP:HB2 | 31       | 0.17          |
| (2,264) | 1:13:A:CYS:HB3 | 1:4:A:HCS:HA   | 15       | 0.17          |
| (2,243) | 1:15:A:TYR:H   | 1:15:A:TYR:HB2 | 2        | 0.17          |
| (2,243) | 1:15:A:TYR:H   | 1:15:A:TYR:HB2 | 6        | 0.17          |
| (2,243) | 1:15:A:TYR:H   | 1:15:A:TYR:HB2 | 10       | 0.17          |
| (2,243) | 1:15:A:TYR:H   | 1:15:A:TYR:HB2 | 14       | 0.17          |
| (2,243) | 1:15:A:TYR:H   | 1:15:A:TYR:HB2 | 22       | 0.17          |
| (2,243) | 1:15:A:TYR:H   | 1:15:A:TYR:HB2 | 24       | 0.17          |
| (2,243) | 1:15:A:TYR:H   | 1:15:A:TYR:HB2 | 32       | 0.17          |
| (2,243) | 1:15:A:TYR:H   | 1:15:A:TYR:HB2 | 33       | 0.17          |
| (2,198) | 1:8:A:ARG:H    | 1:7:A:HIS:HB2  | 11       | 0.17          |
| (2,198) | 1:8:A:ARG:H    | 1:7:A:HIS:HB2  | 30       | 0.17          |
| (2,180) | 1:14:A:TRP:HZ3 | 1:15:A:TYR:HB3 | 18       | 0.17          |
| (2,179) | 1:14:A:TRP:HD1 | 1:12:A:PRO:HB3 | 12       | 0.17          |
| (2,179) | 1:14:A:TRP:HD1 | 1:12:A:PRO:HB3 | 16       | 0.17          |
| (2,179) | 1:14:A:TRP:HD1 | 1:12:A:PRO:HB3 | 34       | 0.17          |
| (2,128) | 1:14:A:TRP:HD1 | 1:12:A:PRO:HG3 | 2        | 0.17          |
| (2,128) | 1:14:A:TRP:HD1 | 1:12:A:PRO:HG3 | 3        | 0.17          |
| (2,99)  | 1:14:A:TRP:H   | 1:13:A:CYS:HB2 | 32       | 0.17          |
| (2,30)  | 1:15:A:TYR:HE1 | 1:13:A:CYS:HB2 | 7        | 0.17          |
| (2,30)  | 1:15:A:TYR:HE2 | 1:13:A:CYS:HB2 | 7        | 0.17          |
| (1,21)  | 1:4:A:HCS:HG3  | 1:3:A:ILE:HG21 | 24       | 0.17          |
| (1,21)  | 1:4:A:HCS:HG3  | 1:3:A:ILE:HG22 | 24       | 0.17          |
| (1,21)  | 1:4:A:HCS:HG3  | 1:3:A:ILE:HG23 | 24       | 0.17          |
| (1,10)  | 1:15:A:TYR:HD1 | 1:8:A:ARG:HB2  | 3        | 0.17          |
| (1,10)  | 1:15:A:TYR:HD2 | 1:8:A:ARG:HB2  | 3        | 0.17          |
| (1,10)  | 1:15:A:TYR:HD1 | 1:8:A:ARG:HB2  | 24       | 0.17          |
| (1,10)  | 1:15:A:TYR:HD2 | 1:8:A:ARG:HB2  | 24       | 0.17          |
| (1,10)  | 1:15:A:TYR:HD1 | 1:8:A:ARG:HB2  | 31       | 0.17          |
| (1,10)  | 1:15:A:TYR:HD2 | 1:8:A:ARG:HB2  | 31       | 0.17          |
| (1,5)   | 1:11:A:TRP:HD1 | 1:12:A:PRO:HB2 | 8        | 0.17          |
| (1,5)   | 1:11:A:TRP:HD1 | 1:12:A:PRO:HB2 | 13       | 0.17          |
| (1,5)   | 1:11:A:TRP:HD1 | 1:12:A:PRO:HB2 | 19       | 0.17          |
| (1,5)   | 1:11:A:TRP:HD1 | 1:12:A:PRO:HB2 | 25       | 0.17          |
| (2,354) | 1:16:A:ARG:HG3 | 1:16:A:ARG:HB2 | 27       | 0.16          |
| (2,294) | 1:10:A:ASP:H   | 1:10:A:ASP:HB2 | 18       | 0.16          |
| (2,294) | 1:10:A:ASP:H   | 1:10:A:ASP:HB2 | 19       | 0.16          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (2,294) | 1:10:A:ASP:H   | 1:10:A:ASP:HB2 | 29       | 0.16          |
| (2,243) | 1:15:A:TYR:H   | 1:15:A:TYR:HB2 | 21       | 0.16          |
| (2,228) | 1:11:A:TRP:HB2 | 1:8:A:ARG:HB2  | 35       | 0.16          |
| (2,198) | 1:8:A:ARG:H    | 1:7:A:HIS:HB2  | 12       | 0.16          |
| (2,198) | 1:8:A:ARG:H    | 1:7:A:HIS:HB2  | 24       | 0.16          |
| (2,193) | 1:7:A:HIS:HD2  | 1:8:A:ARG:HB3  | 31       | 0.16          |
| (2,180) | 1:14:A:TRP:HZ3 | 1:15:A:TYR:HB3 | 3        | 0.16          |
| (2,180) | 1:14:A:TRP:HZ3 | 1:15:A:TYR:HB3 | 27       | 0.16          |
| (2,179) | 1:14:A:TRP:HD1 | 1:12:A:PRO:HB3 | 13       | 0.16          |
| (2,179) | 1:14:A:TRP:HD1 | 1:12:A:PRO:HB3 | 21       | 0.16          |
| (2,142) | 1:14:A:TRP:HD1 | 1:13:A:CYS:HB3 | 24       | 0.16          |
| (2,128) | 1:14:A:TRP:HD1 | 1:12:A:PRO:HG3 | 7        | 0.16          |
| (2,99)  | 1:14:A:TRP:H   | 1:13:A:CYS:HB2 | 19       | 0.16          |
| (2,99)  | 1:14:A:TRP:H   | 1:13:A:CYS:HB2 | 29       | 0.16          |
| (2,99)  | 1:14:A:TRP:H   | 1:13:A:CYS:HB2 | 35       | 0.16          |
| (2,30)  | 1:15:A:TYR:HE1 | 1:13:A:CYS:HB2 | 1        | 0.16          |
| (2,30)  | 1:15:A:TYR:HE2 | 1:13:A:CYS:HB2 | 1        | 0.16          |
| (2,30)  | 1:15:A:TYR:HE1 | 1:13:A:CYS:HB2 | 24       | 0.16          |
| (2,30)  | 1:15:A:TYR:HE2 | 1:13:A:CYS:HB2 | 24       | 0.16          |
| (1,29)  | 1:11:A:TRP:HD1 | 1:1:A:PRO:HG3  | 17       | 0.16          |
| (1,10)  | 1:15:A:TYR:HD1 | 1:8:A:ARG:HB2  | 8        | 0.16          |
| (1,10)  | 1:15:A:TYR:HD2 | 1:8:A:ARG:HB2  | 8        | 0.16          |
| (1,10)  | 1:15:A:TYR:HD1 | 1:8:A:ARG:HB2  | 11       | 0.16          |
| (1,10)  | 1:15:A:TYR:HD2 | 1:8:A:ARG:HB2  | 11       | 0.16          |
| (1,10)  | 1:15:A:TYR:HD1 | 1:8:A:ARG:HB2  | 32       | 0.16          |
| (1,10)  | 1:15:A:TYR:HD2 | 1:8:A:ARG:HB2  | 32       | 0.16          |
| (1,5)   | 1:11:A:TRP:HD1 | 1:12:A:PRO:HB2 | 7        | 0.16          |
| (1,5)   | 1:11:A:TRP:HD1 | 1:12:A:PRO:HB2 | 12       | 0.16          |
| (1,5)   | 1:11:A:TRP:HD1 | 1:12:A:PRO:HB2 | 16       | 0.16          |
| (1,5)   | 1:11:A:TRP:HD1 | 1:12:A:PRO:HB2 | 26       | 0.16          |
| (1,5)   | 1:11:A:TRP:HD1 | 1:12:A:PRO:HB2 | 31       | 0.16          |
| (1,5)   | 1:11:A:TRP:HD1 | 1:12:A:PRO:HB2 | 33       | 0.16          |
| (2,294) | 1:10:A:ASP:H   | 1:10:A:ASP:HB2 | 10       | 0.15          |
| (2,294) | 1:10:A:ASP:H   | 1:10:A:ASP:HB2 | 32       | 0.15          |
| (2,198) | 1:8:A:ARG:H    | 1:7:A:HIS:HB2  | 25       | 0.15          |
| (2,193) | 1:7:A:HIS:HD2  | 1:8:A:ARG:HB3  | 7        | 0.15          |
| (2,193) | 1:7:A:HIS:HD2  | 1:8:A:ARG:HB3  | 30       | 0.15          |
| (2,193) | 1:7:A:HIS:HD2  | 1:8:A:ARG:HB3  | 32       | 0.15          |
| (2,179) | 1:14:A:TRP:HD1 | 1:12:A:PRO:HB3 | 1        | 0.15          |
| (2,179) | 1:14:A:TRP:HD1 | 1:12:A:PRO:HB3 | 2        | 0.15          |
| (2,179) | 1:14:A:TRP:HD1 | 1:12:A:PRO:HB3 | 3        | 0.15          |
| (2,179) | 1:14:A:TRP:HD1 | 1:12:A:PRO:HB3 | 17       | 0.15          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (2,179) | 1:14:A:TRP:HD1 | 1:12:A:PRO:HB3 | 26       | 0.15          |
| (2,179) | 1:14:A:TRP:HD1 | 1:12:A:PRO:HB3 | 30       | 0.15          |
| (2,179) | 1:14:A:TRP:HD1 | 1:12:A:PRO:HB3 | 33       | 0.15          |
| (2,179) | 1:14:A:TRP:HD1 | 1:12:A:PRO:HB3 | 35       | 0.15          |
| (2,142) | 1:14:A:TRP:HD1 | 1:13:A:CYS:HB3 | 33       | 0.15          |
| (2,128) | 1:14:A:TRP:HD1 | 1:12:A:PRO:HG3 | 11       | 0.15          |
| (2,99)  | 1:14:A:TRP:H   | 1:13:A:CYS:HB2 | 10       | 0.15          |
| (2,99)  | 1:14:A:TRP:H   | 1:13:A:CYS:HB2 | 17       | 0.15          |
| (2,99)  | 1:14:A:TRP:H   | 1:13:A:CYS:HB2 | 21       | 0.15          |
| (2,99)  | 1:14:A:TRP:H   | 1:13:A:CYS:HB2 | 26       | 0.15          |
| (1,26)  | 1:9:A:PRO:HD3  | 1:3:A:ILE:HG21 | 29       | 0.15          |
| (1,26)  | 1:9:A:PRO:HD3  | 1:3:A:ILE:HG22 | 29       | 0.15          |
| (1,26)  | 1:9:A:PRO:HD3  | 1:3:A:ILE:HG23 | 29       | 0.15          |
| (1,10)  | 1:15:A:TYR:HD1 | 1:8:A:ARG:HB2  | 35       | 0.15          |
| (1,10)  | 1:15:A:TYR:HD2 | 1:8:A:ARG:HB2  | 35       | 0.15          |
| (1,5)   | 1:11:A:TRP:HD1 | 1:12:A:PRO:HB2 | 29       | 0.15          |
| (3,45)  | 1:13:A:CYS:HA  | 1:4:A:HCS:HG2  | 12       | 0.14          |
| (3,45)  | 1:13:A:CYS:HA  | 1:4:A:HCS:HG2  | 21       | 0.14          |
| (3,45)  | 1:13:A:CYS:HA  | 1:4:A:HCS:HG2  | 32       | 0.14          |
| (3,45)  | 1:13:A:CYS:HA  | 1:4:A:HCS:HG2  | 34       | 0.14          |
| (2,294) | 1:10:A:ASP:H   | 1:10:A:ASP:HB2 | 16       | 0.14          |
| (2,193) | 1:7:A:HIS:HD2  | 1:8:A:ARG:HB3  | 11       | 0.14          |
| (2,180) | 1:14:A:TRP:HZ3 | 1:15:A:TYR:HB3 | 23       | 0.14          |
| (2,180) | 1:14:A:TRP:HZ3 | 1:15:A:TYR:HB3 | 26       | 0.14          |
| (2,179) | 1:14:A:TRP:HD1 | 1:12:A:PRO:HB3 | 5        | 0.14          |
| (2,179) | 1:14:A:TRP:HD1 | 1:12:A:PRO:HB3 | 6        | 0.14          |
| (2,179) | 1:14:A:TRP:HD1 | 1:12:A:PRO:HB3 | 8        | 0.14          |
| (2,179) | 1:14:A:TRP:HD1 | 1:12:A:PRO:HB3 | 18       | 0.14          |
| (2,179) | 1:14:A:TRP:HD1 | 1:12:A:PRO:HB3 | 20       | 0.14          |
| (2,179) | 1:14:A:TRP:HD1 | 1:12:A:PRO:HB3 | 23       | 0.14          |
| (2,179) | 1:14:A:TRP:HD1 | 1:12:A:PRO:HB3 | 25       | 0.14          |
| (2,179) | 1:14:A:TRP:HD1 | 1:12:A:PRO:HB3 | 28       | 0.14          |
| (2,179) | 1:14:A:TRP:HD1 | 1:12:A:PRO:HB3 | 32       | 0.14          |
| (2,99)  | 1:14:A:TRP:H   | 1:13:A:CYS:HB2 | 8        | 0.14          |
| (2,99)  | 1:14:A:TRP:H   | 1:13:A:CYS:HB2 | 11       | 0.14          |
| (2,99)  | 1:14:A:TRP:H   | 1:13:A:CYS:HB2 | 14       | 0.14          |
| (2,99)  | 1:14:A:TRP:H   | 1:13:A:CYS:HB2 | 28       | 0.14          |
| (2,66)  | 1:2:A:SER:HB3  | 1:13:A:CYS:HB3 | 21       | 0.14          |
| (2,48)  | 1:13:A:CYS:HB3 | 1:2:A:SER:HB2  | 20       | 0.14          |
| (2,30)  | 1:15:A:TYR:HE1 | 1:13:A:CYS:HB2 | 22       | 0.14          |
| (2,30)  | 1:15:A:TYR:HE2 | 1:13:A:CYS:HB2 | 22       | 0.14          |
| (1,26)  | 1:9:A:PRO:HD3  | 1:3:A:ILE:HD11 | 30       | 0.14          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,26)  | 1:9:A:PRO:HD3  | 1:3:A:ILE:HD12 | 30       | 0.14          |
| (1,26)  | 1:9:A:PRO:HD3  | 1:3:A:ILE:HD13 | 30       | 0.14          |
| (1,18)  | 1:5:A:HIS:HB3  | 1:3:A:ILE:HG21 | 25       | 0.14          |
| (1,18)  | 1:5:A:HIS:HB3  | 1:3:A:ILE:HG22 | 25       | 0.14          |
| (1,18)  | 1:5:A:HIS:HB3  | 1:3:A:ILE:HG23 | 25       | 0.14          |
| (1,10)  | 1:15:A:TYR:HD1 | 1:8:A:ARG:HB2  | 30       | 0.14          |
| (1,10)  | 1:15:A:TYR:HD2 | 1:8:A:ARG:HB2  | 30       | 0.14          |
| (1,5)   | 1:11:A:TRP:HD1 | 1:12:A:PRO:HB2 | 11       | 0.14          |
| (3,45)  | 1:13:A:CYS:HA  | 1:4:A:HCS:HG2  | 7        | 0.13          |
| (3,45)  | 1:13:A:CYS:HA  | 1:4:A:HCS:HG2  | 14       | 0.13          |
| (3,45)  | 1:13:A:CYS:HA  | 1:4:A:HCS:HG2  | 15       | 0.13          |
| (3,45)  | 1:13:A:CYS:HA  | 1:4:A:HCS:HG2  | 18       | 0.13          |
| (3,45)  | 1:13:A:CYS:HA  | 1:4:A:HCS:HG2  | 20       | 0.13          |
| (3,45)  | 1:13:A:CYS:HA  | 1:4:A:HCS:HG2  | 22       | 0.13          |
| (3,45)  | 1:13:A:CYS:HA  | 1:4:A:HCS:HG2  | 35       | 0.13          |
| (3,10)  | 1:11:A:TRP:HE3 | 1:7:A:HIS:HD2  | 6        | 0.13          |
| (2,180) | 1:14:A:TRP:HZ3 | 1:15:A:TYR:HB3 | 7        | 0.13          |
| (2,180) | 1:14:A:TRP:HZ3 | 1:15:A:TYR:HB3 | 13       | 0.13          |
| (2,180) | 1:14:A:TRP:HZ3 | 1:15:A:TYR:HB3 | 29       | 0.13          |
| (2,180) | 1:14:A:TRP:HZ3 | 1:15:A:TYR:HB3 | 34       | 0.13          |
| (2,179) | 1:14:A:TRP:HD1 | 1:12:A:PRO:HB3 | 4        | 0.13          |
| (2,179) | 1:14:A:TRP:HD1 | 1:12:A:PRO:HB3 | 7        | 0.13          |
| (2,179) | 1:14:A:TRP:HD1 | 1:12:A:PRO:HB3 | 9        | 0.13          |
| (2,179) | 1:14:A:TRP:HD1 | 1:12:A:PRO:HB3 | 10       | 0.13          |
| (2,179) | 1:14:A:TRP:HD1 | 1:12:A:PRO:HB3 | 14       | 0.13          |
| (2,179) | 1:14:A:TRP:HD1 | 1:12:A:PRO:HB3 | 15       | 0.13          |
| (2,179) | 1:14:A:TRP:HD1 | 1:12:A:PRO:HB3 | 22       | 0.13          |
| (2,179) | 1:14:A:TRP:HD1 | 1:12:A:PRO:HB3 | 27       | 0.13          |
| (2,179) | 1:14:A:TRP:HD1 | 1:12:A:PRO:HB3 | 29       | 0.13          |
| (2,179) | 1:14:A:TRP:HD1 | 1:12:A:PRO:HB3 | 31       | 0.13          |
| (2,128) | 1:14:A:TRP:HD1 | 1:12:A:PRO:HG3 | 13       | 0.13          |
| (2,128) | 1:14:A:TRP:HD1 | 1:12:A:PRO:HG3 | 21       | 0.13          |
| (2,128) | 1:14:A:TRP:HD1 | 1:12:A:PRO:HG3 | 25       | 0.13          |
| (2,128) | 1:14:A:TRP:HD1 | 1:12:A:PRO:HG3 | 34       | 0.13          |
| (2,99)  | 1:14:A:TRP:H   | 1:13:A:CYS:HB2 | 3        | 0.13          |
| (2,99)  | 1:14:A:TRP:H   | 1:13:A:CYS:HB2 | 4        | 0.13          |
| (2,99)  | 1:14:A:TRP:H   | 1:13:A:CYS:HB2 | 6        | 0.13          |
| (2,99)  | 1:14:A:TRP:H   | 1:13:A:CYS:HB2 | 7        | 0.13          |
| (2,99)  | 1:14:A:TRP:H   | 1:13:A:CYS:HB2 | 12       | 0.13          |
| (2,99)  | 1:14:A:TRP:H   | 1:13:A:CYS:HB2 | 27       | 0.13          |
| (2,99)  | 1:14:A:TRP:H   | 1:13:A:CYS:HB2 | 30       | 0.13          |
| (2,99)  | 1:14:A:TRP:H   | 1:13:A:CYS:HB2 | 31       | 0.13          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (2,30)  | 1:15:A:TYR:HE1 | 1:13:A:CYS:HB2 | 34       | 0.13          |
| (2,30)  | 1:15:A:TYR:HE2 | 1:13:A:CYS:HB2 | 34       | 0.13          |
| (1,5)   | 1:11:A:TRP:HD1 | 1:12:A:PRO:HB2 | 5        | 0.13          |
| (1,5)   | 1:11:A:TRP:HD1 | 1:12:A:PRO:HB2 | 15       | 0.13          |
| (1,5)   | 1:11:A:TRP:HD1 | 1:12:A:PRO:HB2 | 18       | 0.13          |
| (1,5)   | 1:11:A:TRP:HD1 | 1:12:A:PRO:HB2 | 23       | 0.13          |
| (3,45)  | 1:13:A:CYS:HA  | 1:4:A:HCS:HG2  | 1        | 0.12          |
| (3,45)  | 1:13:A:CYS:HA  | 1:4:A:HCS:HG2  | 3        | 0.12          |
| (3,45)  | 1:13:A:CYS:HA  | 1:4:A:HCS:HG2  | 4        | 0.12          |
| (3,45)  | 1:13:A:CYS:HA  | 1:4:A:HCS:HG2  | 8        | 0.12          |
| (3,45)  | 1:13:A:CYS:HA  | 1:4:A:HCS:HG2  | 9        | 0.12          |
| (3,45)  | 1:13:A:CYS:HA  | 1:4:A:HCS:HG2  | 11       | 0.12          |
| (3,45)  | 1:13:A:CYS:HA  | 1:4:A:HCS:HG2  | 17       | 0.12          |
| (3,45)  | 1:13:A:CYS:HA  | 1:4:A:HCS:HG2  | 26       | 0.12          |
| (3,45)  | 1:13:A:CYS:HA  | 1:4:A:HCS:HG2  | 27       | 0.12          |
| (3,45)  | 1:13:A:CYS:HA  | 1:4:A:HCS:HG2  | 28       | 0.12          |
| (3,45)  | 1:13:A:CYS:HA  | 1:4:A:HCS:HG2  | 29       | 0.12          |
| (3,6)   | 1:14:A:TRP:HD1 | 1:16:A:ARG:HD3 | 16       | 0.12          |
| (2,354) | 1:16:A:ARG:HG3 | 1:16:A:ARG:HB2 | 32       | 0.12          |
| (2,193) | 1:7:A:HIS:HD2  | 1:8:A:ARG:HB3  | 21       | 0.12          |
| (2,180) | 1:14:A:TRP:HZ3 | 1:15:A:TYR:HB3 | 19       | 0.12          |
| (2,179) | 1:14:A:TRP:HD1 | 1:12:A:PRO:HB3 | 11       | 0.12          |
| (2,179) | 1:14:A:TRP:HD1 | 1:12:A:PRO:HB3 | 24       | 0.12          |
| (2,142) | 1:14:A:TRP:HD1 | 1:13:A:CYS:HB3 | 20       | 0.12          |
| (2,139) | 1:14:A:TRP:HD1 | 1:13:A:CYS:HA  | 19       | 0.12          |
| (2,128) | 1:14:A:TRP:HD1 | 1:12:A:PRO:HG3 | 1        | 0.12          |
| (2,100) | 1:8:A:ARG:H    | 1:8:A:ARG:HD3  | 28       | 0.12          |
| (2,99)  | 1:14:A:TRP:H   | 1:13:A:CYS:HB2 | 5        | 0.12          |
| (2,99)  | 1:14:A:TRP:H   | 1:13:A:CYS:HB2 | 16       | 0.12          |
| (2,99)  | 1:14:A:TRP:H   | 1:13:A:CYS:HB2 | 20       | 0.12          |
| (2,99)  | 1:14:A:TRP:H   | 1:13:A:CYS:HB2 | 22       | 0.12          |
| (2,99)  | 1:14:A:TRP:H   | 1:13:A:CYS:HB2 | 23       | 0.12          |
| (2,99)  | 1:14:A:TRP:H   | 1:13:A:CYS:HB2 | 24       | 0.12          |
| (2,30)  | 1:15:A:TYR:HE1 | 1:13:A:CYS:HB2 | 25       | 0.12          |
| (2,30)  | 1:15:A:TYR:HE2 | 1:13:A:CYS:HB2 | 25       | 0.12          |
| (2,13)  | 1:11:A:TRP:HH2 | 1:6:A:VAL:HG11 | 1        | 0.12          |
| (2,13)  | 1:11:A:TRP:HH2 | 1:6:A:VAL:HG12 | 1        | 0.12          |
| (2,13)  | 1:11:A:TRP:HH2 | 1:6:A:VAL:HG13 | 1        | 0.12          |
| (1,24)  | 1:6:A:VAL:HA   | 1:7:A:HIS:HB2  | 29       | 0.12          |
| (1,18)  | 1:5:A:HIS:HB3  | 1:3:A:ILE:HG21 | 7        | 0.12          |
| (1,18)  | 1:5:A:HIS:HB3  | 1:3:A:ILE:HG22 | 7        | 0.12          |
| (1,18)  | 1:5:A:HIS:HB3  | 1:3:A:ILE:HG23 | 7        | 0.12          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,18)  | 1:5:A:HIS:HB3  | 1:3:A:ILE:HG21 | 16       | 0.12          |
| (1,18)  | 1:5:A:HIS:HB3  | 1:3:A:ILE:HG22 | 16       | 0.12          |
| (1,18)  | 1:5:A:HIS:HB3  | 1:3:A:ILE:HG23 | 16       | 0.12          |
| (1,18)  | 1:5:A:HIS:HB3  | 1:3:A:ILE:HG21 | 26       | 0.12          |
| (1,18)  | 1:5:A:HIS:HB3  | 1:3:A:ILE:HG22 | 26       | 0.12          |
| (1,18)  | 1:5:A:HIS:HB3  | 1:3:A:ILE:HG23 | 26       | 0.12          |
| (1,10)  | 1:15:A:TYR:HD1 | 1:8:A:ARG:HB2  | 5        | 0.12          |
| (1,10)  | 1:15:A:TYR:HD2 | 1:8:A:ARG:HB2  | 5        | 0.12          |
| (1,10)  | 1:15:A:TYR:HD1 | 1:8:A:ARG:HB2  | 9        | 0.12          |
| (1,10)  | 1:15:A:TYR:HD2 | 1:8:A:ARG:HB2  | 9        | 0.12          |
| (1,10)  | 1:15:A:TYR:HD1 | 1:8:A:ARG:HB2  | 17       | 0.12          |
| (1,10)  | 1:15:A:TYR:HD2 | 1:8:A:ARG:HB2  | 17       | 0.12          |
| (1,10)  | 1:15:A:TYR:HD1 | 1:8:A:ARG:HB2  | 27       | 0.12          |
| (1,10)  | 1:15:A:TYR:HD2 | 1:8:A:ARG:HB2  | 27       | 0.12          |
| (1,10)  | 1:15:A:TYR:HD1 | 1:8:A:ARG:HB2  | 28       | 0.12          |
| (1,10)  | 1:15:A:TYR:HD2 | 1:8:A:ARG:HB2  | 28       | 0.12          |
| (1,5)   | 1:11:A:TRP:HD1 | 1:12:A:PRO:HB2 | 27       | 0.12          |
| (1,5)   | 1:11:A:TRP:HD1 | 1:12:A:PRO:HB2 | 34       | 0.12          |
| (3,45)  | 1:13:A:CYS:HA  | 1:4:A:HCS:HG2  | 6        | 0.11          |
| (3,45)  | 1:13:A:CYS:HA  | 1:4:A:HCS:HG2  | 10       | 0.11          |
| (3,45)  | 1:13:A:CYS:HA  | 1:4:A:HCS:HG2  | 19       | 0.11          |
| (3,45)  | 1:13:A:CYS:HA  | 1:4:A:HCS:HG2  | 31       | 0.11          |
| (3,24)  | 1:14:A:TRP:HD1 | 1:15:A:TYR:HA  | 1        | 0.11          |
| (3,24)  | 1:14:A:TRP:HD1 | 1:15:A:TYR:HA  | 14       | 0.11          |
| (3,24)  | 1:14:A:TRP:HD1 | 1:15:A:TYR:HA  | 33       | 0.11          |
| (3,6)   | 1:14:A:TRP:HD1 | 1:16:A:ARG:HD3 | 22       | 0.11          |
| (2,354) | 1:16:A:ARG:HG3 | 1:16:A:ARG:HB2 | 14       | 0.11          |
| (2,342) | 1:4:A:HCS:H    | 1:3:A:ILE:HB   | 12       | 0.11          |
| (2,342) | 1:4:A:HCS:H    | 1:3:A:ILE:HB   | 14       | 0.11          |
| (2,340) | 1:9:A:PRO:HD2  | 1:8:A:ARG:HB2  | 22       | 0.11          |
| (2,237) | 1:6:A:VAL:HA   | 1:6:A:VAL:HG21 | 15       | 0.11          |
| (2,237) | 1:6:A:VAL:HA   | 1:6:A:VAL:HG22 | 15       | 0.11          |
| (2,237) | 1:6:A:VAL:HA   | 1:6:A:VAL:HG23 | 15       | 0.11          |
| (2,237) | 1:6:A:VAL:HA   | 1:6:A:VAL:HG21 | 18       | 0.11          |
| (2,237) | 1:6:A:VAL:HA   | 1:6:A:VAL:HG22 | 18       | 0.11          |
| (2,237) | 1:6:A:VAL:HA   | 1:6:A:VAL:HG23 | 18       | 0.11          |
| (2,193) | 1:7:A:HIS:HD2  | 1:8:A:ARG:HB3  | 4        | 0.11          |
| (2,193) | 1:7:A:HIS:HD2  | 1:8:A:ARG:HB3  | 6        | 0.11          |
| (2,193) | 1:7:A:HIS:HD2  | 1:8:A:ARG:HB3  | 34       | 0.11          |
| (2,180) | 1:14:A:TRP:HZ3 | 1:15:A:TYR:HB3 | 25       | 0.11          |
| (2,179) | 1:14:A:TRP:HD1 | 1:12:A:PRO:HB3 | 19       | 0.11          |
| (2,139) | 1:14:A:TRP:HD1 | 1:13:A:CYS:HA  | 29       | 0.11          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (2,128) | 1:14:A:TRP:HD1 | 1:12:A:PRO:HG3 | 4        | 0.11          |
| (2,100) | 1:8:A:ARG:H    | 1:8:A:ARG:HD3  | 33       | 0.11          |
| (2,100) | 1:8:A:ARG:H    | 1:8:A:ARG:HD3  | 35       | 0.11          |
| (2,99)  | 1:14:A:TRP:H   | 1:13:A:CYS:HB2 | 2        | 0.11          |
| (2,99)  | 1:14:A:TRP:H   | 1:13:A:CYS:HB2 | 9        | 0.11          |
| (2,99)  | 1:14:A:TRP:H   | 1:13:A:CYS:HB2 | 15       | 0.11          |
| (2,99)  | 1:14:A:TRP:H   | 1:13:A:CYS:HB2 | 25       | 0.11          |
| (2,99)  | 1:14:A:TRP:H   | 1:13:A:CYS:HB2 | 33       | 0.11          |
| (2,37)  | 1:7:A:HIS:HD2  | 1:11:A:TRP:HZ2 | 10       | 0.11          |
| (2,21)  | 1:11:A:TRP:HH2 | 1:8:A:ARG:HD2  | 27       | 0.11          |
| (2,13)  | 1:11:A:TRP:HH2 | 1:6:A:VAL:HG11 | 2        | 0.11          |
| (2,13)  | 1:11:A:TRP:HH2 | 1:6:A:VAL:HG12 | 2        | 0.11          |
| (2,13)  | 1:11:A:TRP:HH2 | 1:6:A:VAL:HG13 | 2        | 0.11          |
| (2,13)  | 1:11:A:TRP:HH2 | 1:6:A:VAL:HG11 | 20       | 0.11          |
| (2,13)  | 1:11:A:TRP:HH2 | 1:6:A:VAL:HG12 | 20       | 0.11          |
| (2,13)  | 1:11:A:TRP:HH2 | 1:6:A:VAL:HG13 | 20       | 0.11          |
| (1,32)  | 1:3:A:ILE:HD11 | 1:9:A:PRO:HD3  | 6        | 0.11          |
| (1,32)  | 1:3:A:ILE:HD12 | 1:9:A:PRO:HD3  | 6        | 0.11          |
| (1,32)  | 1:3:A:ILE:HD13 | 1:9:A:PRO:HD3  | 6        | 0.11          |
| (1,32)  | 1:3:A:ILE:HD11 | 1:9:A:PRO:HD3  | 21       | 0.11          |
| (1,32)  | 1:3:A:ILE:HD12 | 1:9:A:PRO:HD3  | 21       | 0.11          |
| (1,32)  | 1:3:A:ILE:HD13 | 1:9:A:PRO:HD3  | 21       | 0.11          |
| (1,29)  | 1:11:A:TRP:HD1 | 1:1:A:PRO:HG3  | 2        | 0.11          |
| (1,29)  | 1:11:A:TRP:HD1 | 1:1:A:PRO:HG3  | 32       | 0.11          |
| (1,25)  | 1:9:A:PRO:HD2  | 1:3:A:ILE:HD11 | 15       | 0.11          |
| (1,25)  | 1:9:A:PRO:HD2  | 1:3:A:ILE:HD12 | 15       | 0.11          |
| (1,25)  | 1:9:A:PRO:HD2  | 1:3:A:ILE:HD13 | 15       | 0.11          |
| (1,24)  | 1:6:A:VAL:HA   | 1:7:A:HIS:HB2  | 22       | 0.11          |
| (1,19)  | 1:7:A:HIS:HB2  | 1:6:A:VAL:HG11 | 15       | 0.11          |
| (1,19)  | 1:7:A:HIS:HB2  | 1:6:A:VAL:HG12 | 15       | 0.11          |
| (1,19)  | 1:7:A:HIS:HB2  | 1:6:A:VAL:HG13 | 15       | 0.11          |
| (1,10)  | 1:15:A:TYR:HD1 | 1:8:A:ARG:HB2  | 15       | 0.11          |
| (1,10)  | 1:15:A:TYR:HD2 | 1:8:A:ARG:HB2  | 15       | 0.11          |
| (3,45)  | 1:13:A:CYS:HA  | 1:4:A:HCS:HG2  | 33       | 0.1           |
| (3,6)   | 1:14:A:TRP:HD1 | 1:16:A:ARG:HD3 | 1        | 0.1           |
| (3,6)   | 1:14:A:TRP:HD1 | 1:16:A:ARG:HD3 | 11       | 0.1           |
| (2,193) | 1:7:A:HIS:HD2  | 1:8:A:ARG:HB3  | 9        | 0.1           |
| (2,180) | 1:14:A:TRP:HZ3 | 1:15:A:TYR:HB3 | 12       | 0.1           |
| (2,139) | 1:14:A:TRP:HD1 | 1:13:A:CYS:HA  | 18       | 0.1           |
| (2,139) | 1:14:A:TRP:HD1 | 1:13:A:CYS:HA  | 21       | 0.1           |
| (2,100) | 1:8:A:ARG:H    | 1:8:A:ARG:HD3  | 20       | 0.1           |
| (2,100) | 1:8:A:ARG:H    | 1:8:A:ARG:HD3  | 27       | 0.1           |

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| Key    | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|--------|----------------|----------------|----------|---------------|
| (2,99) | 1:14:A:TRP:H   | 1:13:A:CYS:HB2 | 1        | 0.1           |
| (2,99) | 1:14:A:TRP:H   | 1:13:A:CYS:HB2 | 18       | 0.1           |
| (2,37) | 1:7:A:HIS:HD2  | 1:11:A:TRP:HZ2 | 2        | 0.1           |
| (2,30) | 1:15:A:TYR:HE1 | 1:13:A:CYS:HB2 | 26       | 0.1           |
| (2,30) | 1:15:A:TYR:HE2 | 1:13:A:CYS:HB2 | 26       | 0.1           |
| (2,13) | 1:11:A:TRP:HH2 | 1:6:A:VAL:HG11 | 15       | 0.1           |
| (2,13) | 1:11:A:TRP:HH2 | 1:6:A:VAL:HG12 | 15       | 0.1           |
| (2,13) | 1:11:A:TRP:HH2 | 1:6:A:VAL:HG13 | 15       | 0.1           |
| (2,13) | 1:11:A:TRP:HH2 | 1:6:A:VAL:HG11 | 33       | 0.1           |
| (2,13) | 1:11:A:TRP:HH2 | 1:6:A:VAL:HG12 | 33       | 0.1           |
| (2,13) | 1:11:A:TRP:HH2 | 1:6:A:VAL:HG13 | 33       | 0.1           |
| (1,5)  | 1:11:A:TRP:HD1 | 1:12:A:PRO:HB2 | 1        | 0.1           |



## 10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found