



# Full wwPDB NMR Structure Validation Report ⓘ

Aug 30, 2026 – 01:14 am BST

PDB ID : 9RPU / pdb\_00009rpu  
BMRB ID : 35005  
Title : PIN1 WW Domain Binding Mode with SPY-tide  
Authors : Jiang, M.; Sun, M.; Mott, H.; Creixell, P.  
Deposited on : 2025-06-25

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 1.8.4, CSD as541be (2020)  
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 : v1.2.1  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.50

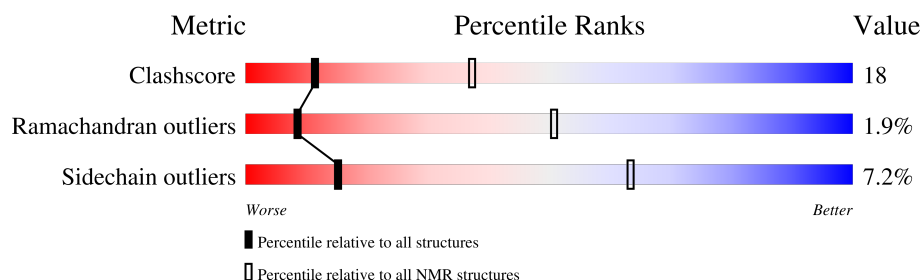
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 68%.

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     | 37     |                  |
| 2   | B     | 12     |                  |

## 2 Ensemble composition and analysis

This entry contains 25 models. Model 6 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *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:7-A:37, B:84-B:84, B:86-B:90 (37) | 0.37              | 6            |

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

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

The models can be grouped into 4 clusters and 2 single-model clusters were found.

| Cluster number        | Models                                              |
|-----------------------|-----------------------------------------------------|
| 1                     | 2, 4, 6, 10, 12, 13, 14, 15, 16, 19, 21, 22, 23, 25 |
| 2                     | 1, 7, 9, 20                                         |
| 3                     | 5, 17, 24                                           |
| 4                     | 3, 18                                               |
| Single-model clusters | 8; 11                                               |

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

There are 2 unique types of molecules in this entry. The entry contains 745 atoms, of which 356 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Peptidyl-prolyl cis-trans isomerase NIMA-interacting 1.

| Mol | Chain | Residues | Atoms |     |     |    |    |   | Trace |
|-----|-------|----------|-------|-----|-----|----|----|---|-------|
| 1   | A     | 37       | Total | C   | H   | N  | O  | S | 0     |
|     |       |          | 599   | 191 | 291 | 59 | 57 | 1 |       |

- Molecule 2 is a protein called SPY-tide SPYpSPFPE.

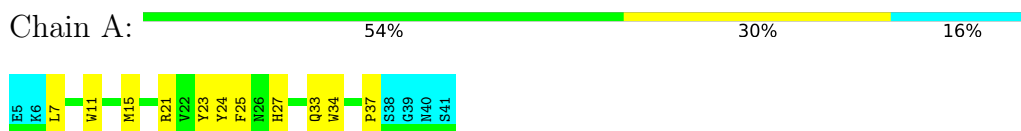
| Mol | Chain | Residues | Atoms |    |    |    |    |   | Trace |
|-----|-------|----------|-------|----|----|----|----|---|-------|
| 2   | B     | 12       | Total | C  | H  | N  | O  | P | 1     |
|     |       |          | 146   | 50 | 65 | 11 | 19 | 1 |       |

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

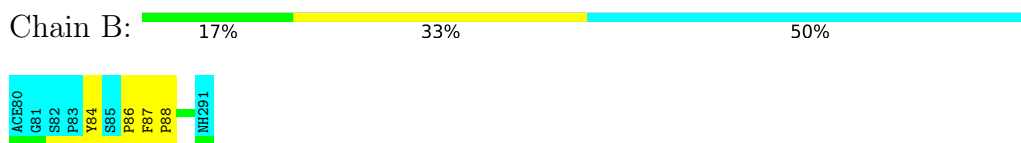
### 4.1 Average score per residue in the NMR ensemble

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: Peptidyl-prolyl cis-trans isomerase NIMA-interacting 1



- Molecule 2: SPY-tide SPYpSPFPE



### 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: Peptidyl-prolyl cis-trans isomerase NIMA-interacting 1



- Molecule 2: SPY-tide SPYpSPFPE



### 4.2.2 Score per residue for model 2

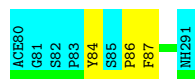
- Molecule 1: Peptidyl-prolyl cis-trans isomerase NIMA-interacting 1

Chain A:  49% 35% 16%



- Molecule 2: SPY-tide SPYpSPFPE

Chain B:  25% 25% 50%



### 4.2.3 Score per residue for model 3

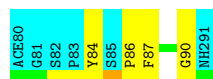
- Molecule 1: Peptidyl-prolyl cis-trans isomerase NIMA-interacting 1

Chain A:  49% 35% 16%



- Molecule 2: SPY-tide SPYpSPFPE

Chain B:  17% 33% 50%



### 4.2.4 Score per residue for model 4

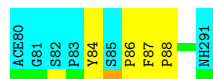
- Molecule 1: Peptidyl-prolyl cis-trans isomerase NIMA-interacting 1

Chain A:  57% 22% 5% 16%



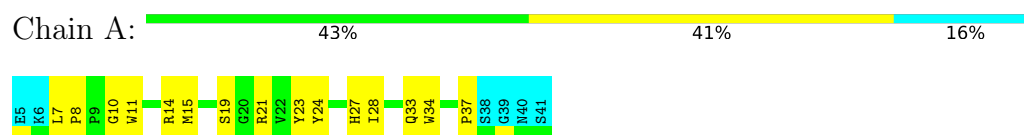
- Molecule 2: SPY-tide SPYpSPFPE

Chain B:  17% 33% 50%

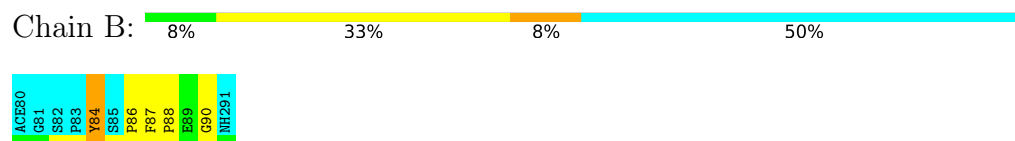


### 4.2.5 Score per residue for model 5

- Molecule 1: Peptidyl-prolyl cis-trans isomerase NIMA-interacting 1

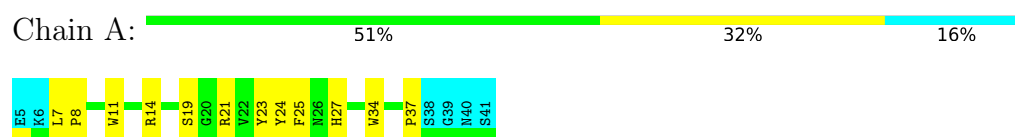


- Molecule 2: SPY-tide SPYpSPFPE

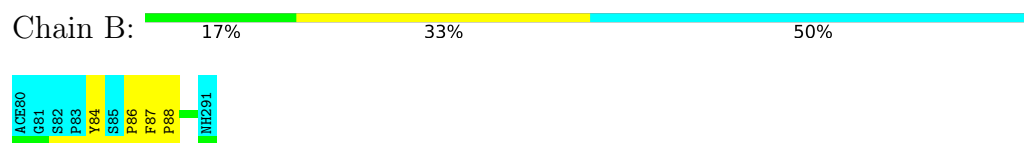


### 4.2.6 Score per residue for model 6 (medoid)

- Molecule 1: Peptidyl-prolyl cis-trans isomerase NIMA-interacting 1

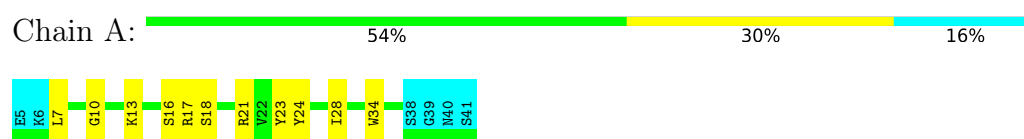


- Molecule 2: SPY-tide SPYpSPFPE

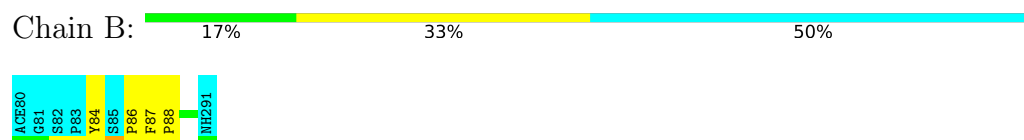


### 4.2.7 Score per residue for model 7

- Molecule 1: Peptidyl-prolyl cis-trans isomerase NIMA-interacting 1



- Molecule 2: SPY-tide SPYpSPFPE



### 4.2.8 Score per residue for model 8

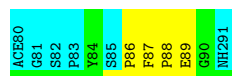
- Molecule 1: Peptidyl-prolyl cis-trans isomerase NIMA-interacting 1

Chain A: 



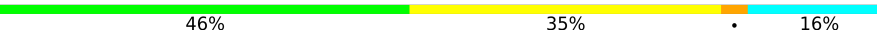
- Molecule 2: SPY-tide SPYpSPFPE

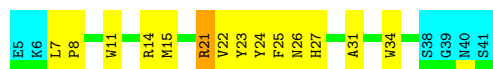
Chain B: 



### 4.2.9 Score per residue for model 9

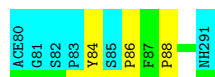
- Molecule 1: Peptidyl-prolyl cis-trans isomerase NIMA-interacting 1

Chain A: 



- Molecule 2: SPY-tide SPYpSPFPE

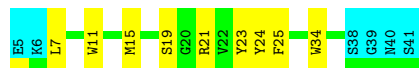
Chain B: 



### 4.2.10 Score per residue for model 10

- Molecule 1: Peptidyl-prolyl cis-trans isomerase NIMA-interacting 1

Chain A: 



- Molecule 2: SPY-tide SPYpSPFPE

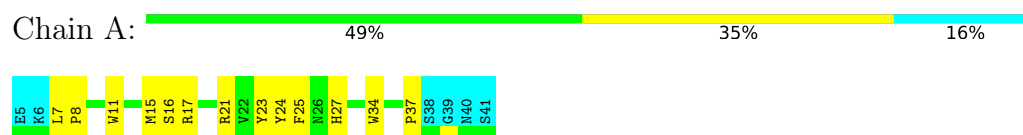
Chain B: 



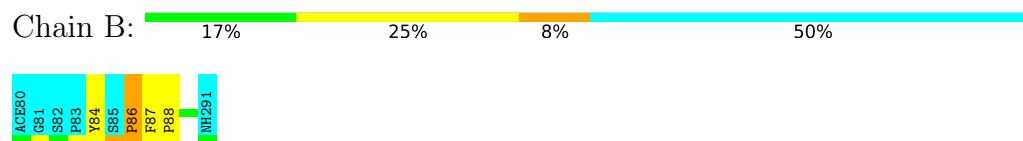


### 4.2.11 Score per residue for model 11

- Molecule 1: Peptidyl-prolyl cis-trans isomerase NIMA-interacting 1

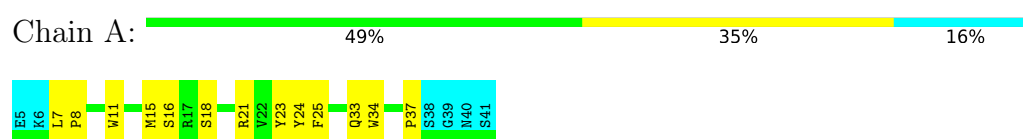


- Molecule 2: SPY-tide SPYpSPFPE

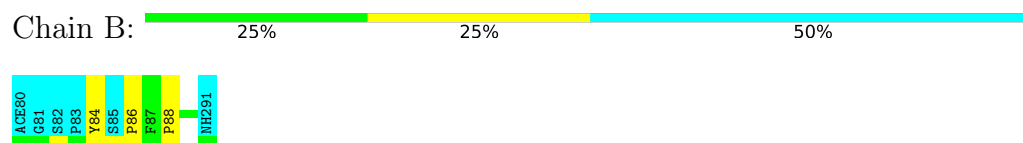


### 4.2.12 Score per residue for model 12

- Molecule 1: Peptidyl-prolyl cis-trans isomerase NIMA-interacting 1



- Molecule 2: SPY-tide SPYpSPFPE

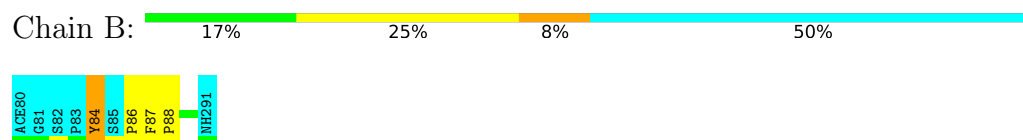


### 4.2.13 Score per residue for model 13

- Molecule 1: Peptidyl-prolyl cis-trans isomerase NIMA-interacting 1

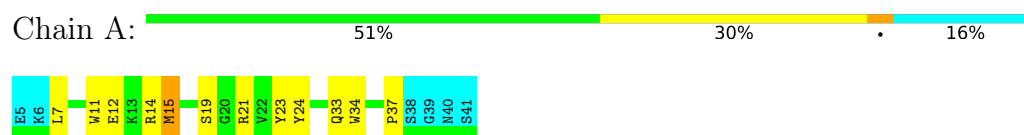


- Molecule 2: SPY-tide SPYpSPFPE

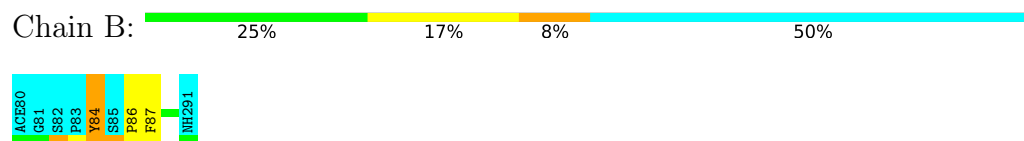


#### 4.2.14 Score per residue for model 14

- Molecule 1: Peptidyl-prolyl cis-trans isomerase NIMA-interacting 1

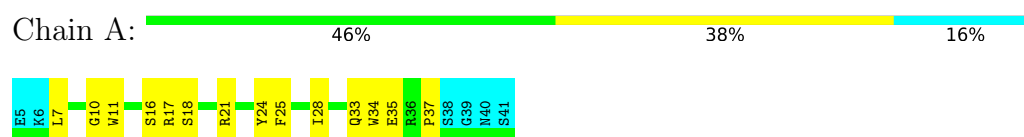


- Molecule 2: SPY-tide SPYpSPFPE

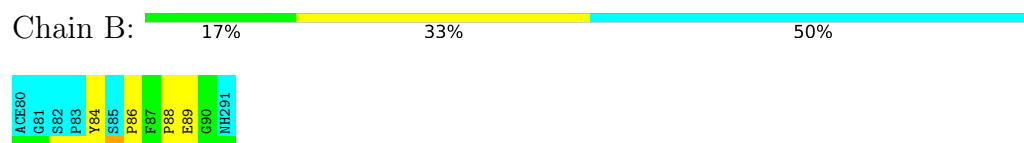


#### 4.2.15 Score per residue for model 15

- Molecule 1: Peptidyl-prolyl cis-trans isomerase NIMA-interacting 1



- Molecule 2: SPY-tide SPYpSPFPE

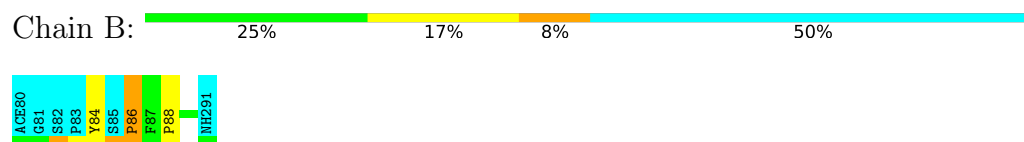


#### 4.2.16 Score per residue for model 16

- Molecule 1: Peptidyl-prolyl cis-trans isomerase NIMA-interacting 1

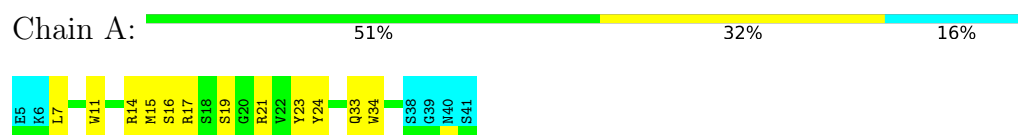


- Molecule 2: SPY-tide SPYpSPFPE

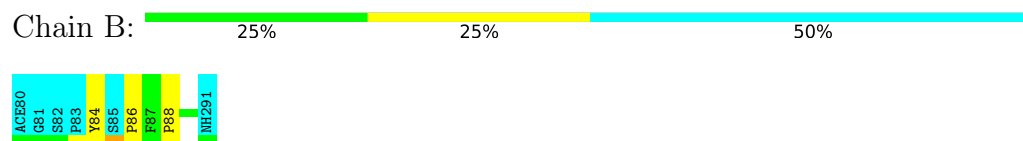


### 4.2.17 Score per residue for model 17

- Molecule 1: Peptidyl-prolyl cis-trans isomerase NIMA-interacting 1

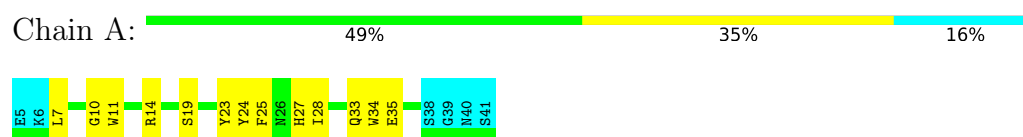


- Molecule 2: SPY-tide SPYpSPFPE

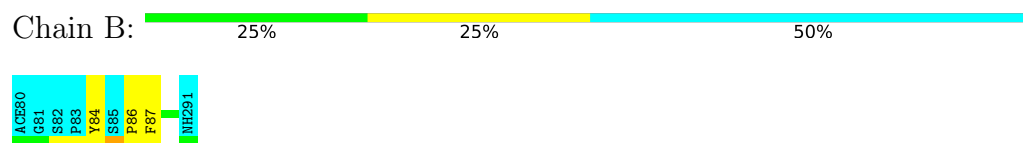


### 4.2.18 Score per residue for model 18

- Molecule 1: Peptidyl-prolyl cis-trans isomerase NIMA-interacting 1



- Molecule 2: SPY-tide SPYpSPFPE

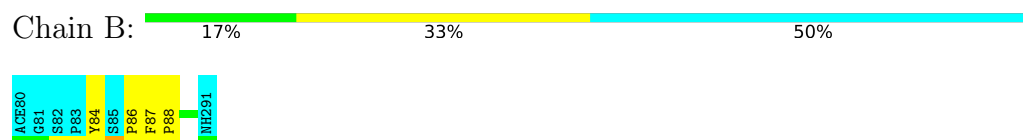


### 4.2.19 Score per residue for model 19

- Molecule 1: Peptidyl-prolyl cis-trans isomerase NIMA-interacting 1



- Molecule 2: SPY-tide SPYpSPFPE



### 4.2.20 Score per residue for model 20

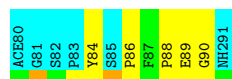
- Molecule 1: Peptidyl-prolyl cis-trans isomerase NIMA-interacting 1

Chain A: 



- Molecule 2: SPY-tide SPYpSPFPE

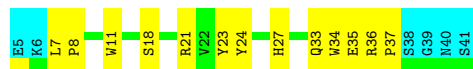
Chain B: 



### 4.2.21 Score per residue for model 21

- Molecule 1: Peptidyl-prolyl cis-trans isomerase NIMA-interacting 1

Chain A: 



- Molecule 2: SPY-tide SPYpSPFPE

Chain B: 



### 4.2.22 Score per residue for model 22

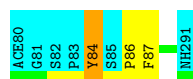
- Molecule 1: Peptidyl-prolyl cis-trans isomerase NIMA-interacting 1

Chain A: 



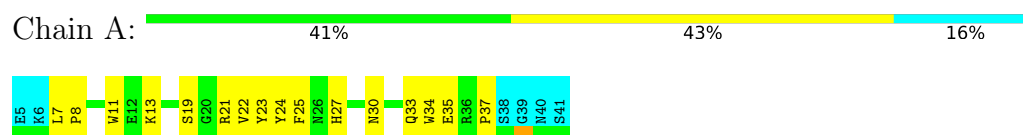
- Molecule 2: SPY-tide SPYpSPFPE

Chain B: 

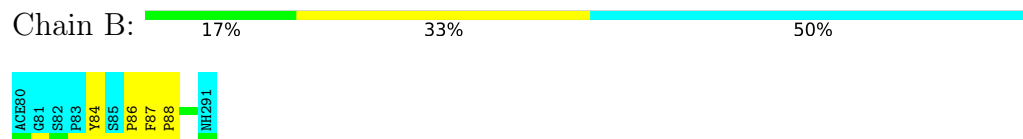


### 4.2.23 Score per residue for model 23

- Molecule 1: Peptidyl-prolyl cis-trans isomerase NIMA-interacting 1

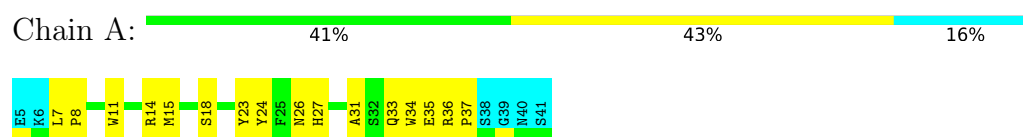


- Molecule 2: SPY-tide SPYpSPFPE

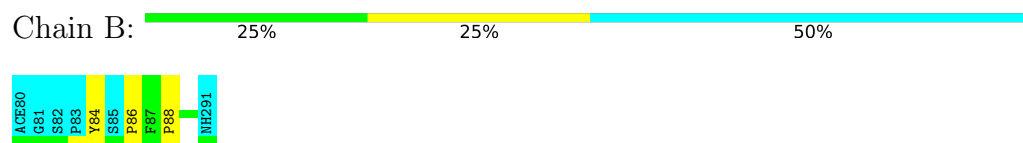


### 4.2.24 Score per residue for model 24

- Molecule 1: Peptidyl-prolyl cis-trans isomerase NIMA-interacting 1

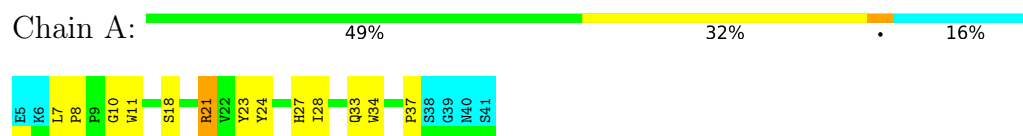


- Molecule 2: SPY-tide SPYpSPFPE

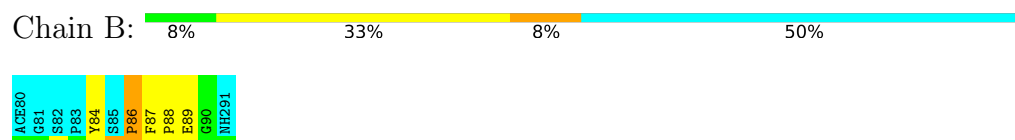


### 4.2.25 Score per residue for model 25

- Molecule 1: Peptidyl-prolyl cis-trans isomerase NIMA-interacting 1



- Molecule 2: SPY-tide SPYpSPFPE



## 5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 25 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 | 2.3     |

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

|                                              |                |
|----------------------------------------------|----------------|
| Chemical shift file(s)                       | working_cs.cif |
| Number of chemical shift lists               | 1              |
| Total number of shifts                       | 429            |
| Number of shifts mapped to atoms             | 429            |
| Number of unparsed shifts                    | 0              |
| Number of shifts with mapping errors         | 0              |
| Number of shifts with mapping warnings       | 0              |
| Assignment completeness (well-defined parts) | 68%            |

## 6 Model quality

### 6.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SEP, ACE, NH2

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

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     | 265   | 251      | 250      | 10±2    |
| 2   | B     | 50    | 41       | 41       | 4±1     |
| All | All   | 7875  | 7300     | 7275     | 271     |

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 18.

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

| Atom-1         | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|----------------|-----------------|----------|-------------|--------|-------|
|                |                 |          |             | Worst  | Total |
| 1:A:10:GLY:HA3 | 1:A:28:ILE:HD11 | 0.86     | 1.45        | 25     | 7     |
| 1:A:18:SER:HB2 | 2:B:88:PRO:HB3  | 0.80     | 1.52        | 15     | 7     |
| 1:A:7:LEU:HD23 | 1:A:11:TRP:HB3  | 0.72     | 1.61        | 10     | 11    |
| 1:A:15:MET:HA  | 1:A:15:MET:HE2  | 0.70     | 1.61        | 24     | 8     |
| 1:A:23:TYR:HB3 | 1:A:34:TRP:CE3  | 0.68     | 2.24        | 11     | 14    |
| 1:A:7:LEU:HD21 | 1:A:24:TYR:CD2  | 0.68     | 2.23        | 11     | 7     |
| 1:A:33:GLN:NE2 | 1:A:37:PRO:HG3  | 0.64     | 2.07        | 13     | 12    |
| 2:B:84:TYR:O   | 2:B:86:PRO:HD3  | 0.64     | 1.92        | 9      | 23    |
| 1:A:21:ARG:HE  | 2:B:89:GLU:HG3  | 0.62     | 1.53        | 20     | 3     |
| 1:A:7:LEU:HD11 | 1:A:24:TYR:CD1  | 0.62     | 2.29        | 8      | 8     |
| 1:A:7:LEU:HD21 | 1:A:24:TYR:CD1  | 0.62     | 2.29        | 18     | 5     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:34:TRP:CZ2  | 2:B:86:PRO:HD2  | 0.61     | 2.30        | 5      | 10    |
| 1:A:8:PRO:HG2   | 1:A:11:TRP:CD1  | 0.61     | 2.30        | 9      | 8     |
| 1:A:33:GLN:HE21 | 1:A:37:PRO:HG3  | 0.60     | 1.57        | 23     | 4     |
| 1:A:34:TRP:NE1  | 2:B:86:PRO:HG2  | 0.60     | 2.12        | 14     | 24    |
| 1:A:14:ARG:HB2  | 1:A:23:TYR:CZ   | 0.59     | 2.33        | 9      | 9     |
| 1:A:23:TYR:HB3  | 1:A:34:TRP:CZ3  | 0.58     | 2.34        | 18     | 18    |
| 1:A:7:LEU:HD11  | 1:A:24:TYR:CD2  | 0.57     | 2.35        | 7      | 5     |
| 1:A:25:PHE:CE2  | 2:B:84:TYR:HA   | 0.57     | 2.35        | 22     | 7     |
| 2:B:86:PRO:O    | 2:B:88:PRO:HD3  | 0.57     | 1.99        | 11     | 1     |
| 1:A:34:TRP:CZ2  | 2:B:88:PRO:HA   | 0.57     | 2.35        | 8      | 12    |
| 1:A:21:ARG:NE   | 2:B:89:GLU:HG3  | 0.56     | 2.15        | 15     | 2     |
| 1:A:16:SER:HG   | 1:A:34:TRP:HH2  | 0.55     | 1.43        | 12     | 2     |
| 1:A:33:GLN:HE21 | 1:A:37:PRO:HD3  | 0.54     | 1.62        | 19     | 3     |
| 1:A:18:SER:HB2  | 2:B:88:PRO:CB   | 0.54     | 2.32        | 24     | 7     |
| 1:A:8:PRO:HD2   | 1:A:37:PRO:HG2  | 0.53     | 1.79        | 11     | 1     |
| 1:A:25:PHE:CE2  | 1:A:27:HIS:HB3  | 0.53     | 2.38        | 23     | 1     |
| 1:A:15:MET:HE1  | 1:A:22:VAL:HG22 | 0.52     | 1.81        | 9      | 1     |
| 1:A:25:PHE:CE1  | 2:B:84:TYR:HA   | 0.52     | 2.40        | 1      | 7     |
| 1:A:21:ARG:HA   | 1:A:21:ARG:NE   | 0.52     | 2.20        | 9      | 3     |
| 1:A:7:LEU:HD12  | 1:A:11:TRP:HB3  | 0.47     | 1.86        | 19     | 1     |
| 1:A:7:LEU:HD21  | 1:A:24:TYR:HD1  | 0.47     | 1.68        | 2      | 2     |
| 1:A:27:HIS:H    | 1:A:27:HIS:CD2  | 0.47     | 2.27        | 23     | 1     |
| 1:A:21:ARG:HD2  | 2:B:89:GLU:OE1  | 0.46     | 2.11        | 1      | 1     |
| 1:A:13:LYS:HE3  | 1:A:22:VAL:HG11 | 0.46     | 1.87        | 23     | 1     |
| 1:A:16:SER:OG   | 1:A:34:TRP:HH2  | 0.46     | 1.93        | 12     | 6     |
| 1:A:21:ARG:HA   | 1:A:21:ARG:HE   | 0.45     | 1.71        | 5      | 1     |
| 1:A:25:PHE:CD1  | 1:A:32:SER:HB3  | 0.45     | 2.46        | 3      | 1     |
| 1:A:21:ARG:HD2  | 2:B:89:GLU:HB2  | 0.45     | 1.88        | 25     | 1     |
| 1:A:16:SER:CB   | 1:A:21:ARG:HB3  | 0.45     | 2.41        | 17     | 1     |
| 1:A:21:ARG:HG2  | 1:A:34:TRP:CZ3  | 0.45     | 2.47        | 22     | 1     |
| 1:A:15:MET:N    | 1:A:15:MET:SD   | 0.45     | 2.90        | 10     | 1     |
| 1:A:33:GLN:HG3  | 1:A:35:GLU:O    | 0.44     | 2.12        | 24     | 5     |
| 1:A:7:LEU:CD2   | 1:A:37:PRO:HD2  | 0.44     | 2.42        | 21     | 1     |
| 1:A:25:PHE:CD2  | 2:B:84:TYR:HA   | 0.43     | 2.47        | 22     | 1     |
| 1:A:8:PRO:HD2   | 1:A:11:TRP:CD1  | 0.43     | 2.48        | 21     | 2     |
| 1:A:7:LEU:HD22  | 1:A:37:PRO:HD2  | 0.43     | 1.91        | 6      | 1     |
| 1:A:18:SER:HB3  | 2:B:88:PRO:CB   | 0.43     | 2.43        | 7      | 1     |
| 1:A:7:LEU:HD21  | 1:A:24:TYR:HD2  | 0.43     | 1.71        | 15     | 2     |
| 1:A:16:SER:OG   | 2:B:88:PRO:HB3  | 0.42     | 2.15        | 11     | 1     |
| 1:A:7:LEU:HD11  | 1:A:36:ARG:HG3  | 0.42     | 1.92        | 13     | 1     |
| 1:A:15:MET:HA   | 1:A:15:MET:CE   | 0.41     | 2.42        | 5      | 1     |

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| Atom-1         | Atom-2         | Clash(Å) | Distance(Å) | Models |       |
|----------------|----------------|----------|-------------|--------|-------|
|                |                |          |             | Worst  | Total |
| 1:A:26:ASN:HB3 | 1:A:31:ALA:HB3 | 0.41     | 1.93        | 9      | 2     |
| 1:A:14:ARG:HB2 | 1:A:23:TYR:CE1 | 0.41     | 2.50        | 17     | 1     |
| 1:A:7:LEU:HD23 | 1:A:11:TRP:CB  | 0.41     | 2.42        | 25     | 1     |
| 1:A:21:ARG:NE  | 1:A:21:ARG:HA  | 0.41     | 2.31        | 4      | 1     |
| 1:A:21:ARG:HG3 | 1:A:34:TRP:CZ3 | 0.40     | 2.51        | 6      | 1     |
| 1:A:26:ASN:HB3 | 1:A:31:ALA:O   | 0.40     | 2.16        | 22     | 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     | 31/37 (84%)    | 29±1 (93±2%) | 2±1 (5±3%)   | 0±0 (1±2%) | 11          | 58 |
| 2   | B     | 6/12 (50%)     | 2±1 (35±11%) | 4±1 (61±10%) | 0±0 (5±7%) | 3           | 25 |
| All | All   | 925/1225 (76%) | 775 (84%)    | 132 (14%)    | 18 (2%)    | 8           | 51 |

All 4 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     | 19  | SER  | 11             |
| 2   | B     | 90  | GLY  | 3              |
| 2   | B     | 86  | PRO  | 3              |
| 2   | B     | 87  | PHE  | 1              |

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

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

| Mol | Chain | Analysed    | Rotameric    | Outliers   | Percentiles |    |
|-----|-------|-------------|--------------|------------|-------------|----|
| 1   | A     | 28/33 (85%) | 27±1 (95±3%) | 1±1 (5±3%) | 22          | 72 |

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| Mol | Chain | Analysed       | Rotameric    | Outliers     | Percentiles |    |
|-----|-------|----------------|--------------|--------------|-------------|----|
| 2   | B     | 5/7 (71%)      | 4±1 (82±13%) | 1±1 (18±13%) | 4           | 37 |
| All | All   | 825/1000 (82%) | 766 (93%)    | 59 (7%)      | 15          | 63 |

All 8 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) |
|-----|-------|-----|------|----------------|
| 2   | B     | 87  | PHE  | 17             |
| 1   | A     | 21  | ARG  | 14             |
| 1   | A     | 27  | HIS  | 13             |
| 1   | A     | 15  | MET  | 5              |
| 2   | B     | 84  | TYR  | 5              |
| 1   | A     | 12  | GLU  | 2              |
| 1   | A     | 33  | GLN  | 2              |
| 1   | A     | 13  | LYS  | 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       |
| 2   | SEP  | B     | 85  | 2    | 8,9,10       | 0.94±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        |
| 2   | SEP  | B     | 85  | 2    | 8,12,14     | 1.38±0.17 | 1±0 (12±2%) |

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 |
|-----|------|-------|-----|------|---------|------------|-------|
| 2   | SEP  | B     | 85  | 2    | -       | 0±0,5,8,10 | -     |

There are no bond-length outliers.

All unique angle outliers are listed below.

| Mol | Chain | Res | Type | Atoms    | Z    | Observed(°) | Ideal(°) | Models |       |
|-----|-------|-----|------|----------|------|-------------|----------|--------|-------|
|     |       |     |      |          |      |             |          | Worst  | Total |
| 2   | B     | 85  | SEP  | OG-CB-CA | 4.25 | 112.28      | 108.14   | 17     | 24    |

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 ⓘ

There are no chain breaks in this entry.

## 7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 68% for the well-defined parts and 68% for the entire structure.

### 7.1 Chemical shift list 1

File name: working\_cs.cif

Chemical shift list name: *default*

#### 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                  | 429 |
| Number of shifts mapped to atoms        | 429 |
| Number of unparsed shifts               | 0   |
| Number of shifts with mapping errors    | 0   |
| Number of shifts with mapping warnings  | 0   |
| Number of shift outliers (ShiftChecker) | 5   |

#### 7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

| Nucleus                | # values | Correction $\pm$ precision, ppm | Suggested action           |
|------------------------|----------|---------------------------------|----------------------------|
| $^{13}\text{C}_\alpha$ | 32       | $0.51 \pm 0.16$                 | Should be checked          |
| $^{13}\text{C}_\beta$  | 40       | $-0.20 \pm 0.39$                | None needed ( $< 0.5$ ppm) |
| $^{13}\text{C}'$       | 0        | —                               | None (insufficient data)   |
| $^{15}\text{N}$        | 26       | $-0.06 \pm 1.35$                | None needed ( $< 0.5$ ppm) |

#### 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 68%, i.e. 356 atoms were assigned a chemical shift out of a possible 524. 2 out of 2 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total         | $^1\text{H}$  | $^{13}\text{C}$ | $^{15}\text{N}$ |
|-----------|---------------|---------------|-----------------|-----------------|
| Backbone  | 117/178 (66%) | 69/72 (96%)   | 26/74 (35%)     | 22/32 (69%)     |
| Sidechain | 201/267 (75%) | 136/171 (80%) | 65/80 (81%)     | 0/16 (0%)       |

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|          | Total         | <sup>1</sup> H | <sup>13</sup> C | <sup>15</sup> N |
|----------|---------------|----------------|-----------------|-----------------|
| Aromatic | 38/79 (48%)   | 36/38 (95%)    | 0/37 (0%)       | 2/4 (50%)       |
| Overall  | 356/524 (68%) | 241/281 (86%)  | 91/191 (48%)    | 24/52 (46%)     |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 68%, i.e. 419 atoms were assigned a chemical shift out of a possible 614. 2 out of 2 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total         | <sup>1</sup> H | <sup>13</sup> C | <sup>15</sup> N |
|-----------|---------------|----------------|-----------------|-----------------|
| Backbone  | 143/223 (64%) | 85/91 (93%)    | 32/92 (35%)     | 26/40 (65%)     |
| Sidechain | 238/312 (76%) | 163/199 (82%)  | 75/95 (79%)     | 0/18 (0%)       |
| Aromatic  | 38/79 (48%)   | 36/38 (95%)    | 0/37 (0%)       | 2/4 (50%)       |
| Overall   | 419/614 (68%) | 284/328 (87%)  | 107/224 (48%)   | 28/62 (45%)     |

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

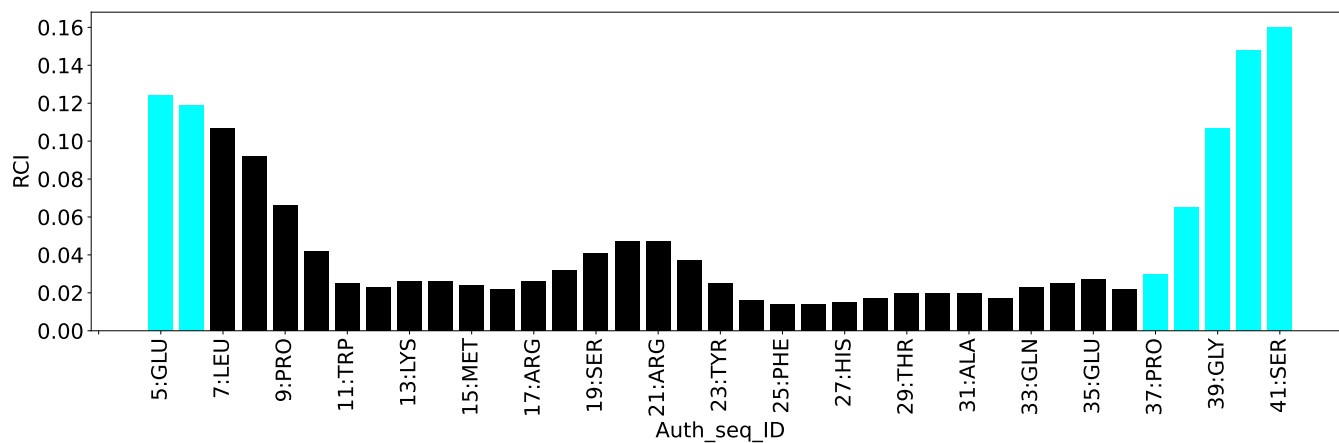
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

| List Id | Chain | Res | Type | Atom | Shift, ppm | Expected range, ppm | Z-score |
|---------|-------|-----|------|------|------------|---------------------|---------|
| 1       | A     | 11  | TRP  | CE2  | 41.94      | 105.29 – 170.61     | -14.7   |
| 1       | A     | 26  | ASN  | HB3  | -0.76      | 1.12 – 4.38         | -10.8   |
| 1       | A     | 14  | ARG  | HB2  | -0.17      | 0.52 – 3.08         | -7.7    |
| 1       | A     | 37  | PRO  | HG2  | -0.22      | 0.41 – 3.45         | -7.1    |
| 1       | A     | 26  | ASN  | HD21 | 4.12       | 4.94 – 9.72         | -6.7    |

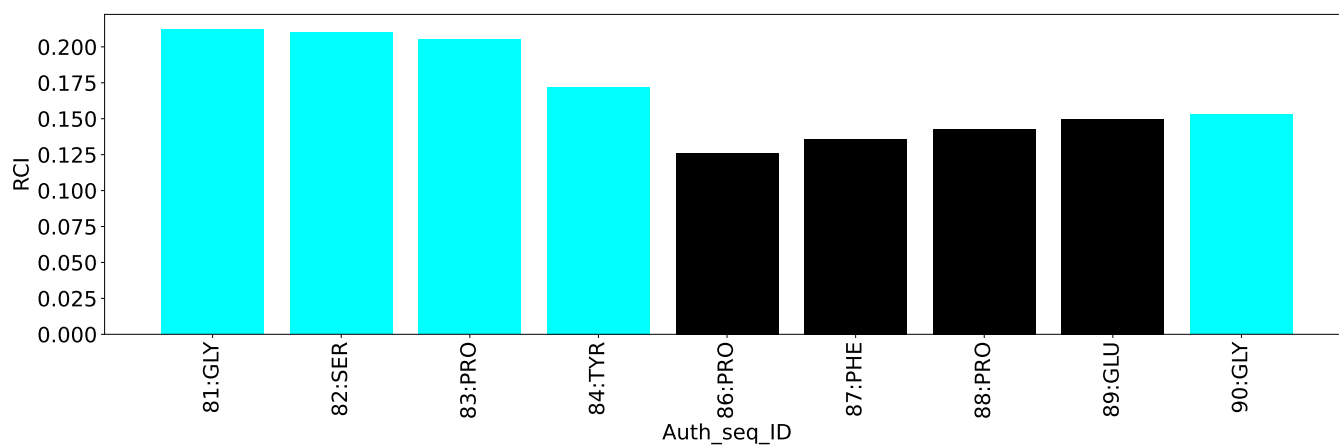
#### 7.1.5 Random Coil Index (RCI) plots [i](#)

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:



Random coil index (RCI) for chain B:



## 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                                | 886   |
| Intra-residue ( $ i-j =0$ )                              | 156   |
| Sequential ( $ i-j =1$ )                                 | 232   |
| Medium range ( $ i-j >1$ and $ i-j <5$ )                 | 102   |
| Long range ( $ i-j \geq 5$ )                             | 298   |
| Inter-chain                                              | 98    |
| Hydrogen bond restraints                                 | 0     |
| Disulfide bond restraints                                | 0     |
| Total dihedral-angle restraints                          | 48    |
| Number of unmapped restraints                            | 0     |
| Number of restraints per residue                         | 19.1  |
| Number of long range restraints per residue <sup>1</sup> | 6.1   |

<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)  | 18.2                                   | 0.2     |
| 0.2-0.5 (Medium) | 29.4                                   | 0.5     |
| >0.5 (Large)     | 39.0                                   | 2.76    |



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

Dihedral-angle violations less than 1° are not included in the calculation.

| Bins (°)           | Average number of violations per model | Max (°) |
|--------------------|----------------------------------------|---------|
| 1.0-10.0 (Small)   | 13.6                                   | 5.41    |
| 10.0-20.0 (Medium) | None                                   | None    |
| >20.0 (Large)      | None                                   | None    |

## 9 Distance violation analysis ⓘ

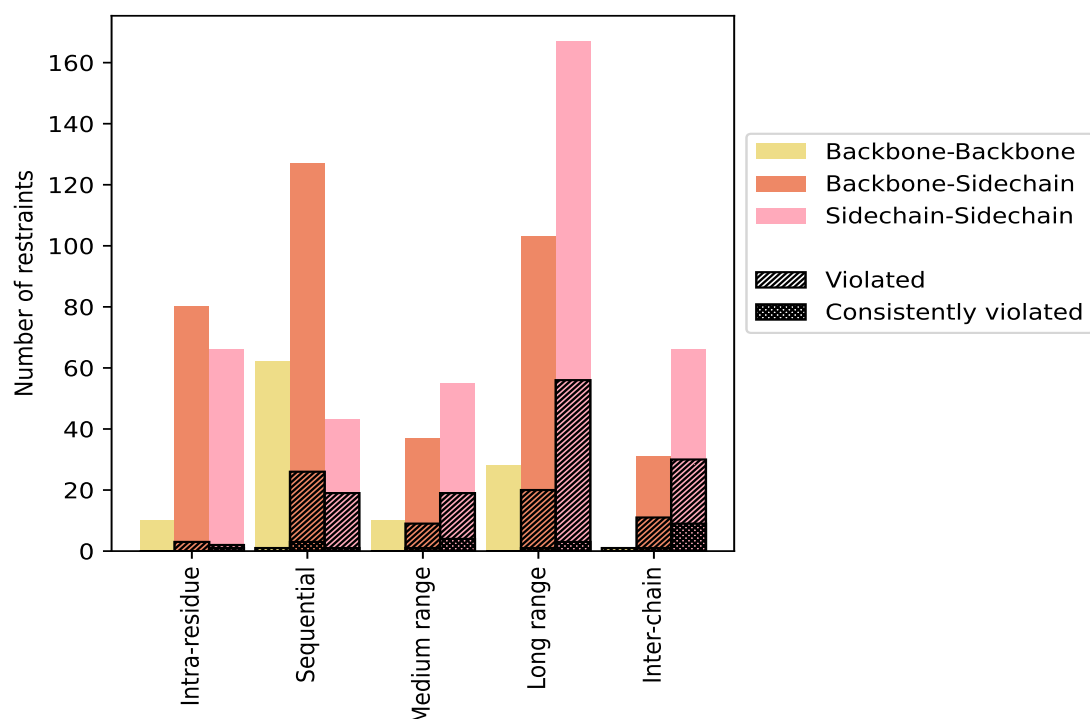
### 9.1 Summary of distance violations ⓘ

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

| Restrains type                                             | Count               | % <sup>1</sup>        | Violated <sup>3</sup> |                      |                      | Consistently Violated <sup>4</sup> |                      |                     |
|------------------------------------------------------------|---------------------|-----------------------|-----------------------|----------------------|----------------------|------------------------------------|----------------------|---------------------|
|                                                            |                     |                       | Count                 | % <sup>2</sup>       | % <sup>1</sup>       | Count                              | % <sup>2</sup>       | % <sup>1</sup>      |
| <a href="#">Intra-residue ( i-j =0)</a>                    | <a href="#">156</a> | <a href="#">17.6</a>  | <a href="#">5</a>     | <a href="#">3.2</a>  | <a href="#">0.6</a>  | <a href="#">1</a>                  | <a href="#">0.6</a>  | <a href="#">0.1</a> |
| Backbone-Backbone                                          | 10                  | 1.1                   | 0                     | 0.0                  | 0.0                  | 0                                  | 0.0                  | 0.0                 |
| Backbone-Sidechain                                         | 80                  | 9.0                   | 3                     | 3.8                  | 0.3                  | 0                                  | 0.0                  | 0.0                 |
| Sidechain-Sidechain                                        | 66                  | 7.4                   | 2                     | 3.0                  | 0.2                  | 1                                  | 1.5                  | 0.1                 |
| <a href="#">Sequential ( i-j =1)</a>                       | <a href="#">232</a> | <a href="#">26.2</a>  | <a href="#">46</a>    | <a href="#">19.8</a> | <a href="#">5.2</a>  | <a href="#">4</a>                  | <a href="#">1.7</a>  | <a href="#">0.5</a> |
| Backbone-Backbone                                          | 62                  | 7.0                   | 1                     | 1.6                  | 0.1                  | 0                                  | 0.0                  | 0.0                 |
| Backbone-Sidechain                                         | 127                 | 14.3                  | 26                    | 20.5                 | 2.9                  | 3                                  | 2.4                  | 0.3                 |
| Sidechain-Sidechain                                        | 43                  | 4.9                   | 19                    | 44.2                 | 2.1                  | 1                                  | 2.3                  | 0.1                 |
| <a href="#">Medium range ( i-j &gt;1 &amp;  i-j &lt;5)</a> | <a href="#">102</a> | <a href="#">11.5</a>  | <a href="#">28</a>    | <a href="#">27.5</a> | <a href="#">3.2</a>  | <a href="#">5</a>                  | <a href="#">4.9</a>  | <a href="#">0.6</a> |
| Backbone-Backbone                                          | 10                  | 1.1                   | 0                     | 0.0                  | 0.0                  | 0                                  | 0.0                  | 0.0                 |
| Backbone-Sidechain                                         | 37                  | 4.2                   | 9                     | 24.3                 | 1.0                  | 1                                  | 2.7                  | 0.1                 |
| Sidechain-Sidechain                                        | 55                  | 6.2                   | 19                    | 34.5                 | 2.1                  | 4                                  | 7.3                  | 0.5                 |
| <a href="#">Long range ( i-j ≥5)</a>                       | <a href="#">298</a> | <a href="#">33.6</a>  | <a href="#">76</a>    | <a href="#">25.5</a> | <a href="#">8.6</a>  | <a href="#">4</a>                  | <a href="#">1.3</a>  | <a href="#">0.5</a> |
| Backbone-Backbone                                          | 28                  | 3.2                   | 0                     | 0.0                  | 0.0                  | 0                                  | 0.0                  | 0.0                 |
| Backbone-Sidechain                                         | 103                 | 11.6                  | 20                    | 19.4                 | 2.3                  | 1                                  | 1.0                  | 0.1                 |
| Sidechain-Sidechain                                        | 167                 | 18.8                  | 56                    | 33.5                 | 6.3                  | 3                                  | 1.8                  | 0.3                 |
| <a href="#">Inter-chain</a>                                | <a href="#">98</a>  | <a href="#">11.1</a>  | <a href="#">42</a>    | <a href="#">42.9</a> | <a href="#">4.7</a>  | <a href="#">10</a>                 | <a href="#">10.2</a> | <a href="#">1.1</a> |
| Backbone-Backbone                                          | 1                   | 0.1                   | 1                     | 100.0                | 0.1                  | 0                                  | 0.0                  | 0.0                 |
| Backbone-Sidechain                                         | 31                  | 3.5                   | 11                    | 35.5                 | 1.2                  | 1                                  | 3.2                  | 0.1                 |
| Sidechain-Sidechain                                        | 66                  | 7.4                   | 30                    | 45.5                 | 3.4                  | 9                                  | 13.6                 | 1.0                 |
| <a href="#">Hydrogen bond</a>                              | <a href="#">0</a>   | <a href="#">0.0</a>   | <a href="#">0</a>     | <a href="#">0.0</a>  | <a href="#">0.0</a>  | <a href="#">0</a>                  | <a href="#">0.0</a>  | <a href="#">0.0</a> |
| <a href="#">Disulfide bond</a>                             | <a href="#">0</a>   | <a href="#">0.0</a>   | <a href="#">0</a>     | <a href="#">0.0</a>  | <a href="#">0.0</a>  | <a href="#">0</a>                  | <a href="#">0.0</a>  | <a href="#">0.0</a> |
| <a href="#">Total</a>                                      | <a href="#">886</a> | <a href="#">100.0</a> | <a href="#">197</a>   | <a href="#">22.2</a> | <a href="#">22.2</a> | <a href="#">24</a>                 | <a href="#">2.7</a>  | <a href="#">2.7</a> |
| Backbone-Backbone                                          | 111                 | 12.5                  | 2                     | 1.8                  | 0.2                  | 0                                  | 0.0                  | 0.0                 |
| Backbone-Sidechain                                         | 378                 | 42.7                  | 69                    | 18.3                 | 7.8                  | 6                                  | 1.6                  | 0.7                 |
| Sidechain-Sidechain                                        | 397                 | 44.8                  | 126                   | 31.7                 | 14.2                 | 18                                 | 4.5                  | 2.0                 |

<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        | 3                    | 19              | 13              | 29              | 24              | 88    | 0.65     | 2.07    | 0.48                | 0.48       |
| 2        | 3                    | 17              | 16              | 23              | 21              | 80    | 0.57     | 2.07    | 0.45                | 0.4        |
| 3        | 3                    | 25              | 12              | 31              | 22              | 93    | 0.62     | 2.03    | 0.46                | 0.46       |
| 4        | 3                    | 18              | 16              | 34              | 20              | 91    | 0.6      | 2.41    | 0.49                | 0.43       |
| 5        | 2                    | 18              | 12              | 25              | 26              | 83    | 0.62     | 2.29    | 0.5                 | 0.43       |
| 6        | 3                    | 20              | 12              | 30              | 21              | 86    | 0.57     | 1.97    | 0.43                | 0.4        |
| 7        | 3                    | 17              | 17              | 27              | 22              | 86    | 0.56     | 2.06    | 0.45                | 0.4        |
| 8        | 2                    | 17              | 12              | 29              | 26              | 86    | 0.63     | 2.47    | 0.53                | 0.46       |
| 9        | 2                    | 21              | 15              | 33              | 23              | 94    | 0.6      | 2.4     | 0.49                | 0.41       |
| 10       | 2                    | 18              | 17              | 26              | 20              | 83    | 0.62     | 2.07    | 0.51                | 0.41       |

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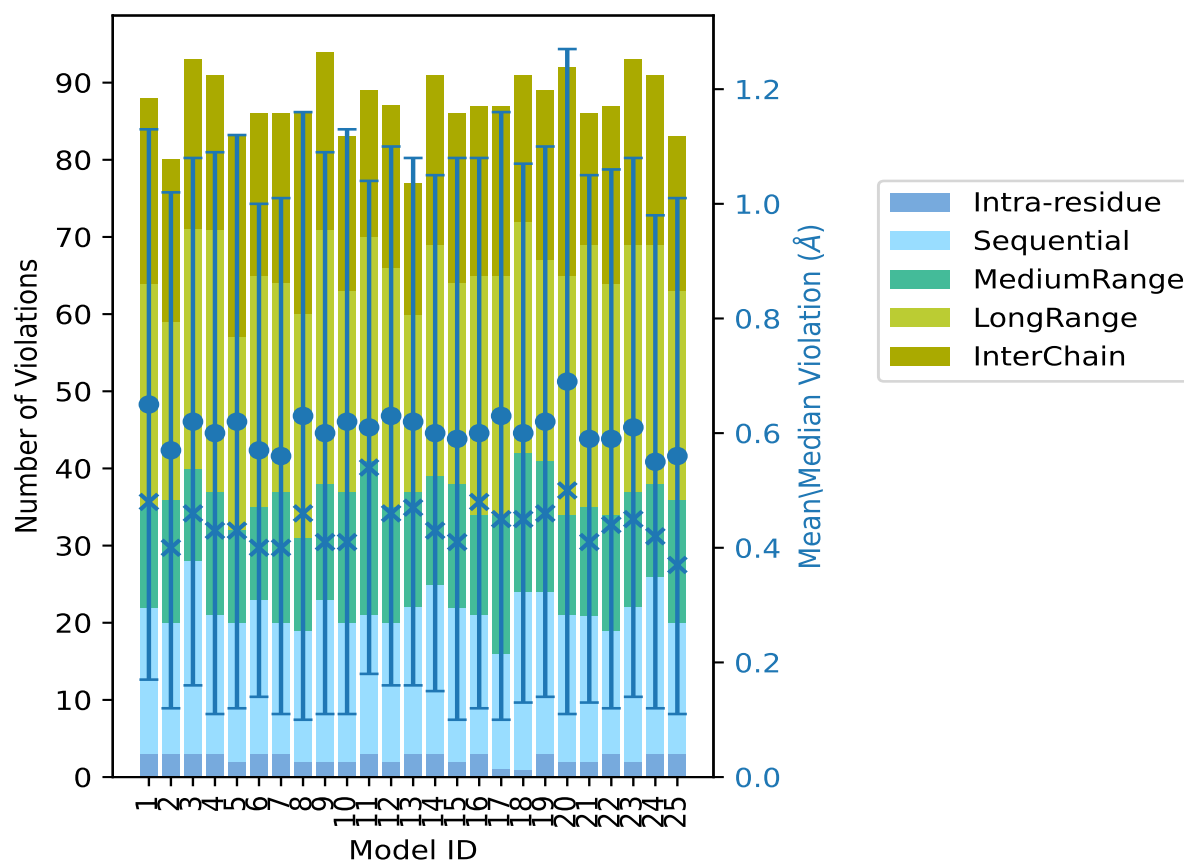
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| Model ID | Number of violations |                 |                 |                 |                 |       | Mean (Å) | Max (Å) | SD <sup>6</sup> (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
|          | IR <sup>1</sup>      | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total |          |         |                     |            |
| 11       | 3                    | 18              | 20              | 29              | 19              | 89    | 0.61     | 1.86    | 0.43                | 0.54       |
| 12       | 2                    | 18              | 15              | 31              | 21              | 87    | 0.63     | 2.1     | 0.47                | 0.46       |
| 13       | 3                    | 19              | 15              | 23              | 17              | 77    | 0.62     | 2.1     | 0.46                | 0.47       |
| 14       | 3                    | 22              | 14              | 30              | 22              | 91    | 0.6      | 2.15    | 0.45                | 0.43       |
| 15       | 2                    | 20              | 16              | 26              | 22              | 86    | 0.59     | 2.05    | 0.49                | 0.41       |
| 16       | 3                    | 18              | 13              | 31              | 22              | 87    | 0.6      | 2.27    | 0.48                | 0.48       |
| 17       | 1                    | 15              | 18              | 31              | 22              | 87    | 0.63     | 2.45    | 0.53                | 0.45       |
| 18       | 1                    | 23              | 18              | 30              | 19              | 91    | 0.6      | 1.95    | 0.47                | 0.45       |
| 19       | 3                    | 21              | 17              | 26              | 22              | 89    | 0.62     | 2.17    | 0.48                | 0.46       |
| 20       | 2                    | 19              | 13              | 31              | 27              | 92    | 0.69     | 2.76    | 0.58                | 0.5        |
| 21       | 2                    | 19              | 14              | 34              | 17              | 86    | 0.59     | 2.32    | 0.46                | 0.41       |
| 22       | 3                    | 16              | 15              | 30              | 23              | 87    | 0.59     | 2.08    | 0.47                | 0.44       |
| 23       | 2                    | 20              | 15              | 32              | 24              | 93    | 0.61     | 2.12    | 0.47                | 0.45       |
| 24       | 3                    | 23              | 12              | 31              | 22              | 91    | 0.55     | 2.5     | 0.43                | 0.42       |
| 25       | 3                    | 17              | 16              | 27              | 20              | 83    | 0.56     | 2.13    | 0.45                | 0.37       |

<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, 689(IR:151, SQ:186, MR:74, LR:222, IC:56) 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>       | %    |
| 2                             | 8               | 2               | 11              | 6               | 29    | 1                        | 4.0  |
| 0                             | 2               | 0               | 8               | 5               | 15    | 2                        | 8.0  |
| 0                             | 5               | 2               | 6               | 1               | 14    | 3                        | 12.0 |
| 0                             | 1               | 2               | 8               | 3               | 14    | 4                        | 16.0 |
| 0                             | 4               | 2               | 3               | 1               | 10    | 5                        | 20.0 |
| 0                             | 3               | 2               | 2               | 0               | 7     | 6                        | 24.0 |

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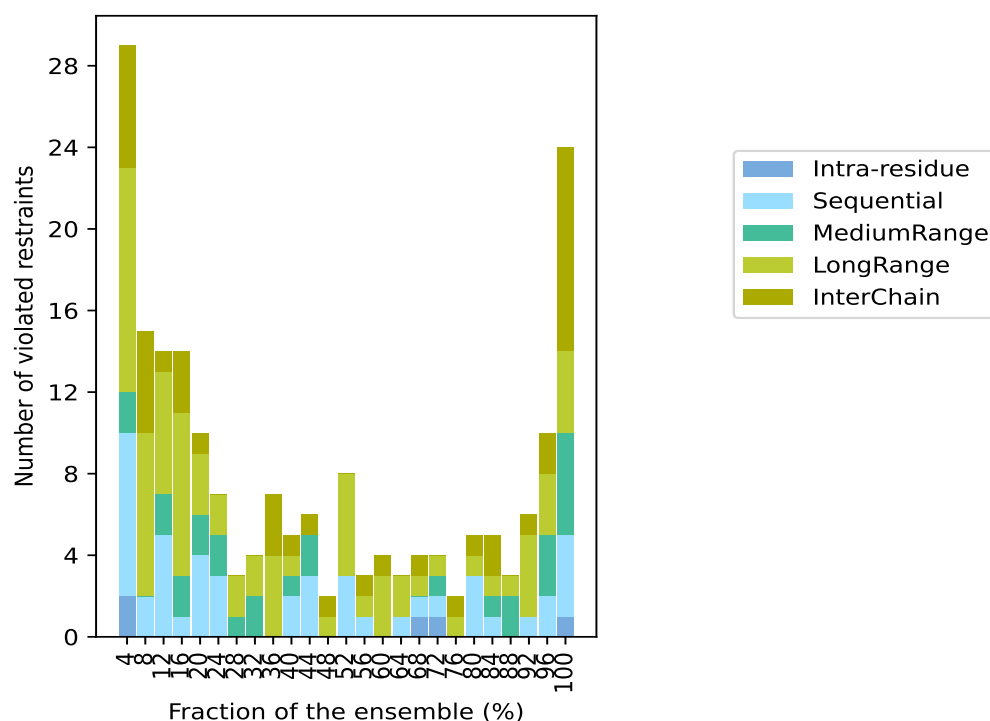
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| Number of violated restraints |                 |                 |                 |                 |       | Fraction of the ensemble |       |
|-------------------------------|-----------------|-----------------|-----------------|-----------------|-------|--------------------------|-------|
| IR <sup>1</sup>               | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total | Count <sup>6</sup>       | %     |
| 0                             | 0               | 1               | 2               | 0               | 3     | 7                        | 28.0  |
| 0                             | 0               | 2               | 2               | 0               | 4     | 8                        | 32.0  |
| 0                             | 0               | 0               | 4               | 3               | 7     | 9                        | 36.0  |
| 0                             | 2               | 1               | 1               | 1               | 5     | 10                       | 40.0  |
| 0                             | 3               | 2               | 0               | 1               | 6     | 11                       | 44.0  |
| 0                             | 0               | 0               | 1               | 1               | 2     | 12                       | 48.0  |
| 0                             | 3               | 0               | 5               | 0               | 8     | 13                       | 52.0  |
| 0                             | 1               | 0               | 1               | 1               | 3     | 14                       | 56.0  |
| 0                             | 0               | 0               | 3               | 1               | 4     | 15                       | 60.0  |
| 0                             | 1               | 0               | 2               | 0               | 3     | 16                       | 64.0  |
| 1                             | 1               | 0               | 1               | 1               | 4     | 17                       | 68.0  |
| 1                             | 1               | 1               | 1               | 0               | 4     | 18                       | 72.0  |
| 0                             | 0               | 0               | 1               | 1               | 2     | 19                       | 76.0  |
| 0                             | 3               | 0               | 1               | 1               | 5     | 20                       | 80.0  |
| 0                             | 1               | 1               | 1               | 2               | 5     | 21                       | 84.0  |
| 0                             | 0               | 2               | 1               | 0               | 3     | 22                       | 88.0  |
| 0                             | 1               | 0               | 4               | 1               | 6     | 23                       | 92.0  |
| 0                             | 2               | 3               | 3               | 2               | 10    | 24                       | 96.0  |
| 1                             | 4               | 5               | 4               | 10              | 24    | 25                       | 100.0 |

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

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

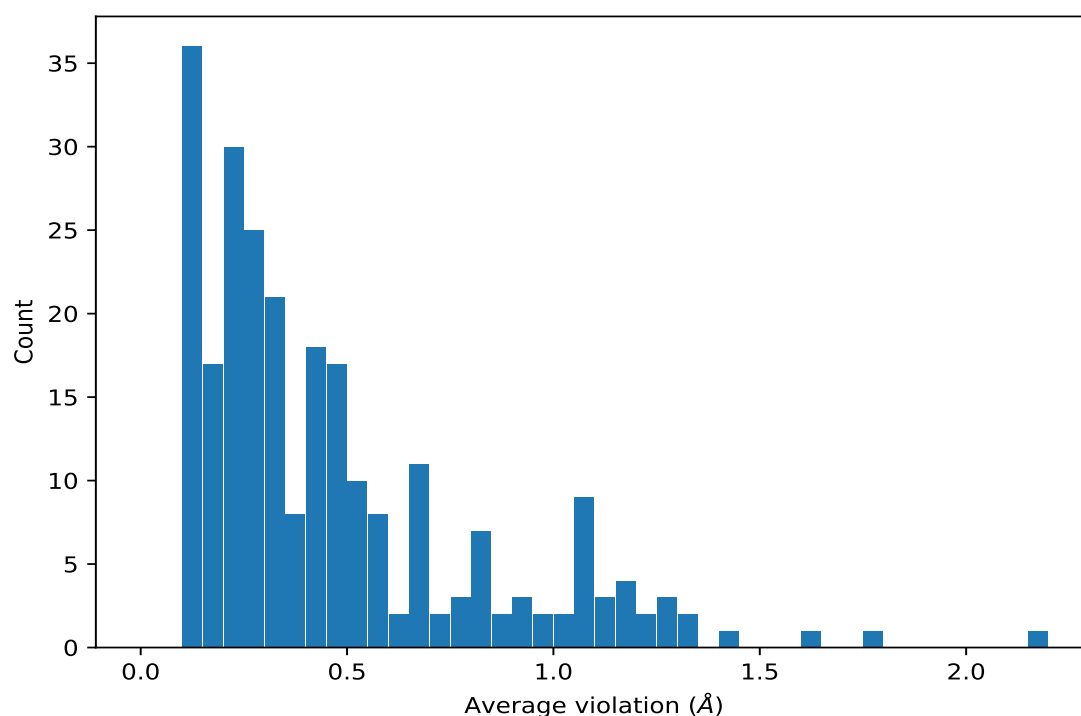
### 9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

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

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



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

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

| Key     | Atom-1          | Atom-2         | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|-----------------|----------------|---------------------|----------|---------------------|------------|
| (1,641) | 2:85:B:SEP:HB2  | 1:17:A:ARG:HB2 | 25                  | 2.15     | 0.18                | 2.1        |
| (1,621) | 1:33:A:GLN:HG2  | 1:37:A:PRO:HD2 | 25                  | 1.79     | 0.2                 | 1.75       |
| (1,333) | 1:34:A:TRP:HE1  | 2:88:B:PRO:HG2 | 25                  | 1.32     | 0.06                | 1.34       |
| (1,751) | 1:33:A:GLN:HE21 | 1:8:A:PRO:HG3  | 25                  | 1.25     | 0.54                | 1.36       |
| (1,453) | 1:11:A:TRP:HE3  | 1:7:A:LEU:HB2  | 25                  | 1.22     | 0.12                | 1.18       |
| (1,175) | 1:30:A:ASN:H    | 1:26:A:ASN:HB2 | 25                  | 1.19     | 0.09                | 1.2        |
| (1,634) | 1:17:A:ARG:HB3  | 1:18:A:SER:HA  | 25                  | 1.15     | 0.06                | 1.17       |
| (1,731) | 2:84:B:TYR:HD1  | 2:83:B:PRO:HB3 | 25                  | 1.11     | 0.07                | 1.12       |
| (1,731) | 2:84:B:TYR:HD2  | 2:83:B:PRO:HB3 | 25                  | 1.11     | 0.07                | 1.12       |
| (1,761) | 1:23:A:TYR:HE1  | 1:21:A:ARG:HB2 | 25                  | 1.09     | 0.44                | 1.08       |
| (1,761) | 1:23:A:TYR:HE2  | 1:21:A:ARG:HB2 | 25                  | 1.09     | 0.44                | 1.08       |
| (1,844) | 1:25:A:PHE:HB3  | 1:14:A:ARG:HB3 | 25                  | 1.07     | 0.28                | 0.99       |
| (1,872) | 2:89:B:GLU:HB2  | 1:16:A:SER:HB3 | 25                  | 0.91     | 0.17                | 0.94       |
| (1,617) | 2:89:B:GLU:HA   | 2:88:B:PRO:HD3 | 25                  | 0.85     | 0.08                | 0.87       |
| (1,837) | 1:21:A:ARG:HA   | 2:88:B:PRO:HB3 | 25                  | 0.82     | 0.16                | 0.84       |
| (1,102) | 1:23:A:TYR:HE1  | 1:25:A:PHE:HB3 | 25                  | 0.69     | 0.26                | 0.82       |

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| Key     | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,102) | 1:23:A:TYR:HE2  | 1:25:A:PHE:HB3  | 25                  | 0.69     | 0.26                | 0.82       |
| (1,465) | 1:23:A:TYR:HE1  | 2:86:B:PRO:HB3  | 25                  | 0.58     | 0.04                | 0.58       |
| (1,465) | 1:23:A:TYR:HE2  | 2:86:B:PRO:HB3  | 25                  | 0.58     | 0.04                | 0.58       |
| (1,516) | 1:11:A:TRP:HH2  | 1:37:A:PRO:HD2  | 25                  | 0.58     | 0.18                | 0.6        |
| (1,876) | 1:27:A:HIS:HD2  | 1:11:A:TRP:H    | 25                  | 0.49     | 0.1                 | 0.49       |
| (1,553) | 1:34:A:TRP:HH2  | 2:86:B:PRO:HB2  | 25                  | 0.47     | 0.05                | 0.47       |
| (1,720) | 2:84:B:TYR:HE1  | 1:23:A:TYR:HE1  | 25                  | 0.41     | 0.17                | 0.4        |
| (1,720) | 2:84:B:TYR:HE1  | 1:23:A:TYR:HE2  | 25                  | 0.41     | 0.17                | 0.4        |
| (1,720) | 2:84:B:TYR:HE2  | 1:23:A:TYR:HE1  | 25                  | 0.41     | 0.17                | 0.4        |
| (1,720) | 2:84:B:TYR:HE2  | 1:23:A:TYR:HE2  | 25                  | 0.41     | 0.17                | 0.4        |
| (1,749) | 1:34:A:TRP:HE1  | 2:88:B:PRO:HB2  | 25                  | 0.36     | 0.08                | 0.37       |
| (1,710) | 1:34:A:TRP:HB3  | 2:86:B:PRO:HD2  | 25                  | 0.34     | 0.05                | 0.33       |
| (1,518) | 1:11:A:TRP:HZ3  | 1:11:A:TRP:HB2  | 25                  | 0.33     | 0.03                | 0.33       |
| (1,114) | 2:87:B:PHE:H    | 2:88:B:PRO:HD2  | 25                  | 0.32     | 0.04                | 0.33       |
| (1,884) | 2:87:B:PHE:HD1  | 1:34:A:TRP:HB3  | 25                  | 0.25     | 0.27                | 0.18       |
| (1,884) | 2:87:B:PHE:HD2  | 1:34:A:TRP:HB3  | 25                  | 0.25     | 0.27                | 0.18       |
| (1,659) | 1:20:A:GLY:H    | 1:16:A:SER:HB2  | 24                  | 1.26     | 0.38                | 1.38       |
| (1,830) | 1:34:A:TRP:HD1  | 1:33:A:GLN:HG2  | 24                  | 0.99     | 0.25                | 1.02       |
| (1,215) | 1:14:A:ARG:H    | 1:13:A:LYS:HG2  | 24                  | 0.96     | 0.11                | 0.99       |
| (1,825) | 2:87:B:PHE:HE1  | 2:81:B:GLY:HA2  | 24                  | 0.93     | 0.68                | 0.9        |
| (1,825) | 2:87:B:PHE:HE2  | 2:81:B:GLY:HA2  | 24                  | 0.93     | 0.68                | 0.9        |
| (1,736) | 1:33:A:GLN:H    | 1:7:A:LEU:HD21  | 24                  | 0.52     | 0.42                | 0.58       |
| (1,736) | 1:33:A:GLN:H    | 1:7:A:LEU:HD22  | 24                  | 0.52     | 0.42                | 0.58       |
| (1,736) | 1:33:A:GLN:H    | 1:7:A:LEU:HD23  | 24                  | 0.52     | 0.42                | 0.58       |
| (1,483) | 1:24:A:TYR:HD1  | 1:37:A:PRO:HB2  | 24                  | 0.4      | 0.23                | 0.3        |
| (1,483) | 1:24:A:TYR:HD2  | 1:37:A:PRO:HB2  | 24                  | 0.4      | 0.23                | 0.3        |
| (1,494) | 1:25:A:PHE:HD1  | 2:83:B:PRO:HG2  | 24                  | 0.39     | 0.04                | 0.4        |
| (1,494) | 1:25:A:PHE:HD2  | 2:83:B:PRO:HG2  | 24                  | 0.39     | 0.04                | 0.4        |
| (1,857) | 1:28:A:ILE:HG13 | 1:31:A:ALA:HB1  | 24                  | 0.35     | 0.24                | 0.17       |
| (1,857) | 1:28:A:ILE:HG13 | 1:31:A:ALA:HB2  | 24                  | 0.35     | 0.24                | 0.17       |
| (1,857) | 1:28:A:ILE:HG13 | 1:31:A:ALA:HB3  | 24                  | 0.35     | 0.24                | 0.17       |
| (1,754) | 1:11:A:TRP:HE3  | 1:13:A:LYS:HB3  | 24                  | 0.26     | 0.06                | 0.26       |
| (1,760) | 2:85:B:SEP:H    | 1:34:A:TRP:HZ2  | 24                  | 0.2      | 0.04                | 0.18       |
| (1,696) | 2:85:B:SEP:HB3  | 2:84:B:TYR:HB3  | 23                  | 0.66     | 0.28                | 0.6        |
| (1,12)  | 1:21:A:ARG:H    | 1:16:A:SER:HB2  | 23                  | 0.62     | 0.34                | 0.54       |
| (1,808) | 1:11:A:TRP:HE3  | 1:37:A:PRO:HD2  | 23                  | 0.37     | 0.17                | 0.33       |
| (1,697) | 2:85:B:SEP:HB3  | 1:17:A:ARG:HA   | 23                  | 0.34     | 0.12                | 0.32       |
| (1,227) | 1:34:A:TRP:HE3  | 1:21:A:ARG:HB2  | 23                  | 0.3      | 0.06                | 0.3        |
| (1,832) | 1:11:A:TRP:HZ2  | 1:37:A:PRO:HD2  | 23                  | 0.27     | 0.09                | 0.26       |
| (1,544) | 1:11:A:TRP:HD1  | 1:7:A:LEU:HB2   | 22                  | 0.45     | 0.14                | 0.44       |
| (1,407) | 1:35:A:GLU:H    | 1:33:A:GLN:HE22 | 22                  | 0.42     | 0.16                | 0.46       |
| (1,770) | 1:25:A:PHE:HE1  | 1:14:A:ARG:HD2  | 22                  | 0.41     | 0.33                | 0.36       |

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| Key     | Atom-1          | Atom-2         | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|-----------------|----------------|---------------------|----------|---------------------|------------|
| (1,770) | 1:25:A:PHE:HE2  | 1:14:A:ARG:HD2 | 22                  | 0.41     | 0.33                | 0.36       |
| (1,137) | 2:85:B:SEP:HB2  | 1:17:A:ARG:HD3 | 21                  | 1.02     | 0.46                | 1.21       |
| (1,674) | 2:86:B:PRO:HD3  | 1:14:A:ARG:HD2 | 21                  | 0.86     | 0.77                | 0.57       |
| (1,841) | 1:5:A:GLU:HA    | 1:6:A:LYS:HB3  | 21                  | 0.81     | 0.3                 | 0.7        |
| (1,820) | 1:21:A:ARG:HB3  | 1:19:A:SER:HA  | 21                  | 0.76     | 0.32                | 0.8        |
| (1,762) | 1:23:A:TYR:HE1  | 1:17:A:ARG:HG3 | 21                  | 0.67     | 0.42                | 0.56       |
| (1,762) | 1:23:A:TYR:HE2  | 1:17:A:ARG:HG3 | 21                  | 0.67     | 0.42                | 0.56       |
| (1,562) | 1:34:A:TRP:HZ2  | 1:16:A:SER:HB3 | 20                  | 0.77     | 0.3                 | 0.81       |
| (1,2)   | 1:13:A:LYS:H    | 1:12:A:GLU:HG2 | 20                  | 0.62     | 0.13                | 0.66       |
| (1,639) | 2:84:B:TYR:HD1  | 1:14:A:ARG:HG2 | 20                  | 0.4      | 0.18                | 0.4        |
| (1,639) | 2:84:B:TYR:HD2  | 1:14:A:ARG:HG2 | 20                  | 0.4      | 0.18                | 0.4        |
| (1,75)  | 1:37:A:PRO:HD3  | 1:36:A:ARG:HD2 | 20                  | 0.34     | 0.15                | 0.3        |
| (1,652) | 1:8:A:PRO:HD2   | 1:9:A:PRO:HA   | 20                  | 0.17     | 0.04                | 0.16       |
| (1,87)  | 1:23:A:TYR:HE1  | 1:16:A:SER:HB3 | 19                  | 0.53     | 0.26                | 0.52       |
| (1,87)  | 1:23:A:TYR:HE2  | 1:16:A:SER:HB3 | 19                  | 0.53     | 0.26                | 0.52       |
| (1,515) | 1:34:A:TRP:HZ3  | 2:88:B:PRO:HB3 | 19                  | 0.14     | 0.03                | 0.13       |
| (1,479) | 1:33:A:GLN:HE21 | 1:35:A:GLU:HB2 | 18                  | 1.19     | 0.51                | 1.19       |
| (1,633) | 1:18:A:SER:HB2  | 1:17:A:ARG:HB3 | 18                  | 0.8      | 0.54                | 0.52       |
| (1,718) | 1:24:A:TYR:HE1  | 1:37:A:PRO:HD2 | 18                  | 0.22     | 0.05                | 0.22       |
| (1,718) | 1:24:A:TYR:HE2  | 1:37:A:PRO:HD2 | 18                  | 0.22     | 0.05                | 0.22       |
| (1,222) | 1:17:A:ARG:HA   | 1:17:A:ARG:HG2 | 18                  | 0.15     | 0.05                | 0.14       |
| (1,683) | 2:83:B:PRO:HD2  | 2:84:B:TYR:HB3 | 17                  | 0.51     | 0.31                | 0.52       |
| (1,254) | 1:11:A:TRP:HE1  | 1:37:A:PRO:HD3 | 17                  | 0.49     | 0.13                | 0.5        |
| (1,836) | 2:88:B:PRO:HA   | 1:17:A:ARG:HG2 | 17                  | 0.41     | 0.22                | 0.49       |
| (1,100) | 1:33:A:GLN:HE22 | 1:33:A:GLN:HG2 | 17                  | 0.15     | 0.01                | 0.14       |
| (1,576) | 1:34:A:TRP:HZ2  | 1:21:A:ARG:HG2 | 16                  | 1.64     | 0.08                | 1.66       |
| (1,506) | 1:25:A:PHE:HE1  | 1:32:A:SER:HB3 | 16                  | 0.23     | 0.06                | 0.24       |
| (1,506) | 1:25:A:PHE:HE2  | 1:32:A:SER:HB3 | 16                  | 0.23     | 0.06                | 0.24       |
| (1,210) | 1:12:A:GLU:H    | 1:11:A:TRP:HB2 | 16                  | 0.13     | 0.02                | 0.12       |
| (1,606) | 1:34:A:TRP:HD1  | 2:89:B:GLU:HG2 | 15                  | 0.71     | 0.23                | 0.73       |
| (1,714) | 1:13:A:LYS:H    | 1:24:A:TYR:HE1 | 15                  | 0.28     | 0.14                | 0.26       |
| (1,714) | 1:13:A:LYS:H    | 1:24:A:TYR:HE2 | 15                  | 0.28     | 0.14                | 0.26       |
| (1,605) | 1:33:A:GLN:HE22 | 1:24:A:TYR:HB3 | 15                  | 0.25     | 0.13                | 0.2        |
| (1,493) | 1:24:A:TYR:HE1  | 1:7:A:LEU:HB3  | 15                  | 0.24     | 0.09                | 0.24       |
| (1,493) | 1:24:A:TYR:HE2  | 1:7:A:LEU:HB3  | 15                  | 0.24     | 0.09                | 0.24       |
| (1,610) | 2:88:B:PRO:HA   | 2:89:B:GLU:HG2 | 14                  | 1.24     | 0.15                | 1.27       |
| (1,8)   | 1:12:A:GLU:H    | 1:7:A:LEU:HD21 | 14                  | 1.06     | 0.32                | 1.12       |
| (1,8)   | 1:12:A:GLU:H    | 1:7:A:LEU:HD22 | 14                  | 1.06     | 0.32                | 1.12       |
| (1,8)   | 1:12:A:GLU:H    | 1:7:A:LEU:HD23 | 14                  | 1.06     | 0.32                | 1.12       |
| (1,468) | 2:85:B:SEP:H    | 1:14:A:ARG:HB3 | 14                  | 0.47     | 0.23                | 0.44       |
| (1,217) | 1:16:A:SER:HB2  | 1:21:A:ARG:HG2 | 13                  | 0.55     | 0.34                | 0.54       |
| (1,343) | 1:25:A:PHE:H    | 1:14:A:ARG:HB3 | 13                  | 0.52     | 0.16                | 0.5        |

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| Key     | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,296) | 1:26:A:ASN:HD22 | 1:10:A:GLY:HA2  | 13                  | 0.46     | 0.26                | 0.41       |
| (1,676) | 1:8:A:PRO:HD3   | 1:7:A:LEU:HD11  | 13                  | 0.45     | 0.23                | 0.37       |
| (1,676) | 1:8:A:PRO:HD3   | 1:7:A:LEU:HD12  | 13                  | 0.45     | 0.23                | 0.37       |
| (1,676) | 1:8:A:PRO:HD3   | 1:7:A:LEU:HD13  | 13                  | 0.45     | 0.23                | 0.37       |
| (1,487) | 1:25:A:PHE:HD1  | 1:14:A:ARG:HB3  | 13                  | 0.43     | 0.07                | 0.47       |
| (1,487) | 1:25:A:PHE:HD2  | 1:14:A:ARG:HB3  | 13                  | 0.43     | 0.07                | 0.47       |
| (1,849) | 1:14:A:ARG:HB3  | 1:15:A:MET:HG3  | 13                  | 0.4      | 0.19                | 0.36       |
| (1,815) | 1:7:A:LEU:HD11  | 1:8:A:PRO:HA    | 13                  | 0.34     | 0.05                | 0.36       |
| (1,815) | 1:7:A:LEU:HD12  | 1:8:A:PRO:HA    | 13                  | 0.34     | 0.05                | 0.36       |
| (1,815) | 1:7:A:LEU:HD13  | 1:8:A:PRO:HA    | 13                  | 0.34     | 0.05                | 0.36       |
| (1,777) | 1:24:A:TYR:HE1  | 1:7:A:LEU:HA    | 13                  | 0.29     | 0.18                | 0.21       |
| (1,777) | 1:24:A:TYR:HE2  | 1:7:A:LEU:HA    | 13                  | 0.29     | 0.18                | 0.21       |
| (1,879) | 2:88:B:PRO:HD2  | 1:17:A:ARG:HD2  | 12                  | 0.4      | 0.19                | 0.38       |
| (1,851) | 1:7:A:LEU:HD11  | 1:37:A:PRO:HD3  | 12                  | 0.32     | 0.2                 | 0.27       |
| (1,851) | 1:7:A:LEU:HD12  | 1:37:A:PRO:HD3  | 12                  | 0.32     | 0.2                 | 0.27       |
| (1,851) | 1:7:A:LEU:HD13  | 1:37:A:PRO:HD3  | 12                  | 0.32     | 0.2                 | 0.27       |
| (1,722) | 2:90:B:GLY:HA2  | 1:21:A:ARG:HG3  | 11                  | 1.3      | 0.77                | 1.31       |
| (1,467) | 1:27:A:HIS:HE1  | 1:28:A:ILE:HG13 | 11                  | 1.19     | 0.35                | 1.3        |
| (1,180) | 1:7:A:LEU:H     | 1:6:A:LYS:HE3   | 11                  | 0.83     | 0.3                 | 0.92       |
| (1,779) | 1:11:A:TRP:HZ3  | 1:7:A:LEU:HD11  | 11                  | 0.5      | 0.15                | 0.45       |
| (1,779) | 1:11:A:TRP:HZ3  | 1:7:A:LEU:HD12  | 11                  | 0.5      | 0.15                | 0.45       |
| (1,779) | 1:11:A:TRP:HZ3  | 1:7:A:LEU:HD13  | 11                  | 0.5      | 0.15                | 0.45       |
| (1,866) | 1:11:A:TRP:HB3  | 1:7:A:LEU:HD21  | 11                  | 0.35     | 0.08                | 0.37       |
| (1,866) | 1:11:A:TRP:HB3  | 1:7:A:LEU:HD22  | 11                  | 0.35     | 0.08                | 0.37       |
| (1,866) | 1:11:A:TRP:HB3  | 1:7:A:LEU:HD23  | 11                  | 0.35     | 0.08                | 0.37       |
| (1,881) | 2:89:B:GLU:HB2  | 2:90:B:GLY:HA2  | 11                  | 0.18     | 0.03                | 0.16       |
| (1,756) | 1:41:A:SER:H    | 1:6:A:LYS:HB2   | 10                  | 0.82     | 0.43                | 0.78       |
| (1,129) | 1:7:A:LEU:HB2   | 1:8:A:PRO:HD3   | 10                  | 0.23     | 0.09                | 0.22       |
| (1,220) | 1:18:A:SER:HA   | 1:17:A:ARG:HD2  | 10                  | 0.2      | 0.05                | 0.2        |
| (1,845) | 1:11:A:TRP:HB2  | 1:7:A:LEU:HB3   | 10                  | 0.12     | 0.01                | 0.12       |
| (1,513) | 1:34:A:TRP:HZ3  | 2:86:B:PRO:HG2  | 10                  | 0.12     | 0.02                | 0.11       |
| (1,322) | 1:17:A:ARG:HD3  | 2:81:B:GLY:HA2  | 9                   | 1.02     | 0.48                | 0.96       |
| (1,783) | 1:34:A:TRP:HZ3  | 2:85:B:SEP:HB2  | 9                   | 0.57     | 0.38                | 0.5        |
| (1,643) | 2:85:B:SEP:HB2  | 1:17:A:ARG:HG2  | 9                   | 0.47     | 0.3                 | 0.42       |
| (1,578) | 1:34:A:TRP:HH2  | 1:21:A:ARG:HD3  | 9                   | 0.27     | 0.13                | 0.26       |
| (1,842) | 1:37:A:PRO:HD2  | 1:7:A:LEU:HD21  | 9                   | 0.21     | 0.03                | 0.21       |
| (1,842) | 1:37:A:PRO:HD2  | 1:7:A:LEU:HD22  | 9                   | 0.21     | 0.03                | 0.21       |
| (1,842) | 1:37:A:PRO:HD2  | 1:7:A:LEU:HD23  | 9                   | 0.21     | 0.03                | 0.21       |
| (1,861) | 1:37:A:PRO:HD2  | 1:7:A:LEU:HD21  | 9                   | 0.21     | 0.03                | 0.21       |
| (1,861) | 1:37:A:PRO:HD2  | 1:7:A:LEU:HD22  | 9                   | 0.21     | 0.03                | 0.21       |
| (1,861) | 1:37:A:PRO:HD2  | 1:7:A:LEU:HD23  | 9                   | 0.21     | 0.03                | 0.21       |
| (1,291) | 1:25:A:PHE:HE1  | 1:32:A:SER:HB2  | 9                   | 0.18     | 0.03                | 0.18       |

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| Key     | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,291) | 1:25:A:PHE:HE2  | 1:32:A:SER:HB2  | 9                   | 0.18     | 0.03                | 0.18       |
| (1,480) | 1:33:A:GLN:HE21 | 1:35:A:GLU:HG2  | 8                   | 0.67     | 0.42                | 0.61       |
| (1,247) | 1:24:A:TYR:HE1  | 1:36:A:ARG:HD2  | 8                   | 0.24     | 0.08                | 0.22       |
| (1,247) | 1:24:A:TYR:HE2  | 1:36:A:ARG:HD2  | 8                   | 0.24     | 0.08                | 0.22       |
| (1,430) | 1:24:A:TYR:HE1  | 1:37:A:PRO:HG2  | 8                   | 0.17     | 0.03                | 0.17       |
| (1,430) | 1:24:A:TYR:HE2  | 1:37:A:PRO:HG2  | 8                   | 0.17     | 0.03                | 0.17       |
| (1,557) | 2:84:B:TYR:HD1  | 2:82:B:SER:HA   | 8                   | 0.13     | 0.02                | 0.12       |
| (1,557) | 2:84:B:TYR:HD2  | 2:82:B:SER:HA   | 8                   | 0.13     | 0.02                | 0.12       |
| (1,798) | 1:34:A:TRP:HZ2  | 1:18:A:SER:HB3  | 7                   | 1.16     | 0.64                | 1.54       |
| (1,604) | 1:33:A:GLN:HE22 | 1:35:A:GLU:HG2  | 7                   | 0.73     | 0.33                | 0.6        |
| (1,682) | 1:23:A:TYR:HB3  | 1:16:A:SER:HB3  | 7                   | 0.32     | 0.14                | 0.29       |
| (1,741) | 1:14:A:ARG:H    | 1:15:A:MET:HG2  | 6                   | 1.29     | 0.14                | 1.35       |
| (1,23)  | 1:36:A:ARG:HD2  | 1:7:A:LEU:HD21  | 6                   | 1.09     | 0.16                | 1.17       |
| (1,23)  | 1:36:A:ARG:HD2  | 1:7:A:LEU:HD22  | 6                   | 1.09     | 0.16                | 1.17       |
| (1,23)  | 1:36:A:ARG:HD2  | 1:7:A:LEU:HD23  | 6                   | 1.09     | 0.16                | 1.17       |
| (1,214) | 1:14:A:ARG:H    | 1:13:A:LYS:HE2  | 6                   | 0.83     | 0.35                | 0.89       |
| (1,94)  | 1:34:A:TRP:HZ3  | 1:21:A:ARG:HG2  | 6                   | 0.2      | 0.04                | 0.22       |
| (1,790) | 1:25:A:PHE:HZ   | 1:27:A:HIS:HB2  | 6                   | 0.18     | 0.06                | 0.17       |
| (1,145) | 1:27:A:HIS:HE1  | 1:25:A:PHE:HD1  | 6                   | 0.14     | 0.05                | 0.12       |
| (1,145) | 1:27:A:HIS:HE1  | 1:25:A:PHE:HD2  | 6                   | 0.14     | 0.05                | 0.12       |
| (1,865) | 1:28:A:ILE:HG21 | 1:27:A:HIS:HB2  | 6                   | 0.11     | 0.01                | 0.11       |
| (1,865) | 1:28:A:ILE:HG22 | 1:27:A:HIS:HB2  | 6                   | 0.11     | 0.01                | 0.11       |
| (1,865) | 1:28:A:ILE:HG23 | 1:27:A:HIS:HB2  | 6                   | 0.11     | 0.01                | 0.11       |
| (1,219) | 1:16:A:SER:HB2  | 1:15:A:MET:HA   | 5                   | 0.87     | 0.07                | 0.87       |
| (1,499) | 1:25:A:PHE:HE1  | 1:12:A:GLU:HG2  | 5                   | 0.68     | 0.48                | 0.52       |
| (1,499) | 1:25:A:PHE:HE2  | 1:12:A:GLU:HG2  | 5                   | 0.68     | 0.48                | 0.52       |
| (1,370) | 1:22:A:VAL:H    | 1:16:A:SER:HB2  | 5                   | 0.46     | 0.08                | 0.45       |
| (1,365) | 1:34:A:TRP:H    | 1:35:A:GLU:HB2  | 5                   | 0.45     | 0.03                | 0.44       |
| (1,704) | 1:16:A:SER:HB3  | 1:17:A:ARG:HA   | 5                   | 0.38     | 0.04                | 0.37       |
| (1,752) | 1:33:A:GLN:HE21 | 1:37:A:PRO:HD3  | 5                   | 0.31     | 0.1                 | 0.34       |
| (1,807) | 1:25:A:PHE:HZ   | 2:83:B:PRO:HB3  | 5                   | 0.24     | 0.13                | 0.2        |
| (1,193) | 1:9:A:PRO:HD3   | 1:8:A:PRO:HG2   | 5                   | 0.23     | 0.06                | 0.26       |
| (1,88)  | 1:33:A:GLN:HE21 | 1:37:A:PRO:HA   | 5                   | 0.21     | 0.07                | 0.18       |
| (1,417) | 1:11:A:TRP:HE3  | 1:26:A:ASN:HB3  | 5                   | 0.14     | 0.03                | 0.14       |
| (1,248) | 2:90:B:GLY:HA2  | 1:18:A:SER:HA   | 4                   | 1.45     | 0.13                | 1.5        |
| (1,342) | 1:25:A:PHE:H    | 1:14:A:ARG:HG2  | 4                   | 0.76     | 0.31                | 0.65       |
| (1,725) | 2:84:B:TYR:HB3  | 1:14:A:ARG:HD2  | 4                   | 0.66     | 0.42                | 0.55       |
| (1,24)  | 1:13:A:LYS:HE2  | 1:22:A:VAL:HG11 | 4                   | 0.57     | 0.3                 | 0.53       |
| (1,24)  | 1:13:A:LYS:HE2  | 1:22:A:VAL:HG12 | 4                   | 0.57     | 0.3                 | 0.53       |
| (1,24)  | 1:13:A:LYS:HE2  | 1:22:A:VAL:HG13 | 4                   | 0.57     | 0.3                 | 0.53       |
| (1,379) | 1:40:A:ASN:H    | 1:9:A:PRO:HD3   | 4                   | 0.48     | 0.3                 | 0.49       |
| (1,501) | 1:24:A:TYR:HE1  | 1:33:A:GLN:HG2  | 4                   | 0.47     | 0.04                | 0.48       |

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| Key     | Atom-1         | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,501) | 1:24:A:TYR:HE2 | 1:33:A:GLN:HG2  | 4                   | 0.47     | 0.04                | 0.48       |
| (1,707) | 1:17:A:ARG:HD3 | 2:88:B:PRO:HD3  | 4                   | 0.37     | 0.21                | 0.36       |
| (1,622) | 1:33:A:GLN:HG2 | 1:24:A:TYR:HB3  | 4                   | 0.3      | 0.13                | 0.3        |
| (1,856) | 1:7:A:LEU:HD11 | 1:36:A:ARG:HG3  | 4                   | 0.29     | 0.2                 | 0.2        |
| (1,856) | 1:7:A:LEU:HD12 | 1:36:A:ARG:HG3  | 4                   | 0.29     | 0.2                 | 0.2        |
| (1,856) | 1:7:A:LEU:HD13 | 1:36:A:ARG:HG3  | 4                   | 0.29     | 0.2                 | 0.2        |
| (1,26)  | 1:22:A:VAL:H   | 1:21:A:ARG:HG3  | 4                   | 0.26     | 0.08                | 0.25       |
| (1,775) | 2:84:B:TYR:HE1 | 2:82:B:SER:HA   | 4                   | 0.16     | 0.02                | 0.16       |
| (1,775) | 2:84:B:TYR:HE2 | 2:82:B:SER:HA   | 4                   | 0.16     | 0.02                | 0.16       |
| (1,258) | 1:33:A:GLN:H   | 1:24:A:TYR:HD1  | 4                   | 0.13     | 0.02                | 0.12       |
| (1,258) | 1:33:A:GLN:H   | 1:24:A:TYR:HD2  | 4                   | 0.13     | 0.02                | 0.12       |
| (1,426) | 1:31:A:ALA:HB1 | 1:26:A:ASN:HB3  | 4                   | 0.11     | 0.01                | 0.11       |
| (1,426) | 1:31:A:ALA:HB2 | 1:26:A:ASN:HB3  | 4                   | 0.11     | 0.01                | 0.11       |
| (1,426) | 1:31:A:ALA:HB3 | 1:26:A:ASN:HB3  | 4                   | 0.11     | 0.01                | 0.11       |
| (1,28)  | 2:85:B:SEP:H   | 2:83:B:PRO:HG2  | 4                   | 0.11     | 0.01                | 0.11       |
| (1,822) | 1:25:A:PHE:HZ  | 1:14:A:ARG:HD2  | 3                   | 0.66     | 0.43                | 0.45       |
| (1,823) | 1:25:A:PHE:HZ  | 1:14:A:ARG:HD2  | 3                   | 0.66     | 0.43                | 0.45       |
| (1,666) | 1:37:A:PRO:HD3 | 1:36:A:ARG:HG3  | 3                   | 0.48     | 0.28                | 0.56       |
| (1,192) | 1:9:A:PRO:HD3  | 1:8:A:PRO:HG3   | 3                   | 0.46     | 0.09                | 0.42       |
| (1,463) | 1:23:A:TYR:HE1 | 1:14:A:ARG:HD2  | 3                   | 0.44     | 0.04                | 0.42       |
| (1,463) | 1:23:A:TYR:HE2 | 1:14:A:ARG:HD2  | 3                   | 0.44     | 0.04                | 0.42       |
| (1,167) | 2:84:B:TYR:HD1 | 2:85:B:SEP:HB2  | 3                   | 0.3      | 0.09                | 0.31       |
| (1,167) | 2:84:B:TYR:HD2 | 2:85:B:SEP:HB2  | 3                   | 0.3      | 0.09                | 0.31       |
| (1,554) | 1:27:A:HIS:HD2 | 1:12:A:GLU:HG2  | 3                   | 0.3      | 0.01                | 0.29       |
| (1,384) | 1:34:A:TRP:HE3 | 1:21:A:ARG:HG2  | 3                   | 0.26     | 0.01                | 0.25       |
| (1,864) | 1:7:A:LEU:HD11 | 1:11:A:TRP:HB3  | 3                   | 0.2      | 0.08                | 0.15       |
| (1,864) | 1:7:A:LEU:HD12 | 1:11:A:TRP:HB3  | 3                   | 0.2      | 0.08                | 0.15       |
| (1,864) | 1:7:A:LEU:HD13 | 1:11:A:TRP:HB3  | 3                   | 0.2      | 0.08                | 0.15       |
| (1,118) | 1:24:A:TYR:HA  | 1:13:A:LYS:HG3  | 3                   | 0.2      | 0.09                | 0.13       |
| (1,547) | 1:11:A:TRP:HD1 | 1:7:A:LEU:HD11  | 3                   | 0.17     | 0.02                | 0.17       |
| (1,547) | 1:11:A:TRP:HD1 | 1:7:A:LEU:HD12  | 3                   | 0.17     | 0.02                | 0.17       |
| (1,547) | 1:11:A:TRP:HD1 | 1:7:A:LEU:HD13  | 3                   | 0.17     | 0.02                | 0.17       |
| (1,466) | 1:27:A:HIS:HE1 | 1:28:A:ILE:HD11 | 3                   | 0.13     | 0.02                | 0.12       |
| (1,466) | 1:27:A:HIS:HE1 | 1:28:A:ILE:HD12 | 3                   | 0.13     | 0.02                | 0.12       |
| (1,466) | 1:27:A:HIS:HE1 | 1:28:A:ILE:HD13 | 3                   | 0.13     | 0.02                | 0.12       |
| (1,372) | 2:81:B:GLY:H   | 2:82:B:SER:HB2  | 3                   | 0.12     | 0.01                | 0.13       |
| (1,594) | 1:25:A:PHE:HZ  | 2:84:B:TYR:HB2  | 3                   | 0.12     | 0.02                | 0.11       |
| (1,875) | 2:84:B:TYR:HD1 | 1:30:A:ASN:HD22 | 2                   | 0.36     | 0.13                | 0.36       |
| (1,875) | 2:84:B:TYR:HD2 | 1:30:A:ASN:HD22 | 2                   | 0.36     | 0.13                | 0.36       |
| (1,362) | 1:7:A:LEU:H    | 1:36:A:ARG:HG3  | 2                   | 0.35     | 0.15                | 0.35       |
| (1,433) | 1:11:A:TRP:HZ3 | 1:37:A:PRO:HG2  | 2                   | 0.34     | 0.06                | 0.34       |
| (1,658) | 1:17:A:ARG:HD3 | 2:88:B:PRO:HD3  | 2                   | 0.28     | 0.07                | 0.28       |

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| Key     | Atom-1         | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,689) | 1:14:A:ARG:HD2 | 2:84:B:TYR:HA   | 2                   | 0.28     | 0.18                | 0.28       |
| (1,769) | 1:25:A:PHE:HE1 | 2:83:B:PRO:HB3  | 2                   | 0.28     | 0.07                | 0.28       |
| (1,769) | 1:25:A:PHE:HE2 | 2:83:B:PRO:HB3  | 2                   | 0.28     | 0.07                | 0.28       |
| (1,281) | 1:16:A:SER:H   | 2:85:B:SEP:HB2  | 2                   | 0.25     | 0.11                | 0.25       |
| (1,715) | 1:16:A:SER:H   | 1:15:A:MET:HE1  | 2                   | 0.24     | 0.03                | 0.24       |
| (1,715) | 1:16:A:SER:H   | 1:15:A:MET:HE2  | 2                   | 0.24     | 0.03                | 0.24       |
| (1,715) | 1:16:A:SER:H   | 1:15:A:MET:HE3  | 2                   | 0.24     | 0.03                | 0.24       |
| (1,776) | 1:24:A:TYR:HD1 | 1:7:A:LEU:HA    | 2                   | 0.22     | 0.05                | 0.22       |
| (1,776) | 1:24:A:TYR:HD2 | 1:7:A:LEU:HA    | 2                   | 0.22     | 0.05                | 0.22       |
| (1,21)  | 1:16:A:SER:H   | 1:15:A:MET:HG2  | 2                   | 0.18     | 0.05                | 0.18       |
| (1,828) | 1:11:A:TRP:HZ2 | 1:29:A:THR:HG21 | 2                   | 0.18     | 0.04                | 0.18       |
| (1,828) | 1:11:A:TRP:HZ2 | 1:29:A:THR:HG22 | 2                   | 0.18     | 0.04                | 0.18       |
| (1,828) | 1:11:A:TRP:HZ2 | 1:29:A:THR:HG23 | 2                   | 0.18     | 0.04                | 0.18       |
| (1,437) | 1:11:A:TRP:HD1 | 1:37:A:PRO:HG3  | 2                   | 0.16     | 0.04                | 0.16       |
| (1,510) | 1:25:A:PHE:HD1 | 1:30:A:ASN:HA   | 2                   | 0.12     | 0.02                | 0.12       |
| (1,510) | 1:25:A:PHE:HD2 | 1:30:A:ASN:HA   | 2                   | 0.12     | 0.02                | 0.12       |
| (1,383) | 1:34:A:TRP:HE3 | 1:22:A:VAL:HG21 | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,383) | 1:34:A:TRP:HE3 | 1:22:A:VAL:HG22 | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,383) | 1:34:A:TRP:HE3 | 1:22:A:VAL:HG23 | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,105) | 1:24:A:TYR:HE1 | 1:7:A:LEU:HD21  | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,105) | 1:24:A:TYR:HE1 | 1:7:A:LEU:HD22  | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,105) | 1:24:A:TYR:HE1 | 1:7:A:LEU:HD23  | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,105) | 1:24:A:TYR:HE2 | 1:7:A:LEU:HD21  | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,105) | 1:24:A:TYR:HE2 | 1:7:A:LEU:HD22  | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,105) | 1:24:A:TYR:HE2 | 1:7:A:LEU:HD23  | 2                   | 0.11     | 0.0                 | 0.11       |

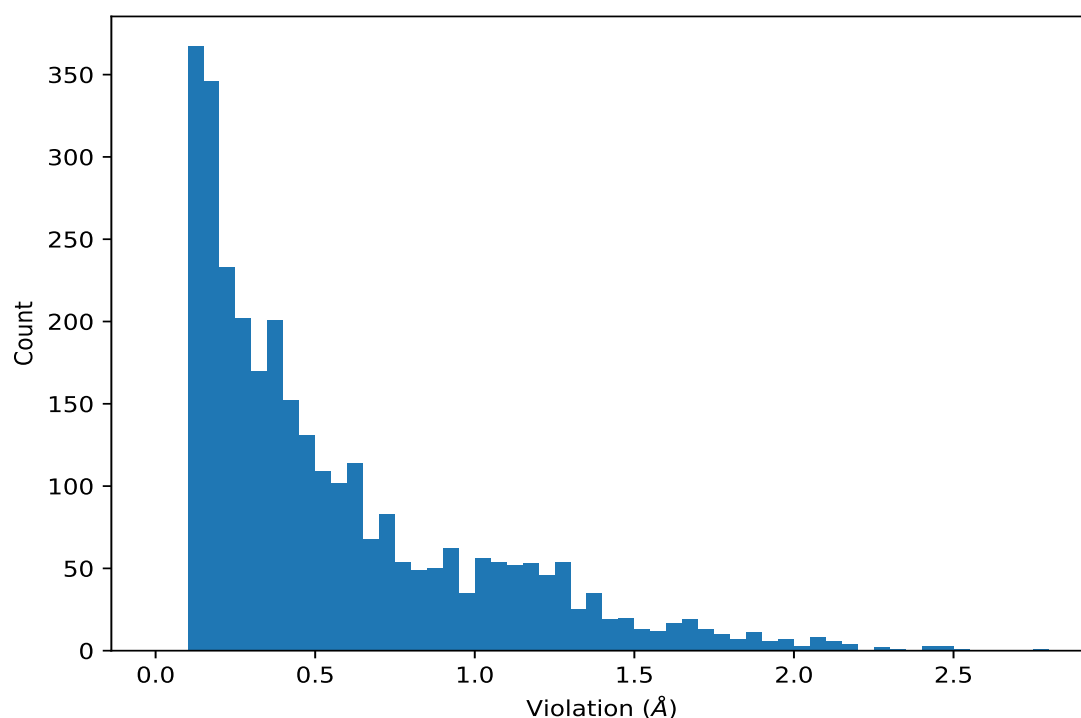
<sup>1</sup>Number of violated models, <sup>2</sup>Standard deviation

## 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) |
|---------|----------------|----------------|----------|---------------|
| (1,674) | 2:86:B:PRO:HD3 | 1:14:A:ARG:HD2 | 20       | 2.76          |
| (1,641) | 2:85:B:SEP:HB2 | 1:17:A:ARG:HB2 | 24       | 2.5           |
| (1,641) | 2:85:B:SEP:HB2 | 1:17:A:ARG:HB2 | 20       | 2.49          |
| (1,722) | 2:90:B:GLY:HA2 | 1:21:A:ARG:HG3 | 8        | 2.47          |
| (1,641) | 2:85:B:SEP:HB2 | 1:17:A:ARG:HB2 | 17       | 2.45          |
| (1,674) | 2:86:B:PRO:HD3 | 1:14:A:ARG:HD2 | 8        | 2.41          |
| (1,641) | 2:85:B:SEP:HB2 | 1:17:A:ARG:HB2 | 4        | 2.41          |
| (1,641) | 2:85:B:SEP:HB2 | 1:17:A:ARG:HB2 | 9        | 2.4           |
| (1,674) | 2:86:B:PRO:HD3 | 1:14:A:ARG:HD2 | 21       | 2.32          |
| (1,641) | 2:85:B:SEP:HB2 | 1:17:A:ARG:HB2 | 5        | 2.29          |
| (1,641) | 2:85:B:SEP:HB2 | 1:17:A:ARG:HB2 | 16       | 2.27          |
| (1,621) | 1:33:A:GLN:HG2 | 1:37:A:PRO:HD2 | 9        | 2.19          |
| (1,621) | 1:33:A:GLN:HG2 | 1:37:A:PRO:HD2 | 4        | 2.18          |
| (1,641) | 2:85:B:SEP:HB2 | 1:17:A:ARG:HB2 | 19       | 2.17          |
| (1,641) | 2:85:B:SEP:HB2 | 1:17:A:ARG:HB2 | 14       | 2.15          |
| (1,641) | 2:85:B:SEP:HB2 | 1:17:A:ARG:HB2 | 8        | 2.14          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,641) | 2:85:B:SEP:HB2  | 1:17:A:ARG:HB2 | 25       | 2.13          |
| (1,751) | 1:33:A:GLN:HE21 | 1:8:A:PRO:HG3  | 17       | 2.12          |
| (1,641) | 2:85:B:SEP:HB2  | 1:17:A:ARG:HB2 | 23       | 2.12          |
| (1,641) | 2:85:B:SEP:HB2  | 1:17:A:ARG:HB2 | 12       | 2.1           |
| (1,641) | 2:85:B:SEP:HB2  | 1:17:A:ARG:HB2 | 13       | 2.1           |
| (1,722) | 2:90:B:GLY:HA2  | 1:21:A:ARG:HG3 | 20       | 2.08          |
| (1,621) | 1:33:A:GLN:HG2  | 1:37:A:PRO:HD2 | 22       | 2.08          |
| (1,641) | 2:85:B:SEP:HB2  | 1:17:A:ARG:HB2 | 1        | 2.07          |
| (1,641) | 2:85:B:SEP:HB2  | 1:17:A:ARG:HB2 | 2        | 2.07          |
| (1,641) | 2:85:B:SEP:HB2  | 1:17:A:ARG:HB2 | 10       | 2.07          |
| (1,641) | 2:85:B:SEP:HB2  | 1:17:A:ARG:HB2 | 21       | 2.07          |
| (1,641) | 2:85:B:SEP:HB2  | 1:17:A:ARG:HB2 | 7        | 2.06          |
| (1,641) | 2:85:B:SEP:HB2  | 1:17:A:ARG:HB2 | 15       | 2.05          |
| (1,621) | 1:33:A:GLN:HG2  | 1:37:A:PRO:HD2 | 14       | 2.04          |
| (1,641) | 2:85:B:SEP:HB2  | 1:17:A:ARG:HB2 | 3        | 2.03          |
| (1,621) | 1:33:A:GLN:HG2  | 1:37:A:PRO:HD2 | 1        | 2.02          |
| (1,761) | 1:23:A:TYR:HE1  | 1:21:A:ARG:HB2 | 20       | 1.99          |
| (1,761) | 1:23:A:TYR:HE2  | 1:21:A:ARG:HB2 | 20       | 1.99          |
| (1,621) | 1:33:A:GLN:HG2  | 1:37:A:PRO:HD2 | 25       | 1.99          |
| (1,751) | 1:33:A:GLN:HE21 | 1:8:A:PRO:HG3  | 13       | 1.98          |
| (1,641) | 2:85:B:SEP:HB2  | 1:17:A:ARG:HB2 | 6        | 1.97          |
| (1,641) | 2:85:B:SEP:HB2  | 1:17:A:ARG:HB2 | 22       | 1.97          |
| (1,641) | 2:85:B:SEP:HB2  | 1:17:A:ARG:HB2 | 18       | 1.95          |
| (1,621) | 1:33:A:GLN:HG2  | 1:37:A:PRO:HD2 | 7        | 1.94          |
| (1,736) | 1:33:A:GLN:H    | 1:7:A:LEU:HD21 | 19       | 1.92          |
| (1,736) | 1:33:A:GLN:H    | 1:7:A:LEU:HD22 | 19       | 1.92          |
| (1,736) | 1:33:A:GLN:H    | 1:7:A:LEU:HD23 | 19       | 1.92          |
| (1,479) | 1:33:A:GLN:HE21 | 1:35:A:GLU:HB2 | 18       | 1.91          |
| (1,722) | 2:90:B:GLY:HA2  | 1:21:A:ARG:HG3 | 5        | 1.9           |
| (1,751) | 1:33:A:GLN:HE21 | 1:8:A:PRO:HG3  | 4        | 1.89          |
| (1,621) | 1:33:A:GLN:HG2  | 1:37:A:PRO:HD2 | 3        | 1.89          |
| (1,322) | 1:17:A:ARG:HD3  | 2:81:B:GLY:HA2 | 5        | 1.89          |
| (1,137) | 2:85:B:SEP:HB2  | 1:17:A:ARG:HD3 | 17       | 1.88          |
| (1,761) | 1:23:A:TYR:HE1  | 1:21:A:ARG:HB2 | 16       | 1.87          |
| (1,761) | 1:23:A:TYR:HE2  | 1:21:A:ARG:HB2 | 16       | 1.87          |
| (1,751) | 1:33:A:GLN:HE21 | 1:8:A:PRO:HG3  | 10       | 1.87          |
| (1,479) | 1:33:A:GLN:HE21 | 1:35:A:GLU:HB2 | 10       | 1.87          |
| (1,722) | 2:90:B:GLY:HA2  | 1:21:A:ARG:HG3 | 1        | 1.86          |
| (1,621) | 1:33:A:GLN:HG2  | 1:37:A:PRO:HD2 | 11       | 1.86          |
| (1,621) | 1:33:A:GLN:HG2  | 1:37:A:PRO:HD2 | 20       | 1.85          |
| (1,751) | 1:33:A:GLN:HE21 | 1:8:A:PRO:HG3  | 8        | 1.82          |
| (1,825) | 2:87:B:PHE:HE1  | 2:81:B:GLY:HA2 | 10       | 1.81          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,825) | 2:87:B:PHE:HE2  | 2:81:B:GLY:HA2 | 10       | 1.81          |
| (1,825) | 2:87:B:PHE:HE1  | 2:81:B:GLY:HA2 | 18       | 1.8           |
| (1,825) | 2:87:B:PHE:HE2  | 2:81:B:GLY:HA2 | 18       | 1.8           |
| (1,825) | 2:87:B:PHE:HE1  | 2:81:B:GLY:HA2 | 19       | 1.8           |
| (1,825) | 2:87:B:PHE:HE2  | 2:81:B:GLY:HA2 | 19       | 1.8           |
| (1,751) | 1:33:A:GLN:HE21 | 1:8:A:PRO:HG3  | 15       | 1.79          |
| (1,722) | 2:90:B:GLY:HA2  | 1:21:A:ARG:HG3 | 16       | 1.79          |
| (1,756) | 1:41:A:SER:H    | 1:6:A:LYS:HB2  | 1        | 1.78          |
| (1,641) | 2:85:B:SEP:HB2  | 1:17:A:ARG:HB2 | 11       | 1.78          |
| (1,479) | 1:33:A:GLN:HE21 | 1:35:A:GLU:HB2 | 23       | 1.77          |
| (1,825) | 2:87:B:PHE:HE1  | 2:81:B:GLY:HA2 | 11       | 1.76          |
| (1,825) | 2:87:B:PHE:HE2  | 2:81:B:GLY:HA2 | 11       | 1.76          |
| (1,621) | 1:33:A:GLN:HG2  | 1:37:A:PRO:HD2 | 13       | 1.76          |
| (1,621) | 1:33:A:GLN:HG2  | 1:37:A:PRO:HD2 | 24       | 1.76          |
| (1,621) | 1:33:A:GLN:HG2  | 1:37:A:PRO:HD2 | 17       | 1.75          |
| (1,479) | 1:33:A:GLN:HE21 | 1:35:A:GLU:HB2 | 5        | 1.74          |
| (1,825) | 2:87:B:PHE:HE1  | 2:81:B:GLY:HA2 | 17       | 1.73          |
| (1,825) | 2:87:B:PHE:HE2  | 2:81:B:GLY:HA2 | 17       | 1.73          |
| (1,479) | 1:33:A:GLN:HE21 | 1:35:A:GLU:HB2 | 15       | 1.73          |
| (1,770) | 1:25:A:PHE:HE1  | 1:14:A:ARG:HD2 | 20       | 1.72          |
| (1,770) | 1:25:A:PHE:HE2  | 1:14:A:ARG:HD2 | 20       | 1.72          |
| (1,621) | 1:33:A:GLN:HG2  | 1:37:A:PRO:HD2 | 2        | 1.71          |
| (1,576) | 1:34:A:TRP:HZ2  | 1:21:A:ARG:HG2 | 10       | 1.71          |
| (1,576) | 1:34:A:TRP:HZ2  | 1:21:A:ARG:HG2 | 14       | 1.71          |
| (1,576) | 1:34:A:TRP:HZ2  | 1:21:A:ARG:HG2 | 25       | 1.71          |
| (1,621) | 1:33:A:GLN:HG2  | 1:37:A:PRO:HD2 | 18       | 1.7           |
| (1,576) | 1:34:A:TRP:HZ2  | 1:21:A:ARG:HG2 | 9        | 1.7           |
| (1,576) | 1:34:A:TRP:HZ2  | 1:21:A:ARG:HG2 | 15       | 1.7           |
| (1,621) | 1:33:A:GLN:HG2  | 1:37:A:PRO:HD2 | 19       | 1.69          |
| (1,576) | 1:34:A:TRP:HZ2  | 1:21:A:ARG:HG2 | 13       | 1.69          |
| (1,659) | 1:20:A:GLY:H    | 1:16:A:SER:HB2 | 20       | 1.68          |
| (1,621) | 1:33:A:GLN:HG2  | 1:37:A:PRO:HD2 | 12       | 1.67          |
| (1,576) | 1:34:A:TRP:HZ2  | 1:21:A:ARG:HG2 | 19       | 1.67          |
| (1,798) | 1:34:A:TRP:HZ2  | 1:18:A:SER:HB3 | 23       | 1.66          |
| (1,751) | 1:33:A:GLN:HE21 | 1:8:A:PRO:HG3  | 18       | 1.66          |
| (1,659) | 1:20:A:GLY:H    | 1:16:A:SER:HB2 | 15       | 1.66          |
| (1,621) | 1:33:A:GLN:HG2  | 1:37:A:PRO:HD2 | 15       | 1.66          |
| (1,576) | 1:34:A:TRP:HZ2  | 1:21:A:ARG:HG2 | 21       | 1.66          |
| (1,576) | 1:34:A:TRP:HZ2  | 1:21:A:ARG:HG2 | 23       | 1.66          |
| (1,825) | 2:87:B:PHE:HE1  | 2:81:B:GLY:HA2 | 12       | 1.65          |
| (1,825) | 2:87:B:PHE:HE2  | 2:81:B:GLY:HA2 | 12       | 1.65          |
| (1,762) | 1:23:A:TYR:HE1  | 1:17:A:ARG:HG3 | 20       | 1.65          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,762) | 1:23:A:TYR:HE2  | 1:17:A:ARG:HG3 | 20       | 1.65          |
| (1,659) | 1:20:A:GLY:H    | 1:16:A:SER:HB2 | 16       | 1.65          |
| (1,576) | 1:34:A:TRP:HZ2  | 1:21:A:ARG:HG2 | 7        | 1.65          |
| (1,576) | 1:34:A:TRP:HZ2  | 1:21:A:ARG:HG2 | 12       | 1.65          |
| (1,479) | 1:33:A:GLN:HE21 | 1:35:A:GLU:HB2 | 12       | 1.65          |
| (1,621) | 1:33:A:GLN:HG2  | 1:37:A:PRO:HD2 | 16       | 1.64          |
| (1,576) | 1:34:A:TRP:HZ2  | 1:21:A:ARG:HG2 | 4        | 1.64          |
| (1,761) | 1:23:A:TYR:HE1  | 1:21:A:ARG:HB2 | 1        | 1.63          |
| (1,761) | 1:23:A:TYR:HE2  | 1:21:A:ARG:HB2 | 1        | 1.63          |
| (1,659) | 1:20:A:GLY:H    | 1:16:A:SER:HB2 | 25       | 1.63          |
| (1,576) | 1:34:A:TRP:HZ2  | 1:21:A:ARG:HG2 | 18       | 1.63          |
| (1,825) | 2:87:B:PHE:HE1  | 2:81:B:GLY:HA2 | 16       | 1.62          |
| (1,825) | 2:87:B:PHE:HE2  | 2:81:B:GLY:HA2 | 16       | 1.62          |
| (1,761) | 1:23:A:TYR:HE1  | 1:21:A:ARG:HB2 | 22       | 1.61          |
| (1,761) | 1:23:A:TYR:HE2  | 1:21:A:ARG:HB2 | 22       | 1.61          |
| (1,674) | 2:86:B:PRO:HD3  | 1:14:A:ARG:HD2 | 6        | 1.61          |
| (1,659) | 1:20:A:GLY:H    | 1:16:A:SER:HB2 | 4        | 1.61          |
| (1,825) | 2:87:B:PHE:HE1  | 2:81:B:GLY:HA2 | 23       | 1.6           |
| (1,825) | 2:87:B:PHE:HE2  | 2:81:B:GLY:HA2 | 23       | 1.6           |
| (1,751) | 1:33:A:GLN:HE21 | 1:8:A:PRO:HG3  | 7        | 1.6           |
| (1,696) | 2:85:B:SEP:HB3  | 2:84:B:TYR:HB3 | 17       | 1.6           |
| (1,621) | 1:33:A:GLN:HG2  | 1:37:A:PRO:HD2 | 10       | 1.6           |
| (1,798) | 1:34:A:TRP:HZ2  | 1:18:A:SER:HB3 | 5        | 1.59          |
| (1,798) | 1:34:A:TRP:HZ2  | 1:18:A:SER:HB3 | 14       | 1.59          |
| (1,621) | 1:33:A:GLN:HG2  | 1:37:A:PRO:HD2 | 21       | 1.59          |
| (1,659) | 1:20:A:GLY:H    | 1:16:A:SER:HB2 | 1        | 1.58          |
| (1,576) | 1:34:A:TRP:HZ2  | 1:21:A:ARG:HG2 | 3        | 1.58          |
| (1,659) | 1:20:A:GLY:H    | 1:16:A:SER:HB2 | 9        | 1.57          |
| (1,621) | 1:33:A:GLN:HG2  | 1:37:A:PRO:HD2 | 6        | 1.57          |
| (1,248) | 2:90:B:GLY:HA2  | 1:18:A:SER:HA  | 8        | 1.57          |
| (1,783) | 1:34:A:TRP:HZ3  | 2:85:B:SEP:HB2 | 17       | 1.56          |
| (1,825) | 2:87:B:PHE:HE1  | 2:81:B:GLY:HA2 | 13       | 1.55          |
| (1,825) | 2:87:B:PHE:HE2  | 2:81:B:GLY:HA2 | 13       | 1.55          |
| (1,621) | 1:33:A:GLN:HG2  | 1:37:A:PRO:HD2 | 23       | 1.55          |
| (1,798) | 1:34:A:TRP:HZ2  | 1:18:A:SER:HB3 | 9        | 1.54          |
| (1,674) | 2:86:B:PRO:HD3  | 1:14:A:ARG:HD2 | 18       | 1.54          |
| (1,751) | 1:33:A:GLN:HE21 | 1:8:A:PRO:HG3  | 20       | 1.53          |
| (1,576) | 1:34:A:TRP:HZ2  | 1:21:A:ARG:HG2 | 2        | 1.53          |
| (1,751) | 1:33:A:GLN:HE21 | 1:8:A:PRO:HG3  | 12       | 1.52          |
| (1,659) | 1:20:A:GLY:H    | 1:16:A:SER:HB2 | 7        | 1.51          |
| (1,248) | 2:90:B:GLY:HA2  | 1:18:A:SER:HA  | 9        | 1.51          |
| (1,137) | 2:85:B:SEP:HB2  | 1:17:A:ARG:HD3 | 5        | 1.51          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,761) | 1:23:A:TYR:HE1  | 1:21:A:ARG:HB2 | 15       | 1.5           |
| (1,761) | 1:23:A:TYR:HE2  | 1:21:A:ARG:HB2 | 15       | 1.5           |
| (1,8)   | 1:12:A:GLU:H    | 1:7:A:LEU:HD21 | 19       | 1.5           |
| (1,8)   | 1:12:A:GLU:H    | 1:7:A:LEU:HD22 | 19       | 1.5           |
| (1,8)   | 1:12:A:GLU:H    | 1:7:A:LEU:HD23 | 19       | 1.5           |
| (1,659) | 1:20:A:GLY:H    | 1:16:A:SER:HB2 | 23       | 1.49          |
| (1,621) | 1:33:A:GLN:HG2  | 1:37:A:PRO:HD2 | 5        | 1.49          |
| (1,248) | 2:90:B:GLY:HA2  | 1:18:A:SER:HA  | 1        | 1.49          |
| (1,659) | 1:20:A:GLY:H    | 1:16:A:SER:HB2 | 6        | 1.48          |
| (1,844) | 1:25:A:PHE:HB3  | 1:14:A:ARG:HB3 | 3        | 1.47          |
| (1,844) | 1:25:A:PHE:HB3  | 1:14:A:ARG:HB3 | 5        | 1.47          |
| (1,844) | 1:25:A:PHE:HB3  | 1:14:A:ARG:HB3 | 16       | 1.47          |
| (1,761) | 1:23:A:TYR:HE1  | 1:21:A:ARG:HB2 | 5        | 1.47          |
| (1,761) | 1:23:A:TYR:HE2  | 1:21:A:ARG:HB2 | 5        | 1.47          |
| (1,751) | 1:33:A:GLN:HE21 | 1:8:A:PRO:HG3  | 21       | 1.47          |
| (1,659) | 1:20:A:GLY:H    | 1:16:A:SER:HB2 | 12       | 1.47          |
| (1,633) | 1:18:A:SER:HB2  | 1:17:A:ARG:HB3 | 10       | 1.47          |
| (1,621) | 1:33:A:GLN:HG2  | 1:37:A:PRO:HD2 | 8        | 1.47          |
| (1,798) | 1:34:A:TRP:HZ2  | 1:18:A:SER:HB3 | 8        | 1.46          |
| (1,659) | 1:20:A:GLY:H    | 1:16:A:SER:HB2 | 22       | 1.46          |
| (1,633) | 1:18:A:SER:HB2  | 1:17:A:ARG:HB3 | 7        | 1.46          |
| (1,633) | 1:18:A:SER:HB2  | 1:17:A:ARG:HB3 | 20       | 1.46          |
| (1,137) | 2:85:B:SEP:HB2  | 1:17:A:ARG:HD3 | 4        | 1.46          |
| (1,830) | 1:34:A:TRP:HD1  | 1:33:A:GLN:HG2 | 3        | 1.45          |
| (1,633) | 1:18:A:SER:HB2  | 1:17:A:ARG:HB3 | 3        | 1.45          |
| (1,610) | 2:88:B:PRO:HA   | 2:89:B:GLU:HG2 | 24       | 1.44          |
| (1,453) | 1:11:A:TRP:HE3  | 1:7:A:LEU:HB2  | 21       | 1.44          |
| (1,322) | 1:17:A:ARG:HD3  | 2:81:B:GLY:HA2 | 22       | 1.44          |
| (1,844) | 1:25:A:PHE:HB3  | 1:14:A:ARG:HB3 | 23       | 1.43          |
| (1,322) | 1:17:A:ARG:HD3  | 2:81:B:GLY:HA2 | 20       | 1.43          |
| (1,137) | 2:85:B:SEP:HB2  | 1:17:A:ARG:HD3 | 20       | 1.43          |
| (1,751) | 1:33:A:GLN:HE21 | 1:8:A:PRO:HG3  | 2        | 1.42          |
| (1,633) | 1:18:A:SER:HB2  | 1:17:A:ARG:HB3 | 1        | 1.42          |
| (1,610) | 2:88:B:PRO:HA   | 2:89:B:GLU:HG2 | 4        | 1.42          |
| (1,499) | 1:25:A:PHE:HE1  | 1:12:A:GLU:HG2 | 11       | 1.42          |
| (1,499) | 1:25:A:PHE:HE2  | 1:12:A:GLU:HG2 | 11       | 1.42          |
| (1,333) | 1:34:A:TRP:HE1  | 2:88:B:PRO:HG2 | 4        | 1.42          |
| (1,333) | 1:34:A:TRP:HE1  | 2:88:B:PRO:HG2 | 20       | 1.42          |
| (1,479) | 1:33:A:GLN:HE21 | 1:35:A:GLU:HB2 | 22       | 1.41          |
| (1,137) | 2:85:B:SEP:HB2  | 1:17:A:ARG:HD3 | 10       | 1.41          |
| (1,844) | 1:25:A:PHE:HB3  | 1:14:A:ARG:HB3 | 9        | 1.4           |
| (1,741) | 1:14:A:ARG:H    | 1:15:A:MET:HG2 | 16       | 1.4           |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,633) | 1:18:A:SER:HB2  | 1:17:A:ARG:HB3  | 17       | 1.4           |
| (1,453) | 1:11:A:TRP:HE3  | 1:7:A:LEU:HB2   | 23       | 1.4           |
| (1,741) | 1:14:A:ARG:H    | 1:15:A:MET:HG2  | 10       | 1.39          |
| (1,576) | 1:34:A:TRP:HZ2  | 1:21:A:ARG:HG2  | 11       | 1.39          |
| (1,333) | 1:34:A:TRP:HE1  | 2:88:B:PRO:HG2  | 22       | 1.39          |
| (1,453) | 1:11:A:TRP:HE3  | 1:7:A:LEU:HB2   | 6        | 1.38          |
| (1,333) | 1:34:A:TRP:HE1  | 2:88:B:PRO:HG2  | 24       | 1.38          |
| (1,761) | 1:23:A:TYR:HE1  | 1:21:A:ARG:HB2  | 6        | 1.37          |
| (1,761) | 1:23:A:TYR:HE2  | 1:21:A:ARG:HB2  | 6        | 1.37          |
| (1,610) | 2:88:B:PRO:HA   | 2:89:B:GLU:HG2  | 3        | 1.37          |
| (1,610) | 2:88:B:PRO:HA   | 2:89:B:GLU:HG2  | 21       | 1.37          |
| (1,453) | 1:11:A:TRP:HE3  | 1:7:A:LEU:HB2   | 19       | 1.37          |
| (1,453) | 1:11:A:TRP:HE3  | 1:7:A:LEU:HB2   | 24       | 1.37          |
| (1,333) | 1:34:A:TRP:HE1  | 2:88:B:PRO:HG2  | 1        | 1.37          |
| (1,333) | 1:34:A:TRP:HE1  | 2:88:B:PRO:HG2  | 6        | 1.37          |
| (1,333) | 1:34:A:TRP:HE1  | 2:88:B:PRO:HG2  | 7        | 1.37          |
| (1,8)   | 1:12:A:GLU:H    | 1:7:A:LEU:HD21  | 8        | 1.37          |
| (1,8)   | 1:12:A:GLU:H    | 1:7:A:LEU:HD22  | 8        | 1.37          |
| (1,8)   | 1:12:A:GLU:H    | 1:7:A:LEU:HD23  | 8        | 1.37          |
| (1,844) | 1:25:A:PHE:HB3  | 1:14:A:ARG:HB3  | 1        | 1.36          |
| (1,761) | 1:23:A:TYR:HE1  | 1:21:A:ARG:HB2  | 10       | 1.36          |
| (1,761) | 1:23:A:TYR:HE2  | 1:21:A:ARG:HB2  | 10       | 1.36          |
| (1,751) | 1:33:A:GLN:HE21 | 1:8:A:PRO:HG3   | 22       | 1.36          |
| (1,741) | 1:14:A:ARG:H    | 1:15:A:MET:HG2  | 6        | 1.36          |
| (1,610) | 2:88:B:PRO:HA   | 2:89:B:GLU:HG2  | 9        | 1.36          |
| (1,333) | 1:34:A:TRP:HE1  | 2:88:B:PRO:HG2  | 2        | 1.36          |
| (1,333) | 1:34:A:TRP:HE1  | 2:88:B:PRO:HG2  | 12       | 1.36          |
| (1,175) | 1:30:A:ASN:H    | 1:26:A:ASN:HB2  | 24       | 1.36          |
| (1,825) | 2:87:B:PHE:HE1  | 2:81:B:GLY:HA2  | 3        | 1.35          |
| (1,825) | 2:87:B:PHE:HE2  | 2:81:B:GLY:HA2  | 3        | 1.35          |
| (1,751) | 1:33:A:GLN:HE21 | 1:8:A:PRO:HG3   | 1        | 1.35          |
| (1,610) | 2:88:B:PRO:HA   | 2:89:B:GLU:HG2  | 14       | 1.35          |
| (1,479) | 1:33:A:GLN:HE21 | 1:35:A:GLU:HB2  | 3        | 1.35          |
| (1,467) | 1:27:A:HIS:HE1  | 1:28:A:ILE:HG13 | 19       | 1.35          |
| (1,453) | 1:11:A:TRP:HE3  | 1:7:A:LEU:HB2   | 8        | 1.35          |
| (1,333) | 1:34:A:TRP:HE1  | 2:88:B:PRO:HG2  | 15       | 1.35          |
| (1,333) | 1:34:A:TRP:HE1  | 2:88:B:PRO:HG2  | 16       | 1.35          |
| (1,844) | 1:25:A:PHE:HB3  | 1:14:A:ARG:HB3  | 17       | 1.34          |
| (1,604) | 1:33:A:GLN:HE22 | 1:35:A:GLU:HG2  | 17       | 1.34          |
| (1,333) | 1:34:A:TRP:HE1  | 2:88:B:PRO:HG2  | 10       | 1.34          |
| (1,333) | 1:34:A:TRP:HE1  | 2:88:B:PRO:HG2  | 25       | 1.34          |
| (1,12)  | 1:21:A:ARG:H    | 1:16:A:SER:HB2  | 15       | 1.34          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,741) | 1:14:A:ARG:H    | 1:15:A:MET:HG2  | 3        | 1.33          |
| (1,467) | 1:27:A:HIS:HE1  | 1:28:A:ILE:HG13 | 8        | 1.33          |
| (1,453) | 1:11:A:TRP:HE3  | 1:7:A:LEU:HB2   | 16       | 1.33          |
| (1,333) | 1:34:A:TRP:HE1  | 2:88:B:PRO:HG2  | 17       | 1.33          |
| (1,333) | 1:34:A:TRP:HE1  | 2:88:B:PRO:HG2  | 21       | 1.33          |
| (1,333) | 1:34:A:TRP:HE1  | 2:88:B:PRO:HG2  | 23       | 1.33          |
| (1,844) | 1:25:A:PHE:HB3  | 1:14:A:ARG:HB3  | 14       | 1.32          |
| (1,725) | 2:84:B:TYR:HB3  | 1:14:A:ARG:HD2  | 20       | 1.32          |
| (1,830) | 1:34:A:TRP:HD1  | 1:33:A:GLN:HG2  | 11       | 1.31          |
| (1,722) | 2:90:B:GLY:HA2  | 1:21:A:ARG:HG3  | 17       | 1.31          |
| (1,467) | 1:27:A:HIS:HE1  | 1:28:A:ILE:HG13 | 14       | 1.31          |
| (1,333) | 1:34:A:TRP:HE1  | 2:88:B:PRO:HG2  | 9        | 1.31          |
| (1,175) | 1:30:A:ASN:H    | 1:26:A:ASN:HB2  | 25       | 1.31          |
| (1,841) | 1:5:A:GLU:HA    | 1:6:A:LYS:HB3   | 11       | 1.3           |
| (1,659) | 1:20:A:GLY:H    | 1:16:A:SER:HB2  | 14       | 1.3           |
| (1,467) | 1:27:A:HIS:HE1  | 1:28:A:ILE:HG13 | 1        | 1.3           |
| (1,467) | 1:27:A:HIS:HE1  | 1:28:A:ILE:HG13 | 6        | 1.3           |
| (1,467) | 1:27:A:HIS:HE1  | 1:28:A:ILE:HG13 | 9        | 1.3           |
| (1,453) | 1:11:A:TRP:HE3  | 1:7:A:LEU:HB2   | 1        | 1.3           |
| (1,214) | 1:14:A:ARG:H    | 1:13:A:LYS:HE2  | 9        | 1.3           |
| (1,841) | 1:5:A:GLU:HA    | 1:6:A:LYS:HB3   | 22       | 1.29          |
| (1,762) | 1:23:A:TYR:HE1  | 1:17:A:ARG:HG3  | 23       | 1.29          |
| (1,762) | 1:23:A:TYR:HE2  | 1:17:A:ARG:HG3  | 23       | 1.29          |
| (1,751) | 1:33:A:GLN:HE21 | 1:8:A:PRO:HG3   | 3        | 1.29          |
| (1,633) | 1:18:A:SER:HB2  | 1:17:A:ARG:HB3  | 18       | 1.29          |
| (1,467) | 1:27:A:HIS:HE1  | 1:28:A:ILE:HG13 | 12       | 1.29          |
| (1,467) | 1:27:A:HIS:HE1  | 1:28:A:ILE:HG13 | 22       | 1.29          |
| (1,453) | 1:11:A:TRP:HE3  | 1:7:A:LEU:HB2   | 3        | 1.29          |
| (1,333) | 1:34:A:TRP:HE1  | 2:88:B:PRO:HG2  | 5        | 1.29          |
| (1,333) | 1:34:A:TRP:HE1  | 2:88:B:PRO:HG2  | 19       | 1.29          |
| (1,175) | 1:30:A:ASN:H    | 1:26:A:ASN:HB2  | 16       | 1.29          |
| (1,137) | 2:85:B:SEP:HB2  | 1:17:A:ARG:HD3  | 13       | 1.29          |
| (1,8)   | 1:12:A:GLU:H    | 1:7:A:LEU:HD21  | 9        | 1.29          |
| (1,8)   | 1:12:A:GLU:H    | 1:7:A:LEU:HD22  | 9        | 1.29          |
| (1,8)   | 1:12:A:GLU:H    | 1:7:A:LEU:HD23  | 9        | 1.29          |
| (1,830) | 1:34:A:TRP:HD1  | 1:33:A:GLN:HG2  | 2        | 1.28          |
| (1,761) | 1:23:A:TYR:HE1  | 1:21:A:ARG:HB2  | 24       | 1.28          |
| (1,761) | 1:23:A:TYR:HE2  | 1:21:A:ARG:HB2  | 24       | 1.28          |
| (1,610) | 2:88:B:PRO:HA   | 2:89:B:GLU:HG2  | 18       | 1.28          |
| (1,467) | 1:27:A:HIS:HE1  | 1:28:A:ILE:HG13 | 10       | 1.28          |
| (1,453) | 1:11:A:TRP:HE3  | 1:7:A:LEU:HB2   | 5        | 1.28          |
| (1,453) | 1:11:A:TRP:HE3  | 1:7:A:LEU:HB2   | 12       | 1.28          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,333) | 1:34:A:TRP:HE1  | 2:88:B:PRO:HG2 | 13       | 1.28          |
| (1,137) | 2:85:B:SEP:HB2  | 1:17:A:ARG:HD3 | 22       | 1.28          |
| (1,8)   | 1:12:A:GLU:H    | 1:7:A:LEU:HD21 | 6        | 1.28          |
| (1,8)   | 1:12:A:GLU:H    | 1:7:A:LEU:HD22 | 6        | 1.28          |
| (1,8)   | 1:12:A:GLU:H    | 1:7:A:LEU:HD23 | 6        | 1.28          |
| (1,884) | 2:87:B:PHE:HD1  | 1:34:A:TRP:HB3 | 8        | 1.27          |
| (1,884) | 2:87:B:PHE:HD2  | 1:34:A:TRP:HB3 | 8        | 1.27          |
| (1,844) | 1:25:A:PHE:HB3  | 1:14:A:ARG:HB3 | 24       | 1.27          |
| (1,820) | 1:21:A:ARG:HB3  | 1:19:A:SER:HA  | 4        | 1.27          |
| (1,722) | 2:90:B:GLY:HA2  | 1:21:A:ARG:HG3 | 6        | 1.27          |
| (1,659) | 1:20:A:GLY:H    | 1:16:A:SER:HB2 | 21       | 1.27          |
| (1,342) | 1:25:A:PHE:H    | 1:14:A:ARG:HG2 | 20       | 1.27          |
| (1,322) | 1:17:A:ARG:HD3  | 2:81:B:GLY:HA2 | 3        | 1.27          |
| (1,175) | 1:30:A:ASN:H    | 1:26:A:ASN:HB2 | 4        | 1.27          |
| (1,175) | 1:30:A:ASN:H    | 1:26:A:ASN:HB2 | 12       | 1.27          |
| (1,175) | 1:30:A:ASN:H    | 1:26:A:ASN:HB2 | 13       | 1.27          |
| (1,823) | 1:25:A:PHE:HZ   | 1:14:A:ARG:HD2 | 20       | 1.26          |
| (1,822) | 1:25:A:PHE:HZ   | 1:14:A:ARG:HD2 | 20       | 1.26          |
| (1,333) | 1:34:A:TRP:HE1  | 2:88:B:PRO:HG2 | 3        | 1.26          |
| (1,333) | 1:34:A:TRP:HE1  | 2:88:B:PRO:HG2 | 14       | 1.26          |
| (1,180) | 1:7:A:LEU:H     | 1:6:A:LYS:HE3  | 2        | 1.26          |
| (1,175) | 1:30:A:ASN:H    | 1:26:A:ASN:HB2 | 1        | 1.26          |
| (1,175) | 1:30:A:ASN:H    | 1:26:A:ASN:HB2 | 6        | 1.26          |
| (1,175) | 1:30:A:ASN:H    | 1:26:A:ASN:HB2 | 23       | 1.26          |
| (1,137) | 2:85:B:SEP:HB2  | 1:17:A:ARG:HD3 | 8        | 1.26          |
| (1,12)  | 1:21:A:ARG:H    | 1:16:A:SER:HB2 | 16       | 1.26          |
| (1,820) | 1:21:A:ARG:HB3  | 1:19:A:SER:HA  | 25       | 1.25          |
| (1,751) | 1:33:A:GLN:HE21 | 1:8:A:PRO:HG3  | 19       | 1.25          |
| (1,634) | 1:17:A:ARG:HB3  | 1:18:A:SER:HA  | 12       | 1.25          |
| (1,610) | 2:88:B:PRO:HA   | 2:89:B:GLU:HG2 | 19       | 1.25          |
| (1,479) | 1:33:A:GLN:HE21 | 1:35:A:GLU:HB2 | 7        | 1.25          |
| (1,217) | 1:16:A:SER:HB2  | 1:21:A:ARG:HG2 | 15       | 1.25          |
| (1,830) | 1:34:A:TRP:HD1  | 1:33:A:GLN:HG2 | 18       | 1.24          |
| (1,820) | 1:21:A:ARG:HB3  | 1:19:A:SER:HA  | 9        | 1.24          |
| (1,761) | 1:23:A:TYR:HE1  | 1:21:A:ARG:HB2 | 12       | 1.24          |
| (1,761) | 1:23:A:TYR:HE2  | 1:21:A:ARG:HB2 | 12       | 1.24          |
| (1,741) | 1:14:A:ARG:H    | 1:15:A:MET:HG2 | 25       | 1.24          |
| (1,634) | 1:17:A:ARG:HB3  | 1:18:A:SER:HA  | 13       | 1.24          |
| (1,333) | 1:34:A:TRP:HE1  | 2:88:B:PRO:HG2 | 11       | 1.24          |
| (1,175) | 1:30:A:ASN:H    | 1:26:A:ASN:HB2 | 14       | 1.24          |
| (1,841) | 1:5:A:GLU:HA    | 1:6:A:LYS:HB3  | 3        | 1.23          |
| (1,756) | 1:41:A:SER:H    | 1:6:A:LYS:HB2  | 17       | 1.23          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,634) | 1:17:A:ARG:HB3  | 1:18:A:SER:HA   | 4        | 1.23          |
| (1,634) | 1:17:A:ARG:HB3  | 1:18:A:SER:HA   | 15       | 1.23          |
| (1,175) | 1:30:A:ASN:H    | 1:26:A:ASN:HB2  | 10       | 1.23          |
| (1,175) | 1:30:A:ASN:H    | 1:26:A:ASN:HB2  | 19       | 1.23          |
| (1,8)   | 1:12:A:GLU:H    | 1:7:A:LEU:HD21  | 5        | 1.23          |
| (1,8)   | 1:12:A:GLU:H    | 1:7:A:LEU:HD22  | 5        | 1.23          |
| (1,8)   | 1:12:A:GLU:H    | 1:7:A:LEU:HD23  | 5        | 1.23          |
| (1,762) | 1:23:A:TYR:HE1  | 1:17:A:ARG:HG3  | 11       | 1.22          |
| (1,762) | 1:23:A:TYR:HE2  | 1:17:A:ARG:HG3  | 11       | 1.22          |
| (1,453) | 1:11:A:TRP:HE3  | 1:7:A:LEU:HB2   | 7        | 1.22          |
| (1,248) | 2:90:B:GLY:HA2  | 1:18:A:SER:HA   | 19       | 1.22          |
| (1,137) | 2:85:B:SEP:HB2  | 1:17:A:ARG:HD3  | 3        | 1.22          |
| (1,634) | 1:17:A:ARG:HB3  | 1:18:A:SER:HA   | 3        | 1.21          |
| (1,634) | 1:17:A:ARG:HB3  | 1:18:A:SER:HA   | 10       | 1.21          |
| (1,634) | 1:17:A:ARG:HB3  | 1:18:A:SER:HA   | 24       | 1.21          |
| (1,467) | 1:27:A:HIS:HE1  | 1:28:A:ILE:HG13 | 11       | 1.21          |
| (1,180) | 1:7:A:LEU:H     | 1:6:A:LYS:HE3   | 24       | 1.21          |
| (1,137) | 2:85:B:SEP:HB2  | 1:17:A:ARG:HD3  | 14       | 1.21          |
| (1,137) | 2:85:B:SEP:HB2  | 1:17:A:ARG:HD3  | 23       | 1.21          |
| (1,23)  | 1:36:A:ARG:HD2  | 1:7:A:LEU:HD21  | 18       | 1.21          |
| (1,23)  | 1:36:A:ARG:HD2  | 1:7:A:LEU:HD22  | 18       | 1.21          |
| (1,23)  | 1:36:A:ARG:HD2  | 1:7:A:LEU:HD23  | 18       | 1.21          |
| (1,844) | 1:25:A:PHE:HB3  | 1:14:A:ARG:HB3  | 22       | 1.2           |
| (1,761) | 1:23:A:TYR:HE1  | 1:21:A:ARG:HB2  | 13       | 1.2           |
| (1,761) | 1:23:A:TYR:HE2  | 1:21:A:ARG:HB2  | 13       | 1.2           |
| (1,731) | 2:84:B:TYR:HD1  | 2:83:B:PRO:HB3  | 3        | 1.2           |
| (1,731) | 2:84:B:TYR:HD2  | 2:83:B:PRO:HB3  | 3        | 1.2           |
| (1,731) | 2:84:B:TYR:HD1  | 2:83:B:PRO:HB3  | 17       | 1.2           |
| (1,731) | 2:84:B:TYR:HD2  | 2:83:B:PRO:HB3  | 17       | 1.2           |
| (1,731) | 2:84:B:TYR:HD1  | 2:83:B:PRO:HB3  | 23       | 1.2           |
| (1,731) | 2:84:B:TYR:HD2  | 2:83:B:PRO:HB3  | 23       | 1.2           |
| (1,634) | 1:17:A:ARG:HB3  | 1:18:A:SER:HA   | 22       | 1.2           |
| (1,633) | 1:18:A:SER:HB2  | 1:17:A:ARG:HB3  | 11       | 1.2           |
| (1,480) | 1:33:A:GLN:HE21 | 1:35:A:GLU:HG2  | 12       | 1.2           |
| (1,333) | 1:34:A:TRP:HE1  | 2:88:B:PRO:HG2  | 18       | 1.2           |
| (1,175) | 1:30:A:ASN:H    | 1:26:A:ASN:HB2  | 3        | 1.2           |
| (1,841) | 1:5:A:GLU:HA    | 1:6:A:LYS:HB3   | 20       | 1.19          |
| (1,837) | 1:21:A:ARG:HA   | 2:88:B:PRO:HB3  | 5        | 1.19          |
| (1,634) | 1:17:A:ARG:HB3  | 1:18:A:SER:HA   | 16       | 1.19          |
| (1,610) | 2:88:B:PRO:HA   | 2:89:B:GLU:HG2  | 1        | 1.19          |
| (1,175) | 1:30:A:ASN:H    | 1:26:A:ASN:HB2  | 5        | 1.19          |
| (1,872) | 2:89:B:GLU:HB2  | 1:16:A:SER:HB3  | 19       | 1.18          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,731) | 2:84:B:TYR:HD1  | 2:83:B:PRO:HB3 | 4        | 1.18          |
| (1,731) | 2:84:B:TYR:HD2  | 2:83:B:PRO:HB3 | 4        | 1.18          |
| (1,731) | 2:84:B:TYR:HD1  | 2:83:B:PRO:HB3 | 10       | 1.18          |
| (1,731) | 2:84:B:TYR:HD2  | 2:83:B:PRO:HB3 | 10       | 1.18          |
| (1,731) | 2:84:B:TYR:HD1  | 2:83:B:PRO:HB3 | 12       | 1.18          |
| (1,731) | 2:84:B:TYR:HD2  | 2:83:B:PRO:HB3 | 12       | 1.18          |
| (1,731) | 2:84:B:TYR:HD1  | 2:83:B:PRO:HB3 | 15       | 1.18          |
| (1,731) | 2:84:B:TYR:HD2  | 2:83:B:PRO:HB3 | 15       | 1.18          |
| (1,659) | 1:20:A:GLY:H    | 1:16:A:SER:HB2 | 11       | 1.18          |
| (1,659) | 1:20:A:GLY:H    | 1:16:A:SER:HB2 | 17       | 1.18          |
| (1,634) | 1:17:A:ARG:HB3  | 1:18:A:SER:HA  | 5        | 1.18          |
| (1,634) | 1:17:A:ARG:HB3  | 1:18:A:SER:HA  | 23       | 1.18          |
| (1,610) | 2:88:B:PRO:HA   | 2:89:B:GLU:HG2 | 12       | 1.18          |
| (1,480) | 1:33:A:GLN:HE21 | 1:35:A:GLU:HG2 | 15       | 1.18          |
| (1,453) | 1:11:A:TRP:HE3  | 1:7:A:LEU:HB2  | 2        | 1.18          |
| (1,23)  | 1:36:A:ARG:HD2  | 1:7:A:LEU:HD21 | 2        | 1.18          |
| (1,23)  | 1:36:A:ARG:HD2  | 1:7:A:LEU:HD22 | 2        | 1.18          |
| (1,23)  | 1:36:A:ARG:HD2  | 1:7:A:LEU:HD23 | 2        | 1.18          |
| (1,23)  | 1:36:A:ARG:HD2  | 1:7:A:LEU:HD21 | 22       | 1.18          |
| (1,23)  | 1:36:A:ARG:HD2  | 1:7:A:LEU:HD22 | 22       | 1.18          |
| (1,23)  | 1:36:A:ARG:HD2  | 1:7:A:LEU:HD23 | 22       | 1.18          |
| (1,844) | 1:25:A:PHE:HB3  | 1:14:A:ARG:HB3 | 15       | 1.17          |
| (1,731) | 2:84:B:TYR:HD1  | 2:83:B:PRO:HB3 | 8        | 1.17          |
| (1,731) | 2:84:B:TYR:HD2  | 2:83:B:PRO:HB3 | 8        | 1.17          |
| (1,634) | 1:17:A:ARG:HB3  | 1:18:A:SER:HA  | 17       | 1.17          |
| (1,634) | 1:17:A:ARG:HB3  | 1:18:A:SER:HA  | 20       | 1.17          |
| (1,453) | 1:11:A:TRP:HE3  | 1:7:A:LEU:HB2  | 13       | 1.17          |
| (1,453) | 1:11:A:TRP:HE3  | 1:7:A:LEU:HB2  | 25       | 1.17          |
| (1,175) | 1:30:A:ASN:H    | 1:26:A:ASN:HB2 | 17       | 1.17          |
| (1,8)   | 1:12:A:GLU:H    | 1:7:A:LEU:HD21 | 12       | 1.17          |
| (1,8)   | 1:12:A:GLU:H    | 1:7:A:LEU:HD22 | 12       | 1.17          |
| (1,8)   | 1:12:A:GLU:H    | 1:7:A:LEU:HD23 | 12       | 1.17          |
| (1,830) | 1:34:A:TRP:HD1  | 1:33:A:GLN:HG2 | 4        | 1.16          |
| (1,731) | 2:84:B:TYR:HD1  | 2:83:B:PRO:HB3 | 7        | 1.16          |
| (1,731) | 2:84:B:TYR:HD2  | 2:83:B:PRO:HB3 | 7        | 1.16          |
| (1,659) | 1:20:A:GLY:H    | 1:16:A:SER:HB2 | 2        | 1.16          |
| (1,634) | 1:17:A:ARG:HB3  | 1:18:A:SER:HA  | 7        | 1.16          |
| (1,333) | 1:34:A:TRP:HE1  | 2:88:B:PRO:HG2 | 8        | 1.16          |
| (1,23)  | 1:36:A:ARG:HD2  | 1:7:A:LEU:HD21 | 4        | 1.16          |
| (1,23)  | 1:36:A:ARG:HD2  | 1:7:A:LEU:HD22 | 4        | 1.16          |
| (1,23)  | 1:36:A:ARG:HD2  | 1:7:A:LEU:HD23 | 4        | 1.16          |
| (1,610) | 2:88:B:PRO:HA   | 2:89:B:GLU:HG2 | 22       | 1.15          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,562) | 1:34:A:TRP:HZ2  | 1:16:A:SER:HB3 | 10       | 1.15          |
| (1,453) | 1:11:A:TRP:HE3  | 1:7:A:LEU:HB2  | 18       | 1.15          |
| (1,453) | 1:11:A:TRP:HE3  | 1:7:A:LEU:HB2  | 20       | 1.15          |
| (1,175) | 1:30:A:ASN:H    | 1:26:A:ASN:HB2 | 2        | 1.15          |
| (1,175) | 1:30:A:ASN:H    | 1:26:A:ASN:HB2 | 7        | 1.15          |
| (1,830) | 1:34:A:TRP:HD1  | 1:33:A:GLN:HG2 | 10       | 1.14          |
| (1,761) | 1:23:A:TYR:HE1  | 1:21:A:ARG:HB2 | 2        | 1.14          |
| (1,761) | 1:23:A:TYR:HE2  | 1:21:A:ARG:HB2 | 2        | 1.14          |
| (1,731) | 2:84:B:TYR:HD1  | 2:83:B:PRO:HB3 | 19       | 1.14          |
| (1,731) | 2:84:B:TYR:HD2  | 2:83:B:PRO:HB3 | 19       | 1.14          |
| (1,479) | 1:33:A:GLN:HE21 | 1:35:A:GLU:HB2 | 11       | 1.14          |
| (1,453) | 1:11:A:TRP:HE3  | 1:7:A:LEU:HB2  | 14       | 1.14          |
| (1,175) | 1:30:A:ASN:H    | 1:26:A:ASN:HB2 | 8        | 1.14          |
| (1,175) | 1:30:A:ASN:H    | 1:26:A:ASN:HB2 | 11       | 1.14          |
| (1,872) | 2:89:B:GLU:HB2  | 1:16:A:SER:HB3 | 12       | 1.13          |
| (1,762) | 1:23:A:TYR:HE1  | 1:17:A:ARG:HG3 | 8        | 1.13          |
| (1,762) | 1:23:A:TYR:HE2  | 1:17:A:ARG:HG3 | 8        | 1.13          |
| (1,731) | 2:84:B:TYR:HD1  | 2:83:B:PRO:HB3 | 2        | 1.13          |
| (1,731) | 2:84:B:TYR:HD2  | 2:83:B:PRO:HB3 | 2        | 1.13          |
| (1,659) | 1:20:A:GLY:H    | 1:16:A:SER:HB2 | 10       | 1.13          |
| (1,562) | 1:34:A:TRP:HZ2  | 1:16:A:SER:HB3 | 14       | 1.13          |
| (1,175) | 1:30:A:ASN:H    | 1:26:A:ASN:HB2 | 22       | 1.13          |
| (1,137) | 2:85:B:SEP:HB2  | 1:17:A:ARG:HD3 | 12       | 1.13          |
| (1,8)   | 1:12:A:GLU:H    | 1:7:A:LEU:HD21 | 24       | 1.13          |
| (1,8)   | 1:12:A:GLU:H    | 1:7:A:LEU:HD22 | 24       | 1.13          |
| (1,8)   | 1:12:A:GLU:H    | 1:7:A:LEU:HD23 | 24       | 1.13          |
| (1,731) | 2:84:B:TYR:HD1  | 2:83:B:PRO:HB3 | 1        | 1.12          |
| (1,731) | 2:84:B:TYR:HD2  | 2:83:B:PRO:HB3 | 1        | 1.12          |
| (1,731) | 2:84:B:TYR:HD1  | 2:83:B:PRO:HB3 | 20       | 1.12          |
| (1,731) | 2:84:B:TYR:HD2  | 2:83:B:PRO:HB3 | 20       | 1.12          |
| (1,731) | 2:84:B:TYR:HD1  | 2:83:B:PRO:HB3 | 25       | 1.12          |
| (1,731) | 2:84:B:TYR:HD2  | 2:83:B:PRO:HB3 | 25       | 1.12          |
| (1,634) | 1:17:A:ARG:HB3  | 1:18:A:SER:HA  | 1        | 1.12          |
| (1,453) | 1:11:A:TRP:HE3  | 1:7:A:LEU:HB2  | 22       | 1.12          |
| (1,137) | 2:85:B:SEP:HB2  | 1:17:A:ARG:HD3 | 15       | 1.12          |
| (1,634) | 1:17:A:ARG:HB3  | 1:18:A:SER:HA  | 2        | 1.11          |
| (1,634) | 1:17:A:ARG:HB3  | 1:18:A:SER:HA  | 19       | 1.11          |
| (1,610) | 2:88:B:PRO:HA   | 2:89:B:GLU:HG2 | 23       | 1.11          |
| (1,604) | 1:33:A:GLN:HE22 | 1:35:A:GLU:HG2 | 2        | 1.11          |
| (1,562) | 1:34:A:TRP:HZ2  | 1:16:A:SER:HB3 | 11       | 1.11          |
| (1,480) | 1:33:A:GLN:HE21 | 1:35:A:GLU:HG2 | 2        | 1.11          |
| (1,479) | 1:33:A:GLN:HE21 | 1:35:A:GLU:HB2 | 9        | 1.11          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,175) | 1:30:A:ASN:H   | 1:26:A:ASN:HB2 | 20       | 1.11          |
| (1,87)  | 1:23:A:TYR:HE1 | 1:16:A:SER:HB3 | 20       | 1.11          |
| (1,87)  | 1:23:A:TYR:HE2 | 1:16:A:SER:HB3 | 20       | 1.11          |
| (1,872) | 2:89:B:GLU:HB2 | 1:16:A:SER:HB3 | 4        | 1.1           |
| (1,872) | 2:89:B:GLU:HB2 | 1:16:A:SER:HB3 | 24       | 1.1           |
| (1,830) | 1:34:A:TRP:HD1 | 1:33:A:GLN:HG2 | 13       | 1.1           |
| (1,731) | 2:84:B:TYR:HD1 | 2:83:B:PRO:HB3 | 16       | 1.1           |
| (1,731) | 2:84:B:TYR:HD2 | 2:83:B:PRO:HB3 | 16       | 1.1           |
| (1,634) | 1:17:A:ARG:HB3 | 1:18:A:SER:HA  | 21       | 1.1           |
| (1,606) | 1:34:A:TRP:HD1 | 2:89:B:GLU:HG2 | 3        | 1.1           |
| (1,175) | 1:30:A:ASN:H   | 1:26:A:ASN:HB2 | 9        | 1.1           |
| (1,175) | 1:30:A:ASN:H   | 1:26:A:ASN:HB2 | 18       | 1.1           |
| (1,8)   | 1:12:A:GLU:H   | 1:7:A:LEU:HD21 | 23       | 1.1           |
| (1,8)   | 1:12:A:GLU:H   | 1:7:A:LEU:HD22 | 23       | 1.1           |
| (1,8)   | 1:12:A:GLU:H   | 1:7:A:LEU:HD23 | 23       | 1.1           |
| (1,872) | 2:89:B:GLU:HB2 | 1:16:A:SER:HB3 | 5        | 1.09          |
| (1,872) | 2:89:B:GLU:HB2 | 1:16:A:SER:HB3 | 17       | 1.09          |
| (1,841) | 1:5:A:GLU:HA   | 1:6:A:LYS:HB3  | 9        | 1.09          |
| (1,841) | 1:5:A:GLU:HA   | 1:6:A:LYS:HB3  | 21       | 1.09          |
| (1,634) | 1:17:A:ARG:HB3 | 1:18:A:SER:HA  | 8        | 1.09          |
| (1,453) | 1:11:A:TRP:HE3 | 1:7:A:LEU:HB2  | 4        | 1.09          |
| (1,453) | 1:11:A:TRP:HE3 | 1:7:A:LEU:HB2  | 17       | 1.09          |
| (1,215) | 1:14:A:ARG:H   | 1:13:A:LYS:HG2 | 2        | 1.09          |
| (1,215) | 1:14:A:ARG:H   | 1:13:A:LYS:HG2 | 11       | 1.09          |
| (1,23)  | 1:36:A:ARG:HD2 | 1:7:A:LEU:HD21 | 14       | 1.09          |
| (1,23)  | 1:36:A:ARG:HD2 | 1:7:A:LEU:HD22 | 14       | 1.09          |
| (1,23)  | 1:36:A:ARG:HD2 | 1:7:A:LEU:HD23 | 14       | 1.09          |
| (1,830) | 1:34:A:TRP:HD1 | 1:33:A:GLN:HG2 | 7        | 1.08          |
| (1,830) | 1:34:A:TRP:HD1 | 1:33:A:GLN:HG2 | 19       | 1.08          |
| (1,762) | 1:23:A:TYR:HE1 | 1:17:A:ARG:HG3 | 14       | 1.08          |
| (1,762) | 1:23:A:TYR:HE2 | 1:17:A:ARG:HG3 | 14       | 1.08          |
| (1,761) | 1:23:A:TYR:HE1 | 1:21:A:ARG:HB2 | 17       | 1.08          |
| (1,761) | 1:23:A:TYR:HE2 | 1:21:A:ARG:HB2 | 17       | 1.08          |
| (1,731) | 2:84:B:TYR:HD1 | 2:83:B:PRO:HB3 | 22       | 1.08          |
| (1,731) | 2:84:B:TYR:HD2 | 2:83:B:PRO:HB3 | 22       | 1.08          |
| (1,634) | 1:17:A:ARG:HB3 | 1:18:A:SER:HA  | 11       | 1.08          |
| (1,634) | 1:17:A:ARG:HB3 | 1:18:A:SER:HA  | 14       | 1.08          |
| (1,634) | 1:17:A:ARG:HB3 | 1:18:A:SER:HA  | 18       | 1.08          |
| (1,468) | 2:85:B:SEP:H   | 1:14:A:ARG:HB3 | 17       | 1.08          |
| (1,453) | 1:11:A:TRP:HE3 | 1:7:A:LEU:HB2  | 10       | 1.08          |
| (1,215) | 1:14:A:ARG:H   | 1:13:A:LYS:HG2 | 22       | 1.08          |
| (1,731) | 2:84:B:TYR:HD1 | 2:83:B:PRO:HB3 | 6        | 1.07          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,731) | 2:84:B:TYR:HD2 | 2:83:B:PRO:HB3  | 6        | 1.07          |
| (1,731) | 2:84:B:TYR:HD1 | 2:83:B:PRO:HB3  | 9        | 1.07          |
| (1,731) | 2:84:B:TYR:HD2 | 2:83:B:PRO:HB3  | 9        | 1.07          |
| (1,731) | 2:84:B:TYR:HD1 | 2:83:B:PRO:HB3  | 13       | 1.07          |
| (1,731) | 2:84:B:TYR:HD2 | 2:83:B:PRO:HB3  | 13       | 1.07          |
| (1,634) | 1:17:A:ARG:HB3 | 1:18:A:SER:HA   | 25       | 1.07          |
| (1,453) | 1:11:A:TRP:HE3 | 1:7:A:LEU:HB2   | 15       | 1.07          |
| (1,215) | 1:14:A:ARG:H   | 1:13:A:LYS:HG2  | 3        | 1.07          |
| (1,87)  | 1:23:A:TYR:HE1 | 1:16:A:SER:HB3  | 10       | 1.07          |
| (1,87)  | 1:23:A:TYR:HE2 | 1:16:A:SER:HB3  | 10       | 1.07          |
| (1,844) | 1:25:A:PHE:HB3 | 1:14:A:ARG:HB3  | 18       | 1.06          |
| (1,837) | 1:21:A:ARG:HA  | 2:88:B:PRO:HB3  | 15       | 1.06          |
| (1,761) | 1:23:A:TYR:HE1 | 1:21:A:ARG:HB2  | 18       | 1.06          |
| (1,761) | 1:23:A:TYR:HE2 | 1:21:A:ARG:HB2  | 18       | 1.06          |
| (1,731) | 2:84:B:TYR:HD1 | 2:83:B:PRO:HB3  | 24       | 1.06          |
| (1,731) | 2:84:B:TYR:HD2 | 2:83:B:PRO:HB3  | 24       | 1.06          |
| (1,634) | 1:17:A:ARG:HB3 | 1:18:A:SER:HA   | 6        | 1.06          |
| (1,453) | 1:11:A:TRP:HE3 | 1:7:A:LEU:HB2   | 9        | 1.06          |
| (1,215) | 1:14:A:ARG:H   | 1:13:A:LYS:HG2  | 4        | 1.06          |
| (1,215) | 1:14:A:ARG:H   | 1:13:A:LYS:HG2  | 12       | 1.06          |
| (1,830) | 1:34:A:TRP:HD1 | 1:33:A:GLN:HG2  | 25       | 1.05          |
| (1,825) | 2:87:B:PHE:HE1 | 2:81:B:GLY:HA2  | 4        | 1.05          |
| (1,825) | 2:87:B:PHE:HE2 | 2:81:B:GLY:HA2  | 4        | 1.05          |
| (1,762) | 1:23:A:TYR:HE1 | 1:17:A:ARG:HG3  | 9        | 1.05          |
| (1,762) | 1:23:A:TYR:HE2 | 1:17:A:ARG:HG3  | 9        | 1.05          |
| (1,634) | 1:17:A:ARG:HB3 | 1:18:A:SER:HA   | 9        | 1.05          |
| (1,215) | 1:14:A:ARG:H   | 1:13:A:LYS:HG2  | 19       | 1.05          |
| (1,830) | 1:34:A:TRP:HD1 | 1:33:A:GLN:HG2  | 14       | 1.04          |
| (1,643) | 2:85:B:SEP:HB2 | 1:17:A:ARG:HG2  | 17       | 1.04          |
| (1,617) | 2:89:B:GLU:HA  | 2:88:B:PRO:HD3  | 8        | 1.04          |
| (1,872) | 2:89:B:GLU:HB2 | 1:16:A:SER:HB3  | 2        | 1.03          |
| (1,837) | 1:21:A:ARG:HA  | 2:88:B:PRO:HB3  | 16       | 1.03          |
| (1,830) | 1:34:A:TRP:HD1 | 1:33:A:GLN:HG2  | 15       | 1.03          |
| (1,761) | 1:23:A:TYR:HE1 | 1:21:A:ARG:HB2  | 7        | 1.03          |
| (1,761) | 1:23:A:TYR:HE2 | 1:21:A:ARG:HB2  | 7        | 1.03          |
| (1,731) | 2:84:B:TYR:HD1 | 2:83:B:PRO:HB3  | 5        | 1.03          |
| (1,731) | 2:84:B:TYR:HD2 | 2:83:B:PRO:HB3  | 5        | 1.03          |
| (1,562) | 1:34:A:TRP:HZ2 | 1:16:A:SER:HB3  | 6        | 1.03          |
| (1,453) | 1:11:A:TRP:HE3 | 1:7:A:LEU:HB2   | 11       | 1.03          |
| (1,215) | 1:14:A:ARG:H   | 1:13:A:LYS:HG2  | 13       | 1.03          |
| (1,24)  | 1:13:A:LYS:HE2 | 1:22:A:VAL:HG11 | 12       | 1.03          |
| (1,24)  | 1:13:A:LYS:HE2 | 1:22:A:VAL:HG12 | 12       | 1.03          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,24)  | 1:13:A:LYS:HE2  | 1:22:A:VAL:HG13 | 12       | 1.03          |
| (1,884) | 2:87:B:PHE:HD1  | 1:34:A:TRP:HB3  | 4        | 1.02          |
| (1,884) | 2:87:B:PHE:HD2  | 1:34:A:TRP:HB3  | 4        | 1.02          |
| (1,841) | 1:5:A:GLU:HA    | 1:6:A:LYS:HB3   | 23       | 1.02          |
| (1,837) | 1:21:A:ARG:HA   | 2:88:B:PRO:HB3  | 8        | 1.02          |
| (1,830) | 1:34:A:TRP:HD1  | 1:33:A:GLN:HG2  | 22       | 1.02          |
| (1,756) | 1:41:A:SER:H    | 1:6:A:LYS:HB2   | 25       | 1.02          |
| (1,736) | 1:33:A:GLN:H    | 1:7:A:LEU:HD21  | 8        | 1.02          |
| (1,736) | 1:33:A:GLN:H    | 1:7:A:LEU:HD22  | 8        | 1.02          |
| (1,736) | 1:33:A:GLN:H    | 1:7:A:LEU:HD23  | 8        | 1.02          |
| (1,731) | 2:84:B:TYR:HD1  | 2:83:B:PRO:HB3  | 21       | 1.02          |
| (1,731) | 2:84:B:TYR:HD2  | 2:83:B:PRO:HB3  | 21       | 1.02          |
| (1,499) | 1:25:A:PHE:HE1  | 1:12:A:GLU:HG2  | 4        | 1.02          |
| (1,499) | 1:25:A:PHE:HE2  | 1:12:A:GLU:HG2  | 4        | 1.02          |
| (1,296) | 1:26:A:ASN:HD22 | 1:10:A:GLY:HA2  | 13       | 1.02          |
| (1,215) | 1:14:A:ARG:H    | 1:13:A:LYS:HG2  | 14       | 1.02          |
| (1,215) | 1:14:A:ARG:H    | 1:13:A:LYS:HG2  | 25       | 1.02          |
| (1,180) | 1:7:A:LEU:H     | 1:6:A:LYS:HE3   | 18       | 1.02          |
| (1,175) | 1:30:A:ASN:H    | 1:26:A:ASN:HB2  | 15       | 1.02          |
| (1,8)   | 1:12:A:GLU:H    | 1:7:A:LEU:HD21  | 20       | 1.02          |
| (1,8)   | 1:12:A:GLU:H    | 1:7:A:LEU:HD22  | 20       | 1.02          |
| (1,8)   | 1:12:A:GLU:H    | 1:7:A:LEU:HD23  | 20       | 1.02          |
| (1,872) | 2:89:B:GLU:HB2  | 1:16:A:SER:HB3  | 21       | 1.01          |
| (1,741) | 1:14:A:ARG:H    | 1:15:A:MET:HG2  | 15       | 1.01          |
| (1,731) | 2:84:B:TYR:HD1  | 2:83:B:PRO:HB3  | 11       | 1.01          |
| (1,731) | 2:84:B:TYR:HD2  | 2:83:B:PRO:HB3  | 11       | 1.01          |
| (1,731) | 2:84:B:TYR:HD1  | 2:83:B:PRO:HB3  | 14       | 1.01          |
| (1,731) | 2:84:B:TYR:HD2  | 2:83:B:PRO:HB3  | 14       | 1.01          |
| (1,610) | 2:88:B:PRO:HA   | 2:89:B:GLU:HG2  | 5        | 1.01          |
| (1,606) | 1:34:A:TRP:HD1  | 2:89:B:GLU:HG2  | 21       | 1.01          |
| (1,841) | 1:5:A:GLU:HA    | 1:6:A:LYS:HB3   | 2        | 1.0           |
| (1,562) | 1:34:A:TRP:HZ2  | 1:16:A:SER:HB3  | 22       | 1.0           |
| (1,215) | 1:14:A:ARG:H    | 1:13:A:LYS:HG2  | 23       | 1.0           |
| (1,215) | 1:14:A:ARG:H    | 1:13:A:LYS:HG2  | 24       | 1.0           |
| (1,175) | 1:30:A:ASN:H    | 1:26:A:ASN:HB2  | 21       | 1.0           |
| (1,8)   | 1:12:A:GLU:H    | 1:7:A:LEU:HD21  | 7        | 1.0           |
| (1,8)   | 1:12:A:GLU:H    | 1:7:A:LEU:HD22  | 7        | 1.0           |
| (1,8)   | 1:12:A:GLU:H    | 1:7:A:LEU:HD23  | 7        | 1.0           |
| (1,8)   | 1:12:A:GLU:H    | 1:7:A:LEU:HD21  | 16       | 1.0           |
| (1,8)   | 1:12:A:GLU:H    | 1:7:A:LEU:HD22  | 16       | 1.0           |
| (1,8)   | 1:12:A:GLU:H    | 1:7:A:LEU:HD23  | 16       | 1.0           |
| (1,844) | 1:25:A:PHE:HB3  | 1:14:A:ARG:HB3  | 13       | 0.99          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,820) | 1:21:A:ARG:HB3  | 1:19:A:SER:HA  | 19       | 0.99          |
| (1,562) | 1:34:A:TRP:HZ2  | 1:16:A:SER:HB3 | 17       | 0.99          |
| (1,214) | 1:14:A:ARG:H    | 1:13:A:LYS:HE2 | 12       | 0.99          |
| (1,12)  | 1:21:A:ARG:H    | 1:16:A:SER:HB2 | 20       | 0.99          |
| (1,872) | 2:89:B:GLU:HB2  | 1:16:A:SER:HB3 | 11       | 0.98          |
| (1,830) | 1:34:A:TRP:HD1  | 1:33:A:GLN:HG2 | 9        | 0.98          |
| (1,479) | 1:33:A:GLN:HE21 | 1:35:A:GLU:HB2 | 16       | 0.98          |
| (1,215) | 1:14:A:ARG:H    | 1:13:A:LYS:HG2 | 10       | 0.98          |
| (1,87)  | 1:23:A:TYR:HE1  | 1:16:A:SER:HB3 | 23       | 0.98          |
| (1,87)  | 1:23:A:TYR:HE2  | 1:16:A:SER:HB3 | 23       | 0.98          |
| (1,872) | 2:89:B:GLU:HB2  | 1:16:A:SER:HB3 | 13       | 0.97          |
| (1,872) | 2:89:B:GLU:HB2  | 1:16:A:SER:HB3 | 14       | 0.97          |
| (1,844) | 1:25:A:PHE:HB3  | 1:14:A:ARG:HB3 | 6        | 0.97          |
| (1,837) | 1:21:A:ARG:HA   | 2:88:B:PRO:HB3 | 10       | 0.97          |
| (1,820) | 1:21:A:ARG:HB3  | 1:19:A:SER:HA  | 21       | 0.97          |
| (1,731) | 2:84:B:TYR:HD1  | 2:83:B:PRO:HB3 | 18       | 0.97          |
| (1,731) | 2:84:B:TYR:HD2  | 2:83:B:PRO:HB3 | 18       | 0.97          |
| (1,562) | 1:34:A:TRP:HZ2  | 1:16:A:SER:HB3 | 21       | 0.97          |
| (1,215) | 1:14:A:ARG:H    | 1:13:A:LYS:HG2 | 15       | 0.97          |
| (1,180) | 1:7:A:LEU:H     | 1:6:A:LYS:HE3  | 19       | 0.97          |
| (1,12)  | 1:21:A:ARG:H    | 1:16:A:SER:HB2 | 4        | 0.97          |
| (1,872) | 2:89:B:GLU:HB2  | 1:16:A:SER:HB3 | 22       | 0.96          |
| (1,844) | 1:25:A:PHE:HB3  | 1:14:A:ARG:HB3 | 4        | 0.96          |
| (1,562) | 1:34:A:TRP:HZ2  | 1:16:A:SER:HB3 | 23       | 0.96          |
| (1,322) | 1:17:A:ARG:HD3  | 2:81:B:GLY:HA2 | 23       | 0.96          |
| (1,215) | 1:14:A:ARG:H    | 1:13:A:LYS:HG2 | 18       | 0.96          |
| (1,180) | 1:7:A:LEU:H     | 1:6:A:LYS:HE3  | 15       | 0.96          |
| (1,102) | 1:23:A:TYR:HE1  | 1:25:A:PHE:HB3 | 11       | 0.96          |
| (1,102) | 1:23:A:TYR:HE2  | 1:25:A:PHE:HB3 | 11       | 0.96          |
| (1,8)   | 1:12:A:GLU:H    | 1:7:A:LEU:HD21 | 3        | 0.96          |
| (1,8)   | 1:12:A:GLU:H    | 1:7:A:LEU:HD22 | 3        | 0.96          |
| (1,8)   | 1:12:A:GLU:H    | 1:7:A:LEU:HD23 | 3        | 0.96          |
| (1,844) | 1:25:A:PHE:HB3  | 1:14:A:ARG:HB3 | 11       | 0.95          |
| (1,12)  | 1:21:A:ARG:H    | 1:16:A:SER:HB2 | 25       | 0.95          |
| (1,872) | 2:89:B:GLU:HB2  | 1:16:A:SER:HB3 | 25       | 0.94          |
| (1,844) | 1:25:A:PHE:HB3  | 1:14:A:ARG:HB3 | 2        | 0.94          |
| (1,837) | 1:21:A:ARG:HA   | 2:88:B:PRO:HB3 | 20       | 0.94          |
| (1,820) | 1:21:A:ARG:HB3  | 1:19:A:SER:HA  | 3        | 0.94          |
| (1,696) | 2:85:B:SEP:HB3  | 2:84:B:TYR:HB3 | 14       | 0.94          |
| (1,659) | 1:20:A:GLY:H    | 1:16:A:SER:HB2 | 19       | 0.94          |
| (1,617) | 2:89:B:GLU:HA   | 2:88:B:PRO:HD3 | 13       | 0.94          |
| (1,219) | 1:16:A:SER:HB2  | 1:15:A:MET:HA  | 3        | 0.94          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,844) | 1:25:A:PHE:HB3 | 1:14:A:ARG:HB3 | 20       | 0.93          |
| (1,820) | 1:21:A:ARG:HB3 | 1:19:A:SER:HA  | 15       | 0.93          |
| (1,683) | 2:83:B:PRO:HD2 | 2:84:B:TYR:HB3 | 22       | 0.93          |
| (1,683) | 2:83:B:PRO:HD2 | 2:84:B:TYR:HB3 | 24       | 0.93          |
| (1,617) | 2:89:B:GLU:HA  | 2:88:B:PRO:HD3 | 4        | 0.93          |
| (1,617) | 2:89:B:GLU:HA  | 2:88:B:PRO:HD3 | 6        | 0.93          |
| (1,617) | 2:89:B:GLU:HA  | 2:88:B:PRO:HD3 | 25       | 0.93          |
| (1,610) | 2:88:B:PRO:HA  | 2:89:B:GLU:HG2 | 11       | 0.93          |
| (1,219) | 1:16:A:SER:HB2 | 1:15:A:MET:HA  | 18       | 0.93          |
| (1,215) | 1:14:A:ARG:H   | 1:13:A:LYS:HG2 | 1        | 0.93          |
| (1,102) | 1:23:A:TYR:HE1 | 1:25:A:PHE:HB3 | 17       | 0.93          |
| (1,102) | 1:23:A:TYR:HE2 | 1:25:A:PHE:HB3 | 17       | 0.93          |
| (1,102) | 1:23:A:TYR:HE1 | 1:25:A:PHE:HB3 | 21       | 0.93          |
| (1,102) | 1:23:A:TYR:HE2 | 1:25:A:PHE:HB3 | 21       | 0.93          |
| (1,102) | 1:23:A:TYR:HE1 | 1:25:A:PHE:HB3 | 25       | 0.93          |
| (1,102) | 1:23:A:TYR:HE2 | 1:25:A:PHE:HB3 | 25       | 0.93          |
| (1,841) | 1:5:A:GLU:HA   | 1:6:A:LYS:HB3  | 13       | 0.92          |
| (1,837) | 1:21:A:ARG:HA  | 2:88:B:PRO:HB3 | 22       | 0.92          |
| (1,830) | 1:34:A:TRP:HD1 | 1:33:A:GLN:HG2 | 5        | 0.92          |
| (1,830) | 1:34:A:TRP:HD1 | 1:33:A:GLN:HG2 | 21       | 0.92          |
| (1,820) | 1:21:A:ARG:HB3 | 1:19:A:SER:HA  | 23       | 0.92          |
| (1,683) | 2:83:B:PRO:HD2 | 2:84:B:TYR:HB3 | 5        | 0.92          |
| (1,617) | 2:89:B:GLU:HA  | 2:88:B:PRO:HD3 | 16       | 0.92          |
| (1,617) | 2:89:B:GLU:HA  | 2:88:B:PRO:HD3 | 17       | 0.92          |
| (1,606) | 1:34:A:TRP:HD1 | 2:89:B:GLU:HG2 | 11       | 0.92          |
| (1,215) | 1:14:A:ARG:H   | 1:13:A:LYS:HG2 | 5        | 0.92          |
| (1,214) | 1:14:A:ARG:H   | 1:13:A:LYS:HE2 | 20       | 0.92          |
| (1,180) | 1:7:A:LEU:H    | 1:6:A:LYS:HE3  | 21       | 0.92          |
| (1,102) | 1:23:A:TYR:HE1 | 1:25:A:PHE:HB3 | 5        | 0.92          |
| (1,102) | 1:23:A:TYR:HE2 | 1:25:A:PHE:HB3 | 5        | 0.92          |
| (1,102) | 1:23:A:TYR:HE1 | 1:25:A:PHE:HB3 | 8        | 0.92          |
| (1,102) | 1:23:A:TYR:HE2 | 1:25:A:PHE:HB3 | 8        | 0.92          |
| (1,102) | 1:23:A:TYR:HE1 | 1:25:A:PHE:HB3 | 18       | 0.92          |
| (1,102) | 1:23:A:TYR:HE2 | 1:25:A:PHE:HB3 | 18       | 0.92          |
| (1,762) | 1:23:A:TYR:HE1 | 1:17:A:ARG:HG3 | 25       | 0.91          |
| (1,762) | 1:23:A:TYR:HE2 | 1:17:A:ARG:HG3 | 25       | 0.91          |
| (1,696) | 2:85:B:SEP:HB3 | 2:84:B:TYR:HB3 | 6        | 0.91          |
| (1,683) | 2:83:B:PRO:HD2 | 2:84:B:TYR:HB3 | 6        | 0.91          |
| (1,617) | 2:89:B:GLU:HA  | 2:88:B:PRO:HD3 | 20       | 0.91          |
| (1,516) | 1:11:A:TRP:HH2 | 1:37:A:PRO:HD2 | 14       | 0.91          |
| (1,217) | 1:16:A:SER:HB2 | 1:21:A:ARG:HG2 | 13       | 0.91          |
| (1,215) | 1:14:A:ARG:H   | 1:13:A:LYS:HG2 | 16       | 0.91          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,102) | 1:23:A:TYR:HE1  | 1:25:A:PHE:HB3 | 16       | 0.91          |
| (1,102) | 1:23:A:TYR:HE2  | 1:25:A:PHE:HB3 | 16       | 0.91          |
| (1,872) | 2:89:B:GLU:HB2  | 1:16:A:SER:HB3 | 8        | 0.9           |
| (1,837) | 1:21:A:ARG:HA   | 2:88:B:PRO:HB3 | 1        | 0.9           |
| (1,830) | 1:34:A:TRP:HD1  | 1:33:A:GLN:HG2 | 23       | 0.9           |
| (1,825) | 2:87:B:PHE:HE1  | 2:81:B:GLY:HA2 | 15       | 0.9           |
| (1,825) | 2:87:B:PHE:HE2  | 2:81:B:GLY:HA2 | 15       | 0.9           |
| (1,820) | 1:21:A:ARG:HB3  | 1:19:A:SER:HA  | 7        | 0.9           |
| (1,761) | 1:23:A:TYR:HE1  | 1:21:A:ARG:HB2 | 19       | 0.9           |
| (1,761) | 1:23:A:TYR:HE2  | 1:21:A:ARG:HB2 | 19       | 0.9           |
| (1,617) | 2:89:B:GLU:HA   | 2:88:B:PRO:HD3 | 7        | 0.9           |
| (1,217) | 1:16:A:SER:HB2  | 1:21:A:ARG:HG2 | 19       | 0.9           |
| (1,872) | 2:89:B:GLU:HB2  | 1:16:A:SER:HB3 | 1        | 0.89          |
| (1,825) | 2:87:B:PHE:HE1  | 2:81:B:GLY:HA2 | 5        | 0.89          |
| (1,825) | 2:87:B:PHE:HE2  | 2:81:B:GLY:HA2 | 5        | 0.89          |
| (1,751) | 1:33:A:GLN:HE21 | 1:8:A:PRO:HG3  | 14       | 0.89          |
| (1,617) | 2:89:B:GLU:HA   | 2:88:B:PRO:HD3 | 14       | 0.89          |
| (1,215) | 1:14:A:ARG:H    | 1:13:A:LYS:HG2 | 8        | 0.89          |
| (1,215) | 1:14:A:ARG:H    | 1:13:A:LYS:HG2 | 9        | 0.89          |
| (1,830) | 1:34:A:TRP:HD1  | 1:33:A:GLN:HG2 | 16       | 0.88          |
| (1,722) | 2:90:B:GLY:HA2  | 1:21:A:ARG:HG3 | 24       | 0.88          |
| (1,696) | 2:85:B:SEP:HB3  | 2:84:B:TYR:HB3 | 5        | 0.88          |
| (1,617) | 2:89:B:GLU:HA   | 2:88:B:PRO:HD3 | 15       | 0.88          |
| (1,102) | 1:23:A:TYR:HE1  | 1:25:A:PHE:HB3 | 2        | 0.88          |
| (1,102) | 1:23:A:TYR:HE2  | 1:25:A:PHE:HB3 | 2        | 0.88          |
| (1,102) | 1:23:A:TYR:HE1  | 1:25:A:PHE:HB3 | 13       | 0.88          |
| (1,102) | 1:23:A:TYR:HE2  | 1:25:A:PHE:HB3 | 13       | 0.88          |
| (1,872) | 2:89:B:GLU:HB2  | 1:16:A:SER:HB3 | 16       | 0.87          |
| (1,830) | 1:34:A:TRP:HD1  | 1:33:A:GLN:HG2 | 1        | 0.87          |
| (1,830) | 1:34:A:TRP:HD1  | 1:33:A:GLN:HG2 | 6        | 0.87          |
| (1,617) | 2:89:B:GLU:HA   | 2:88:B:PRO:HD3 | 9        | 0.87          |
| (1,617) | 2:89:B:GLU:HA   | 2:88:B:PRO:HD3 | 10       | 0.87          |
| (1,617) | 2:89:B:GLU:HA   | 2:88:B:PRO:HD3 | 24       | 0.87          |
| (1,219) | 1:16:A:SER:HB2  | 1:15:A:MET:HA  | 13       | 0.87          |
| (1,102) | 1:23:A:TYR:HE1  | 1:25:A:PHE:HB3 | 1        | 0.87          |
| (1,102) | 1:23:A:TYR:HE2  | 1:25:A:PHE:HB3 | 1        | 0.87          |
| (1,872) | 2:89:B:GLU:HB2  | 1:16:A:SER:HB3 | 23       | 0.86          |
| (1,844) | 1:25:A:PHE:HB3  | 1:14:A:ARG:HB3 | 10       | 0.86          |
| (1,837) | 1:21:A:ARG:HA   | 2:88:B:PRO:HB3 | 6        | 0.86          |
| (1,837) | 1:21:A:ARG:HA   | 2:88:B:PRO:HB3 | 23       | 0.86          |
| (1,761) | 1:23:A:TYR:HE1  | 1:21:A:ARG:HB2 | 8        | 0.86          |
| (1,761) | 1:23:A:TYR:HE2  | 1:21:A:ARG:HB2 | 8        | 0.86          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,761) | 1:23:A:TYR:HE1  | 1:21:A:ARG:HB2 | 23       | 0.86          |
| (1,761) | 1:23:A:TYR:HE2  | 1:21:A:ARG:HB2 | 23       | 0.86          |
| (1,674) | 2:86:B:PRO:HD3  | 1:14:A:ARG:HD2 | 23       | 0.86          |
| (1,659) | 1:20:A:GLY:H    | 1:16:A:SER:HB2 | 3        | 0.86          |
| (1,617) | 2:89:B:GLU:HA   | 2:88:B:PRO:HD3 | 1        | 0.86          |
| (1,606) | 1:34:A:TRP:HD1  | 2:89:B:GLU:HG2 | 18       | 0.86          |
| (1,214) | 1:14:A:ARG:H    | 1:13:A:LYS:HE2 | 1        | 0.86          |
| (1,12)  | 1:21:A:ARG:H    | 1:16:A:SER:HB2 | 7        | 0.86          |
| (1,872) | 2:89:B:GLU:HB2  | 1:16:A:SER:HB3 | 18       | 0.85          |
| (1,837) | 1:21:A:ARG:HA   | 2:88:B:PRO:HB3 | 14       | 0.85          |
| (1,837) | 1:21:A:ARG:HA   | 2:88:B:PRO:HB3 | 18       | 0.85          |
| (1,830) | 1:34:A:TRP:HD1  | 1:33:A:GLN:HG2 | 12       | 0.85          |
| (1,736) | 1:33:A:GLN:H    | 1:7:A:LEU:HD21 | 6        | 0.85          |
| (1,736) | 1:33:A:GLN:H    | 1:7:A:LEU:HD22 | 6        | 0.85          |
| (1,736) | 1:33:A:GLN:H    | 1:7:A:LEU:HD23 | 6        | 0.85          |
| (1,696) | 2:85:B:SEP:HB3  | 2:84:B:TYR:HB3 | 21       | 0.85          |
| (1,215) | 1:14:A:ARG:H    | 1:13:A:LYS:HG2 | 17       | 0.85          |
| (1,102) | 1:23:A:TYR:HE1  | 1:25:A:PHE:HB3 | 23       | 0.85          |
| (1,102) | 1:23:A:TYR:HE2  | 1:25:A:PHE:HB3 | 23       | 0.85          |
| (1,12)  | 1:21:A:ARG:H    | 1:16:A:SER:HB2 | 12       | 0.85          |
| (1,872) | 2:89:B:GLU:HB2  | 1:16:A:SER:HB3 | 3        | 0.84          |
| (1,837) | 1:21:A:ARG:HA   | 2:88:B:PRO:HB3 | 13       | 0.84          |
| (1,770) | 1:25:A:PHE:HE1  | 1:14:A:ARG:HD2 | 21       | 0.84          |
| (1,770) | 1:25:A:PHE:HE2  | 1:14:A:ARG:HD2 | 21       | 0.84          |
| (1,751) | 1:33:A:GLN:HE21 | 1:8:A:PRO:HG3  | 25       | 0.84          |
| (1,683) | 2:83:B:PRO:HD2  | 2:84:B:TYR:HB3 | 9        | 0.84          |
| (1,516) | 1:11:A:TRP:HH2  | 1:37:A:PRO:HD2 | 4        | 0.84          |
| (1,483) | 1:24:A:TYR:HD1  | 1:37:A:PRO:HB2 | 22       | 0.84          |
| (1,483) | 1:24:A:TYR:HD2  | 1:37:A:PRO:HB2 | 22       | 0.84          |
| (1,219) | 1:16:A:SER:HB2  | 1:15:A:MET:HA  | 24       | 0.84          |
| (1,12)  | 1:21:A:ARG:H    | 1:16:A:SER:HB2 | 1        | 0.84          |
| (1,844) | 1:25:A:PHE:HB3  | 1:14:A:ARG:HB3 | 7        | 0.83          |
| (1,837) | 1:21:A:ARG:HA   | 2:88:B:PRO:HB3 | 12       | 0.83          |
| (1,820) | 1:21:A:ARG:HB3  | 1:19:A:SER:HA  | 12       | 0.83          |
| (1,736) | 1:33:A:GLN:H    | 1:7:A:LEU:HD21 | 12       | 0.83          |
| (1,736) | 1:33:A:GLN:H    | 1:7:A:LEU:HD22 | 12       | 0.83          |
| (1,736) | 1:33:A:GLN:H    | 1:7:A:LEU:HD23 | 12       | 0.83          |
| (1,639) | 2:84:B:TYR:HD1  | 1:14:A:ARG:HG2 | 20       | 0.83          |
| (1,639) | 2:84:B:TYR:HD2  | 1:14:A:ARG:HG2 | 20       | 0.83          |
| (1,562) | 1:34:A:TRP:HZ2  | 1:16:A:SER:HB3 | 25       | 0.83          |
| (1,516) | 1:11:A:TRP:HH2  | 1:37:A:PRO:HD2 | 25       | 0.83          |
| (1,479) | 1:33:A:GLN:HE21 | 1:35:A:GLU:HB2 | 19       | 0.83          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,696) | 2:85:B:SEP:HB3  | 2:84:B:TYR:HB3 | 22       | 0.82          |
| (1,562) | 1:34:A:TRP:HZ2  | 1:16:A:SER:HB3 | 9        | 0.82          |
| (1,516) | 1:11:A:TRP:HH2  | 1:37:A:PRO:HD2 | 1        | 0.82          |
| (1,215) | 1:14:A:ARG:H    | 1:13:A:LYS:HG2 | 6        | 0.82          |
| (1,102) | 1:23:A:TYR:HE1  | 1:25:A:PHE:HB3 | 14       | 0.82          |
| (1,102) | 1:23:A:TYR:HE2  | 1:25:A:PHE:HB3 | 14       | 0.82          |
| (1,872) | 2:89:B:GLU:HB2  | 1:16:A:SER:HB3 | 15       | 0.81          |
| (1,844) | 1:25:A:PHE:HB3  | 1:14:A:ARG:HB3 | 21       | 0.81          |
| (1,837) | 1:21:A:ARG:HA   | 2:88:B:PRO:HB3 | 9        | 0.81          |
| (1,756) | 1:41:A:SER:H    | 1:6:A:LYS:HB2  | 6        | 0.81          |
| (1,756) | 1:41:A:SER:H    | 1:6:A:LYS:HB2  | 8        | 0.81          |
| (1,674) | 2:86:B:PRO:HD3  | 1:14:A:ARG:HD2 | 4        | 0.81          |
| (1,820) | 1:21:A:ARG:HB3  | 1:19:A:SER:HA  | 11       | 0.8           |
| (1,820) | 1:21:A:ARG:HB3  | 1:19:A:SER:HA  | 14       | 0.8           |
| (1,779) | 1:11:A:TRP:HZ3  | 1:7:A:LEU:HD11 | 14       | 0.8           |
| (1,779) | 1:11:A:TRP:HZ3  | 1:7:A:LEU:HD12 | 14       | 0.8           |
| (1,779) | 1:11:A:TRP:HZ3  | 1:7:A:LEU:HD13 | 14       | 0.8           |
| (1,676) | 1:8:A:PRO:HD3   | 1:7:A:LEU:HD11 | 24       | 0.8           |
| (1,676) | 1:8:A:PRO:HD3   | 1:7:A:LEU:HD12 | 24       | 0.8           |
| (1,676) | 1:8:A:PRO:HD3   | 1:7:A:LEU:HD13 | 24       | 0.8           |
| (1,659) | 1:20:A:GLY:H    | 1:16:A:SER:HB2 | 24       | 0.8           |
| (1,617) | 2:89:B:GLU:HA   | 2:88:B:PRO:HD3 | 5        | 0.8           |
| (1,562) | 1:34:A:TRP:HZ2  | 1:16:A:SER:HB3 | 1        | 0.8           |
| (1,562) | 1:34:A:TRP:HZ2  | 1:16:A:SER:HB3 | 2        | 0.8           |
| (1,379) | 1:40:A:ASN:H    | 1:9:A:PRO:HD3  | 18       | 0.8           |
| (1,296) | 1:26:A:ASN:HD22 | 1:10:A:GLY:HA2 | 3        | 0.8           |
| (1,180) | 1:7:A:LEU:H     | 1:6:A:LYS:HE3  | 20       | 0.8           |
| (1,777) | 1:24:A:TYR:HE1  | 1:7:A:LEU:HA   | 13       | 0.79          |
| (1,777) | 1:24:A:TYR:HE2  | 1:7:A:LEU:HA   | 13       | 0.79          |
| (1,696) | 2:85:B:SEP:HB3  | 2:84:B:TYR:HB3 | 11       | 0.79          |
| (1,696) | 2:85:B:SEP:HB3  | 2:84:B:TYR:HB3 | 13       | 0.79          |
| (1,617) | 2:89:B:GLU:HA   | 2:88:B:PRO:HD3 | 2        | 0.79          |
| (1,617) | 2:89:B:GLU:HA   | 2:88:B:PRO:HD3 | 18       | 0.79          |
| (1,617) | 2:89:B:GLU:HA   | 2:88:B:PRO:HD3 | 19       | 0.79          |
| (1,617) | 2:89:B:GLU:HA   | 2:88:B:PRO:HD3 | 21       | 0.79          |
| (1,617) | 2:89:B:GLU:HA   | 2:88:B:PRO:HD3 | 22       | 0.79          |
| (1,606) | 1:34:A:TRP:HD1  | 2:89:B:GLU:HG2 | 9        | 0.79          |
| (1,606) | 1:34:A:TRP:HD1  | 2:89:B:GLU:HG2 | 19       | 0.79          |
| (1,217) | 1:16:A:SER:HB2  | 1:21:A:ARG:HG2 | 7        | 0.79          |
| (1,215) | 1:14:A:ARG:H    | 1:13:A:LYS:HG2 | 21       | 0.79          |
| (1,820) | 1:21:A:ARG:HB3  | 1:19:A:SER:HA  | 18       | 0.78          |
| (1,779) | 1:11:A:TRP:HZ3  | 1:7:A:LEU:HD11 | 11       | 0.78          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,779) | 1:11:A:TRP:HZ3  | 1:7:A:LEU:HD12 | 11       | 0.78          |
| (1,779) | 1:11:A:TRP:HZ3  | 1:7:A:LEU:HD13 | 11       | 0.78          |
| (1,736) | 1:33:A:GLN:H    | 1:7:A:LEU:HD21 | 20       | 0.78          |
| (1,736) | 1:33:A:GLN:H    | 1:7:A:LEU:HD22 | 20       | 0.78          |
| (1,736) | 1:33:A:GLN:H    | 1:7:A:LEU:HD23 | 20       | 0.78          |
| (1,666) | 1:37:A:PRO:HD3  | 1:36:A:ARG:HG3 | 19       | 0.78          |
| (1,659) | 1:20:A:GLY:H    | 1:16:A:SER:HB2 | 13       | 0.78          |
| (1,617) | 2:89:B:GLU:HA   | 2:88:B:PRO:HD3 | 12       | 0.78          |
| (1,797) | 2:84:B:TYR:HD1  | 1:14:A:ARG:HD2 | 20       | 0.77          |
| (1,797) | 2:84:B:TYR:HD2  | 1:14:A:ARG:HD2 | 20       | 0.77          |
| (1,736) | 1:33:A:GLN:H    | 1:7:A:LEU:HD21 | 16       | 0.77          |
| (1,736) | 1:33:A:GLN:H    | 1:7:A:LEU:HD22 | 16       | 0.77          |
| (1,736) | 1:33:A:GLN:H    | 1:7:A:LEU:HD23 | 16       | 0.77          |
| (1,562) | 1:34:A:TRP:HZ2  | 1:16:A:SER:HB3 | 12       | 0.77          |
| (1,379) | 1:40:A:ASN:H    | 1:9:A:PRO:HD3  | 3        | 0.77          |
| (1,12)  | 1:21:A:ARG:H    | 1:16:A:SER:HB2 | 9        | 0.77          |
| (1,879) | 2:88:B:PRO:HD2  | 1:17:A:ARG:HD2 | 25       | 0.76          |
| (1,837) | 1:21:A:ARG:HA   | 2:88:B:PRO:HB3 | 11       | 0.76          |
| (1,837) | 1:21:A:ARG:HA   | 2:88:B:PRO:HB3 | 19       | 0.76          |
| (1,830) | 1:34:A:TRP:HD1  | 1:33:A:GLN:HG2 | 20       | 0.76          |
| (1,808) | 1:11:A:TRP:HE3  | 1:37:A:PRO:HD2 | 9        | 0.76          |
| (1,756) | 1:41:A:SER:H    | 1:6:A:LYS:HB2  | 12       | 0.76          |
| (1,676) | 1:8:A:PRO:HD3   | 1:7:A:LEU:HD11 | 5        | 0.76          |
| (1,676) | 1:8:A:PRO:HD3   | 1:7:A:LEU:HD12 | 5        | 0.76          |
| (1,676) | 1:8:A:PRO:HD3   | 1:7:A:LEU:HD13 | 5        | 0.76          |
| (1,674) | 2:86:B:PRO:HD3  | 1:14:A:ARG:HD2 | 1        | 0.76          |
| (1,659) | 1:20:A:GLY:H    | 1:16:A:SER:HB2 | 18       | 0.76          |
| (1,137) | 2:85:B:SEP:HB2  | 1:17:A:ARG:HD3 | 1        | 0.76          |
| (1,102) | 1:23:A:TYR:HE1  | 1:25:A:PHE:HB3 | 7        | 0.76          |
| (1,102) | 1:23:A:TYR:HE2  | 1:25:A:PHE:HB3 | 7        | 0.76          |
| (1,720) | 2:84:B:TYR:HE1  | 1:23:A:TYR:HE1 | 17       | 0.75          |
| (1,720) | 2:84:B:TYR:HE1  | 1:23:A:TYR:HE2 | 17       | 0.75          |
| (1,720) | 2:84:B:TYR:HE2  | 1:23:A:TYR:HE1 | 17       | 0.75          |
| (1,720) | 2:84:B:TYR:HE2  | 1:23:A:TYR:HE2 | 17       | 0.75          |
| (1,674) | 2:86:B:PRO:HD3  | 1:14:A:ARG:HD2 | 25       | 0.75          |
| (1,544) | 1:11:A:TRP:HD1  | 1:7:A:LEU:HB2  | 21       | 0.75          |
| (1,296) | 1:26:A:ASN:HD22 | 1:10:A:GLY:HA2 | 4        | 0.75          |
| (1,219) | 1:16:A:SER:HB2  | 1:15:A:MET:HA  | 19       | 0.75          |
| (1,214) | 1:14:A:ARG:H    | 1:13:A:LYS:HE2 | 16       | 0.75          |
| (1,851) | 1:7:A:LEU:HD11  | 1:37:A:PRO:HD3 | 3        | 0.74          |
| (1,851) | 1:7:A:LEU:HD12  | 1:37:A:PRO:HD3 | 3        | 0.74          |
| (1,851) | 1:7:A:LEU:HD13  | 1:37:A:PRO:HD3 | 3        | 0.74          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,844) | 1:25:A:PHE:HB3 | 1:14:A:ARG:HB3 | 8        | 0.74          |
| (1,837) | 1:21:A:ARG:HA  | 2:88:B:PRO:HB3 | 7        | 0.74          |
| (1,837) | 1:21:A:ARG:HA  | 2:88:B:PRO:HB3 | 21       | 0.74          |
| (1,836) | 2:88:B:PRO:HA  | 1:17:A:ARG:HG2 | 24       | 0.74          |
| (1,736) | 1:33:A:GLN:H   | 1:7:A:LEU:HD21 | 3        | 0.74          |
| (1,736) | 1:33:A:GLN:H   | 1:7:A:LEU:HD22 | 3        | 0.74          |
| (1,736) | 1:33:A:GLN:H   | 1:7:A:LEU:HD23 | 3        | 0.74          |
| (1,696) | 2:85:B:SEP:HB3 | 2:84:B:TYR:HB3 | 24       | 0.74          |
| (1,683) | 2:83:B:PRO:HD2 | 2:84:B:TYR:HB3 | 18       | 0.74          |
| (1,606) | 1:34:A:TRP:HD1 | 2:89:B:GLU:HG2 | 23       | 0.74          |
| (1,137) | 2:85:B:SEP:HB2 | 1:17:A:ARG:HD3 | 24       | 0.74          |
| (1,23)  | 1:36:A:ARG:HD2 | 1:7:A:LEU:HD21 | 11       | 0.74          |
| (1,23)  | 1:36:A:ARG:HD2 | 1:7:A:LEU:HD22 | 11       | 0.74          |
| (1,23)  | 1:36:A:ARG:HD2 | 1:7:A:LEU:HD23 | 11       | 0.74          |
| (1,2)   | 1:13:A:LYS:H   | 1:12:A:GLU:HG2 | 19       | 0.74          |
| (1,879) | 2:88:B:PRO:HD2 | 1:17:A:ARG:HD2 | 6        | 0.73          |
| (1,872) | 2:89:B:GLU:HB2 | 1:16:A:SER:HB3 | 7        | 0.73          |
| (1,851) | 1:7:A:LEU:HD11 | 1:37:A:PRO:HD3 | 21       | 0.73          |
| (1,851) | 1:7:A:LEU:HD12 | 1:37:A:PRO:HD3 | 21       | 0.73          |
| (1,851) | 1:7:A:LEU:HD13 | 1:37:A:PRO:HD3 | 21       | 0.73          |
| (1,606) | 1:34:A:TRP:HD1 | 2:89:B:GLU:HG2 | 4        | 0.73          |
| (1,254) | 1:11:A:TRP:HE1 | 1:37:A:PRO:HD3 | 24       | 0.73          |
| (1,180) | 1:7:A:LEU:H    | 1:6:A:LYS:HE3  | 11       | 0.73          |
| (1,8)   | 1:12:A:GLU:H   | 1:7:A:LEU:HD21 | 1        | 0.73          |
| (1,8)   | 1:12:A:GLU:H   | 1:7:A:LEU:HD22 | 1        | 0.73          |
| (1,8)   | 1:12:A:GLU:H   | 1:7:A:LEU:HD23 | 1        | 0.73          |
| (1,872) | 2:89:B:GLU:HB2 | 1:16:A:SER:HB3 | 9        | 0.72          |
| (1,761) | 1:23:A:TYR:HE1 | 1:21:A:ARG:HB2 | 14       | 0.72          |
| (1,761) | 1:23:A:TYR:HE2 | 1:21:A:ARG:HB2 | 14       | 0.72          |
| (1,720) | 2:84:B:TYR:HE1 | 1:23:A:TYR:HE1 | 3        | 0.72          |
| (1,720) | 2:84:B:TYR:HE1 | 1:23:A:TYR:HE2 | 3        | 0.72          |
| (1,720) | 2:84:B:TYR:HE2 | 1:23:A:TYR:HE1 | 3        | 0.72          |
| (1,720) | 2:84:B:TYR:HE2 | 1:23:A:TYR:HE2 | 3        | 0.72          |
| (1,617) | 2:89:B:GLU:HA  | 2:88:B:PRO:HD3 | 23       | 0.72          |
| (1,516) | 1:11:A:TRP:HH2 | 1:37:A:PRO:HD2 | 20       | 0.72          |
| (1,483) | 1:24:A:TYR:HD1 | 1:37:A:PRO:HB2 | 19       | 0.72          |
| (1,483) | 1:24:A:TYR:HD2 | 1:37:A:PRO:HB2 | 19       | 0.72          |
| (1,468) | 2:85:B:SEP:H   | 1:14:A:ARG:HB3 | 1        | 0.72          |
| (1,343) | 1:25:A:PHE:H   | 1:14:A:ARG:HB3 | 9        | 0.72          |
| (1,137) | 2:85:B:SEP:HB2 | 1:17:A:ARG:HD3 | 2        | 0.72          |
| (1,12)  | 1:21:A:ARG:H   | 1:16:A:SER:HB2 | 19       | 0.72          |
| (1,2)   | 1:13:A:LYS:H   | 1:12:A:GLU:HG2 | 6        | 0.72          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,2)   | 1:13:A:LYS:H    | 1:12:A:GLU:HG2 | 7        | 0.72          |
| (1,844) | 1:25:A:PHE:HB3  | 1:14:A:ARG:HB3 | 25       | 0.71          |
| (1,841) | 1:5:A:GLU:HA    | 1:6:A:LYS:HB3  | 19       | 0.71          |
| (1,825) | 2:87:B:PHE:HE1  | 2:81:B:GLY:HA2 | 6        | 0.71          |
| (1,825) | 2:87:B:PHE:HE2  | 2:81:B:GLY:HA2 | 6        | 0.71          |
| (1,808) | 1:11:A:TRP:HE3  | 1:37:A:PRO:HD2 | 7        | 0.71          |
| (1,770) | 1:25:A:PHE:HE1  | 1:14:A:ARG:HD2 | 8        | 0.71          |
| (1,770) | 1:25:A:PHE:HE2  | 1:14:A:ARG:HD2 | 8        | 0.71          |
| (1,761) | 1:23:A:TYR:HE1  | 1:21:A:ARG:HB2 | 11       | 0.71          |
| (1,761) | 1:23:A:TYR:HE2  | 1:21:A:ARG:HB2 | 11       | 0.71          |
| (1,751) | 1:33:A:GLN:HE21 | 1:8:A:PRO:HG3  | 11       | 0.71          |
| (1,617) | 2:89:B:GLU:HA   | 2:88:B:PRO:HD3 | 11       | 0.71          |
| (1,606) | 1:34:A:TRP:HD1  | 2:89:B:GLU:HG2 | 12       | 0.71          |
| (1,451) | 1:11:A:TRP:HE3  | 1:7:A:LEU:HD21 | 19       | 0.71          |
| (1,451) | 1:11:A:TRP:HE3  | 1:7:A:LEU:HD22 | 19       | 0.71          |
| (1,451) | 1:11:A:TRP:HE3  | 1:7:A:LEU:HD23 | 19       | 0.71          |
| (1,343) | 1:25:A:PHE:H    | 1:14:A:ARG:HB3 | 5        | 0.71          |
| (1,343) | 1:25:A:PHE:H    | 1:14:A:ARG:HB3 | 17       | 0.71          |
| (1,342) | 1:25:A:PHE:H    | 1:14:A:ARG:HG2 | 4        | 0.71          |
| (1,322) | 1:17:A:ARG:HD3  | 2:81:B:GLY:HA2 | 4        | 0.71          |
| (1,2)   | 1:13:A:LYS:H    | 1:12:A:GLU:HG2 | 25       | 0.71          |
| (1,841) | 1:5:A:GLU:HA    | 1:6:A:LYS:HB3  | 12       | 0.7           |
| (1,837) | 1:21:A:ARG:HA   | 2:88:B:PRO:HB3 | 25       | 0.7           |
| (1,830) | 1:34:A:TRP:HD1  | 1:33:A:GLN:HG2 | 24       | 0.7           |
| (1,751) | 1:33:A:GLN:HE21 | 1:8:A:PRO:HG3  | 24       | 0.7           |
| (1,736) | 1:33:A:GLN:H    | 1:7:A:LEU:HD21 | 7        | 0.7           |
| (1,736) | 1:33:A:GLN:H    | 1:7:A:LEU:HD22 | 7        | 0.7           |
| (1,736) | 1:33:A:GLN:H    | 1:7:A:LEU:HD23 | 7        | 0.7           |
| (1,725) | 2:84:B:TYR:HB3  | 1:14:A:ARG:HD2 | 8        | 0.7           |
| (1,714) | 1:13:A:LYS:H    | 1:24:A:TYR:HE1 | 9        | 0.7           |
| (1,714) | 1:13:A:LYS:H    | 1:24:A:TYR:HE2 | 9        | 0.7           |
| (1,696) | 2:85:B:SEP:HB3  | 2:84:B:TYR:HB3 | 8        | 0.7           |
| (1,643) | 2:85:B:SEP:HB2  | 1:17:A:ARG:HG2 | 8        | 0.7           |
| (1,606) | 1:34:A:TRP:HD1  | 2:89:B:GLU:HG2 | 14       | 0.7           |
| (1,562) | 1:34:A:TRP:HZ2  | 1:16:A:SER:HB3 | 16       | 0.7           |
| (1,516) | 1:11:A:TRP:HH2  | 1:37:A:PRO:HD2 | 7        | 0.7           |
| (1,102) | 1:23:A:TYR:HE1  | 1:25:A:PHE:HB3 | 3        | 0.7           |
| (1,102) | 1:23:A:TYR:HE2  | 1:25:A:PHE:HB3 | 3        | 0.7           |
| (1,849) | 1:14:A:ARG:HB3  | 1:15:A:MET:HG3 | 20       | 0.69          |
| (1,820) | 1:21:A:ARG:HB3  | 1:19:A:SER:HA  | 13       | 0.69          |
| (1,761) | 1:23:A:TYR:HE1  | 1:21:A:ARG:HB2 | 3        | 0.69          |
| (1,761) | 1:23:A:TYR:HE2  | 1:21:A:ARG:HB2 | 3        | 0.69          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,617) | 2:89:B:GLU:HA   | 2:88:B:PRO:HD3 | 3        | 0.69          |
| (1,544) | 1:11:A:TRP:HD1  | 1:7:A:LEU:HB2  | 1        | 0.69          |
| (1,102) | 1:23:A:TYR:HE1  | 1:25:A:PHE:HB3 | 4        | 0.69          |
| (1,102) | 1:23:A:TYR:HE2  | 1:25:A:PHE:HB3 | 4        | 0.69          |
| (1,2)   | 1:13:A:LYS:H    | 1:12:A:GLU:HG2 | 15       | 0.69          |
| (1,2)   | 1:13:A:LYS:H    | 1:12:A:GLU:HG2 | 18       | 0.69          |
| (1,808) | 1:11:A:TRP:HE3  | 1:37:A:PRO:HD2 | 22       | 0.68          |
| (1,676) | 1:8:A:PRO:HD3   | 1:7:A:LEU:HD11 | 9        | 0.68          |
| (1,676) | 1:8:A:PRO:HD3   | 1:7:A:LEU:HD12 | 9        | 0.68          |
| (1,676) | 1:8:A:PRO:HD3   | 1:7:A:LEU:HD13 | 9        | 0.68          |
| (1,639) | 2:84:B:TYR:HD1  | 1:14:A:ARG:HG2 | 23       | 0.68          |
| (1,639) | 2:84:B:TYR:HD2  | 1:14:A:ARG:HG2 | 23       | 0.68          |
| (1,516) | 1:11:A:TRP:HH2  | 1:37:A:PRO:HD2 | 16       | 0.68          |
| (1,465) | 1:23:A:TYR:HE1  | 2:86:B:PRO:HB3 | 3        | 0.68          |
| (1,465) | 1:23:A:TYR:HE2  | 2:86:B:PRO:HB3 | 3        | 0.68          |
| (1,343) | 1:25:A:PHE:H    | 1:14:A:ARG:HB3 | 16       | 0.68          |
| (1,2)   | 1:13:A:LYS:H    | 1:12:A:GLU:HG2 | 13       | 0.68          |
| (1,2)   | 1:13:A:LYS:H    | 1:12:A:GLU:HG2 | 21       | 0.68          |
| (1,857) | 1:28:A:ILE:HG13 | 1:31:A:ALA:HB1 | 11       | 0.67          |
| (1,857) | 1:28:A:ILE:HG13 | 1:31:A:ALA:HB2 | 11       | 0.67          |
| (1,857) | 1:28:A:ILE:HG13 | 1:31:A:ALA:HB3 | 11       | 0.67          |
| (1,841) | 1:5:A:GLU:HA    | 1:6:A:LYS:HB3  | 17       | 0.67          |
| (1,836) | 2:88:B:PRO:HA   | 1:17:A:ARG:HG2 | 16       | 0.67          |
| (1,643) | 2:85:B:SEP:HB2  | 1:17:A:ARG:HG2 | 11       | 0.67          |
| (1,254) | 1:11:A:TRP:HE1  | 1:37:A:PRO:HD3 | 25       | 0.67          |
| (1,217) | 1:16:A:SER:HB2  | 1:21:A:ARG:HG2 | 18       | 0.67          |
| (1,2)   | 1:13:A:LYS:H    | 1:12:A:GLU:HG2 | 3        | 0.67          |
| (1,2)   | 1:13:A:LYS:H    | 1:12:A:GLU:HG2 | 24       | 0.67          |
| (1,857) | 1:28:A:ILE:HG13 | 1:31:A:ALA:HB1 | 6        | 0.66          |
| (1,857) | 1:28:A:ILE:HG13 | 1:31:A:ALA:HB2 | 6        | 0.66          |
| (1,857) | 1:28:A:ILE:HG13 | 1:31:A:ALA:HB3 | 6        | 0.66          |
| (1,836) | 2:88:B:PRO:HA   | 1:17:A:ARG:HG2 | 4        | 0.66          |
| (1,762) | 1:23:A:TYR:HE1  | 1:17:A:ARG:HG3 | 5        | 0.66          |
| (1,762) | 1:23:A:TYR:HE2  | 1:17:A:ARG:HG3 | 5        | 0.66          |
| (1,736) | 1:33:A:GLN:H    | 1:7:A:LEU:HD21 | 5        | 0.66          |
| (1,736) | 1:33:A:GLN:H    | 1:7:A:LEU:HD22 | 5        | 0.66          |
| (1,736) | 1:33:A:GLN:H    | 1:7:A:LEU:HD23 | 5        | 0.66          |
| (1,674) | 2:86:B:PRO:HD3  | 1:14:A:ARG:HD2 | 19       | 0.66          |
| (1,643) | 2:85:B:SEP:HB2  | 1:17:A:ARG:HG2 | 14       | 0.66          |
| (1,604) | 1:33:A:GLN:HE22 | 1:35:A:GLU:HG2 | 11       | 0.66          |
| (1,516) | 1:11:A:TRP:HH2  | 1:37:A:PRO:HD2 | 17       | 0.66          |
| (1,516) | 1:11:A:TRP:HH2  | 1:37:A:PRO:HD2 | 18       | 0.66          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,483) | 1:24:A:TYR:HD1  | 1:37:A:PRO:HB2  | 3        | 0.66          |
| (1,483) | 1:24:A:TYR:HD2  | 1:37:A:PRO:HB2  | 3        | 0.66          |
| (1,483) | 1:24:A:TYR:HD1  | 1:37:A:PRO:HB2  | 10       | 0.66          |
| (1,483) | 1:24:A:TYR:HD2  | 1:37:A:PRO:HB2  | 10       | 0.66          |
| (1,479) | 1:33:A:GLN:HE21 | 1:35:A:GLU:HB2  | 13       | 0.66          |
| (1,87)  | 1:23:A:TYR:HE1  | 1:16:A:SER:HB3  | 22       | 0.66          |
| (1,87)  | 1:23:A:TYR:HE2  | 1:16:A:SER:HB3  | 22       | 0.66          |
| (1,872) | 2:89:B:GLU:HB2  | 1:16:A:SER:HB3  | 6        | 0.65          |
| (1,857) | 1:28:A:ILE:HG13 | 1:31:A:ALA:HB1  | 10       | 0.65          |
| (1,857) | 1:28:A:ILE:HG13 | 1:31:A:ALA:HB2  | 10       | 0.65          |
| (1,857) | 1:28:A:ILE:HG13 | 1:31:A:ALA:HB3  | 10       | 0.65          |
| (1,849) | 1:14:A:ARG:HB3  | 1:15:A:MET:HG3  | 21       | 0.65          |
| (1,844) | 1:25:A:PHE:HB3  | 1:14:A:ARG:HB3  | 12       | 0.65          |
| (1,762) | 1:23:A:TYR:HE1  | 1:17:A:ARG:HG3  | 1        | 0.65          |
| (1,762) | 1:23:A:TYR:HE2  | 1:17:A:ARG:HG3  | 1        | 0.65          |
| (1,707) | 1:17:A:ARG:HD3  | 2:88:B:PRO:HD3  | 23       | 0.65          |
| (1,516) | 1:11:A:TRP:HH2  | 1:37:A:PRO:HD2  | 24       | 0.65          |
| (1,483) | 1:24:A:TYR:HD1  | 1:37:A:PRO:HB2  | 2        | 0.65          |
| (1,483) | 1:24:A:TYR:HD2  | 1:37:A:PRO:HB2  | 2        | 0.65          |
| (1,407) | 1:35:A:GLU:H    | 1:33:A:GLN:HE22 | 7        | 0.65          |
| (1,2)   | 1:13:A:LYS:H    | 1:12:A:GLU:HG2  | 1        | 0.65          |
| (1,2)   | 1:13:A:LYS:H    | 1:12:A:GLU:HG2  | 5        | 0.65          |
| (1,876) | 1:27:A:HIS:HD2  | 1:11:A:TRP:H    | 17       | 0.64          |
| (1,876) | 1:27:A:HIS:HD2  | 1:11:A:TRP:H    | 20       | 0.64          |
| (1,857) | 1:28:A:ILE:HG13 | 1:31:A:ALA:HB1  | 1        | 0.64          |
| (1,857) | 1:28:A:ILE:HG13 | 1:31:A:ALA:HB2  | 1        | 0.64          |
| (1,857) | 1:28:A:ILE:HG13 | 1:31:A:ALA:HB3  | 1        | 0.64          |
| (1,857) | 1:28:A:ILE:HG13 | 1:31:A:ALA:HB1  | 8        | 0.64          |
| (1,857) | 1:28:A:ILE:HG13 | 1:31:A:ALA:HB2  | 8        | 0.64          |
| (1,857) | 1:28:A:ILE:HG13 | 1:31:A:ALA:HB3  | 8        | 0.64          |
| (1,857) | 1:28:A:ILE:HG13 | 1:31:A:ALA:HB1  | 12       | 0.64          |
| (1,857) | 1:28:A:ILE:HG13 | 1:31:A:ALA:HB2  | 12       | 0.64          |
| (1,857) | 1:28:A:ILE:HG13 | 1:31:A:ALA:HB3  | 12       | 0.64          |
| (1,837) | 1:21:A:ARG:HA   | 2:88:B:PRO:HB3  | 17       | 0.64          |
| (1,676) | 1:8:A:PRO:HD3   | 1:7:A:LEU:HD11  | 6        | 0.64          |
| (1,676) | 1:8:A:PRO:HD3   | 1:7:A:LEU:HD12  | 6        | 0.64          |
| (1,676) | 1:8:A:PRO:HD3   | 1:7:A:LEU:HD13  | 6        | 0.64          |
| (1,676) | 1:8:A:PRO:HD3   | 1:7:A:LEU:HD11  | 23       | 0.64          |
| (1,676) | 1:8:A:PRO:HD3   | 1:7:A:LEU:HD12  | 23       | 0.64          |
| (1,676) | 1:8:A:PRO:HD3   | 1:7:A:LEU:HD13  | 23       | 0.64          |
| (1,639) | 2:84:B:TYR:HD1  | 1:14:A:ARG:HG2  | 17       | 0.64          |
| (1,639) | 2:84:B:TYR:HD2  | 1:14:A:ARG:HG2  | 17       | 0.64          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,562) | 1:34:A:TRP:HZ2  | 1:16:A:SER:HB3  | 4        | 0.64          |
| (1,480) | 1:33:A:GLN:HE21 | 1:35:A:GLU:HG2  | 11       | 0.64          |
| (1,465) | 1:23:A:TYR:HE1  | 2:86:B:PRO:HB3  | 17       | 0.64          |
| (1,465) | 1:23:A:TYR:HE2  | 2:86:B:PRO:HB3  | 17       | 0.64          |
| (1,465) | 1:23:A:TYR:HE1  | 2:86:B:PRO:HB3  | 18       | 0.64          |
| (1,465) | 1:23:A:TYR:HE2  | 2:86:B:PRO:HB3  | 18       | 0.64          |
| (1,102) | 1:23:A:TYR:HE1  | 1:25:A:PHE:HB3  | 9        | 0.64          |
| (1,102) | 1:23:A:TYR:HE2  | 1:25:A:PHE:HB3  | 9        | 0.64          |
| (1,857) | 1:28:A:ILE:HG13 | 1:31:A:ALA:HB1  | 9        | 0.63          |
| (1,857) | 1:28:A:ILE:HG13 | 1:31:A:ALA:HB2  | 9        | 0.63          |
| (1,857) | 1:28:A:ILE:HG13 | 1:31:A:ALA:HB3  | 9        | 0.63          |
| (1,856) | 1:7:A:LEU:HD11  | 1:36:A:ARG:HG3  | 24       | 0.63          |
| (1,856) | 1:7:A:LEU:HD12  | 1:36:A:ARG:HG3  | 24       | 0.63          |
| (1,856) | 1:7:A:LEU:HD13  | 1:36:A:ARG:HG3  | 24       | 0.63          |
| (1,849) | 1:14:A:ARG:HB3  | 1:15:A:MET:HG3  | 2        | 0.63          |
| (1,756) | 1:41:A:SER:H    | 1:6:A:LYS:HB2   | 16       | 0.63          |
| (1,720) | 2:84:B:TYR:HE1  | 1:23:A:TYR:HE1  | 6        | 0.63          |
| (1,720) | 2:84:B:TYR:HE1  | 1:23:A:TYR:HE2  | 6        | 0.63          |
| (1,720) | 2:84:B:TYR:HE2  | 1:23:A:TYR:HE1  | 6        | 0.63          |
| (1,720) | 2:84:B:TYR:HE2  | 1:23:A:TYR:HE2  | 6        | 0.63          |
| (1,606) | 1:34:A:TRP:HD1  | 2:89:B:GLU:HG2  | 22       | 0.63          |
| (1,516) | 1:11:A:TRP:HH2  | 1:37:A:PRO:HD2  | 9        | 0.63          |
| (1,465) | 1:23:A:TYR:HE1  | 2:86:B:PRO:HB3  | 6        | 0.63          |
| (1,465) | 1:23:A:TYR:HE2  | 2:86:B:PRO:HB3  | 6        | 0.63          |
| (1,465) | 1:23:A:TYR:HE1  | 2:86:B:PRO:HB3  | 15       | 0.63          |
| (1,465) | 1:23:A:TYR:HE2  | 2:86:B:PRO:HB3  | 15       | 0.63          |
| (1,407) | 1:35:A:GLU:H    | 1:33:A:GLN:HE22 | 9        | 0.63          |
| (1,2)   | 1:13:A:LYS:H    | 1:12:A:GLU:HG2  | 2        | 0.63          |
| (1,857) | 1:28:A:ILE:HG13 | 1:31:A:ALA:HB1  | 14       | 0.62          |
| (1,857) | 1:28:A:ILE:HG13 | 1:31:A:ALA:HB2  | 14       | 0.62          |
| (1,857) | 1:28:A:ILE:HG13 | 1:31:A:ALA:HB3  | 14       | 0.62          |
| (1,841) | 1:5:A:GLU:HA    | 1:6:A:LYS:HB3   | 14       | 0.62          |
| (1,837) | 1:21:A:ARG:HA   | 2:88:B:PRO:HB3  | 2        | 0.62          |
| (1,736) | 1:33:A:GLN:H    | 1:7:A:LEU:HD21  | 23       | 0.62          |
| (1,736) | 1:33:A:GLN:H    | 1:7:A:LEU:HD22  | 23       | 0.62          |
| (1,736) | 1:33:A:GLN:H    | 1:7:A:LEU:HD23  | 23       | 0.62          |
| (1,544) | 1:11:A:TRP:HD1  | 1:7:A:LEU:HB2   | 2        | 0.62          |
| (1,516) | 1:11:A:TRP:HH2  | 1:37:A:PRO:HD2  | 10       | 0.62          |
| (1,483) | 1:24:A:TYR:HD1  | 1:37:A:PRO:HB2  | 11       | 0.62          |
| (1,483) | 1:24:A:TYR:HD2  | 1:37:A:PRO:HB2  | 11       | 0.62          |
| (1,465) | 1:23:A:TYR:HE1  | 2:86:B:PRO:HB3  | 19       | 0.62          |
| (1,465) | 1:23:A:TYR:HE2  | 2:86:B:PRO:HB3  | 19       | 0.62          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,454) | 1:27:A:HIS:HE1  | 1:12:A:GLU:HB2  | 23       | 0.62          |
| (1,407) | 1:35:A:GLU:H    | 1:33:A:GLN:HE22 | 16       | 0.62          |
| (1,137) | 2:85:B:SEP:HB2  | 1:17:A:ARG:HD3  | 9        | 0.62          |
| (1,2)   | 1:13:A:LYS:H    | 1:12:A:GLU:HG2  | 9        | 0.62          |
| (1,876) | 1:27:A:HIS:HD2  | 1:11:A:TRP:H    | 3        | 0.61          |
| (1,837) | 1:21:A:ARG:HA   | 2:88:B:PRO:HB3  | 24       | 0.61          |
| (1,783) | 1:34:A:TRP:HZ3  | 2:85:B:SEP:HB2  | 5        | 0.61          |
| (1,783) | 1:34:A:TRP:HZ3  | 2:85:B:SEP:HB2  | 13       | 0.61          |
| (1,736) | 1:33:A:GLN:H    | 1:7:A:LEU:HD21  | 9        | 0.61          |
| (1,736) | 1:33:A:GLN:H    | 1:7:A:LEU:HD22  | 9        | 0.61          |
| (1,736) | 1:33:A:GLN:H    | 1:7:A:LEU:HD23  | 9        | 0.61          |
| (1,720) | 2:84:B:TYR:HE1  | 1:23:A:TYR:HE1  | 20       | 0.61          |
| (1,720) | 2:84:B:TYR:HE1  | 1:23:A:TYR:HE2  | 20       | 0.61          |
| (1,720) | 2:84:B:TYR:HE2  | 1:23:A:TYR:HE1  | 20       | 0.61          |
| (1,720) | 2:84:B:TYR:HE2  | 1:23:A:TYR:HE2  | 20       | 0.61          |
| (1,606) | 1:34:A:TRP:HD1  | 2:89:B:GLU:HG2  | 24       | 0.61          |
| (1,544) | 1:11:A:TRP:HD1  | 1:7:A:LEU:HB2   | 3        | 0.61          |
| (1,479) | 1:33:A:GLN:HE21 | 1:35:A:GLU:HB2  | 8        | 0.61          |
| (1,465) | 1:23:A:TYR:HE1  | 2:86:B:PRO:HB3  | 7        | 0.61          |
| (1,465) | 1:23:A:TYR:HE2  | 2:86:B:PRO:HB3  | 7        | 0.61          |
| (1,465) | 1:23:A:TYR:HE1  | 2:86:B:PRO:HB3  | 10       | 0.61          |
| (1,465) | 1:23:A:TYR:HE2  | 2:86:B:PRO:HB3  | 10       | 0.61          |
| (1,254) | 1:11:A:TRP:HE1  | 1:37:A:PRO:HD3  | 21       | 0.61          |
| (1,215) | 1:14:A:ARG:H    | 1:13:A:LYS:HG2  | 20       | 0.61          |
| (1,102) | 1:23:A:TYR:HE1  | 1:25:A:PHE:HB3  | 22       | 0.61          |
| (1,102) | 1:23:A:TYR:HE2  | 1:25:A:PHE:HB3  | 22       | 0.61          |
| (1,87)  | 1:23:A:TYR:HE1  | 1:16:A:SER:HB3  | 2        | 0.61          |
| (1,87)  | 1:23:A:TYR:HE2  | 1:16:A:SER:HB3  | 2        | 0.61          |
| (1,24)  | 1:13:A:LYS:HE2  | 1:22:A:VAL:HG11 | 16       | 0.61          |
| (1,24)  | 1:13:A:LYS:HE2  | 1:22:A:VAL:HG12 | 16       | 0.61          |
| (1,24)  | 1:13:A:LYS:HE2  | 1:22:A:VAL:HG13 | 16       | 0.61          |
| (1,876) | 1:27:A:HIS:HD2  | 1:11:A:TRP:H    | 18       | 0.6           |
| (1,876) | 1:27:A:HIS:HD2  | 1:11:A:TRP:H    | 21       | 0.6           |
| (1,876) | 1:27:A:HIS:HD2  | 1:11:A:TRP:H    | 25       | 0.6           |
| (1,820) | 1:21:A:ARG:HB3  | 1:19:A:SER:HA   | 2        | 0.6           |
| (1,736) | 1:33:A:GLN:H    | 1:7:A:LEU:HD21  | 24       | 0.6           |
| (1,736) | 1:33:A:GLN:H    | 1:7:A:LEU:HD22  | 24       | 0.6           |
| (1,736) | 1:33:A:GLN:H    | 1:7:A:LEU:HD23  | 24       | 0.6           |
| (1,696) | 2:85:B:SEP:HB3  | 2:84:B:TYR:HB3  | 7        | 0.6           |
| (1,696) | 2:85:B:SEP:HB3  | 2:84:B:TYR:HB3  | 18       | 0.6           |
| (1,696) | 2:85:B:SEP:HB3  | 2:84:B:TYR:HB3  | 25       | 0.6           |
| (1,604) | 1:33:A:GLN:HE22 | 1:35:A:GLU:HG2  | 12       | 0.6           |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,516) | 1:11:A:TRP:HH2  | 1:37:A:PRO:HD2  | 12       | 0.6           |
| (1,483) | 1:24:A:TYR:HD1  | 1:37:A:PRO:HB2  | 7        | 0.6           |
| (1,483) | 1:24:A:TYR:HD2  | 1:37:A:PRO:HB2  | 7        | 0.6           |
| (1,468) | 2:85:B:SEP:H    | 1:14:A:ARG:HB3  | 15       | 0.6           |
| (1,465) | 1:23:A:TYR:HE1  | 2:86:B:PRO:HB3  | 5        | 0.6           |
| (1,465) | 1:23:A:TYR:HE2  | 2:86:B:PRO:HB3  | 5        | 0.6           |
| (1,465) | 1:23:A:TYR:HE1  | 2:86:B:PRO:HB3  | 9        | 0.6           |
| (1,465) | 1:23:A:TYR:HE2  | 2:86:B:PRO:HB3  | 9        | 0.6           |
| (1,75)  | 1:37:A:PRO:HD3  | 1:36:A:ARG:HD2  | 7        | 0.6           |
| (1,12)  | 1:21:A:ARG:H    | 1:16:A:SER:HB2  | 24       | 0.6           |
| (1,857) | 1:28:A:ILE:HG13 | 1:31:A:ALA:HB1  | 19       | 0.59          |
| (1,857) | 1:28:A:ILE:HG13 | 1:31:A:ALA:HB2  | 19       | 0.59          |
| (1,857) | 1:28:A:ILE:HG13 | 1:31:A:ALA:HB3  | 19       | 0.59          |
| (1,857) | 1:28:A:ILE:HG13 | 1:31:A:ALA:HB1  | 22       | 0.59          |
| (1,857) | 1:28:A:ILE:HG13 | 1:31:A:ALA:HB2  | 22       | 0.59          |
| (1,857) | 1:28:A:ILE:HG13 | 1:31:A:ALA:HB3  | 22       | 0.59          |
| (1,783) | 1:34:A:TRP:HZ3  | 2:85:B:SEP:HB2  | 3        | 0.59          |
| (1,639) | 2:84:B:TYR:HD1  | 1:14:A:ARG:HG2  | 1        | 0.59          |
| (1,639) | 2:84:B:TYR:HD2  | 1:14:A:ARG:HG2  | 1        | 0.59          |
| (1,465) | 1:23:A:TYR:HE1  | 2:86:B:PRO:HB3  | 2        | 0.59          |
| (1,465) | 1:23:A:TYR:HE2  | 2:86:B:PRO:HB3  | 2        | 0.59          |
| (1,407) | 1:35:A:GLU:H    | 1:33:A:GLN:HE22 | 11       | 0.59          |
| (1,343) | 1:25:A:PHE:H    | 1:14:A:ARG:HB3  | 1        | 0.59          |
| (1,342) | 1:25:A:PHE:H    | 1:14:A:ARG:HG2  | 8        | 0.59          |
| (1,322) | 1:17:A:ARG:HD3  | 2:81:B:GLY:HA2  | 17       | 0.59          |
| (1,254) | 1:11:A:TRP:HE1  | 1:37:A:PRO:HD3  | 20       | 0.59          |
| (1,2)   | 1:13:A:LYS:H    | 1:12:A:GLU:HG2  | 16       | 0.59          |
| (1,876) | 1:27:A:HIS:HD2  | 1:11:A:TRP:H    | 24       | 0.58          |
| (1,762) | 1:23:A:TYR:HE1  | 1:17:A:ARG:HG3  | 19       | 0.58          |
| (1,762) | 1:23:A:TYR:HE2  | 1:17:A:ARG:HG3  | 19       | 0.58          |
| (1,756) | 1:41:A:SER:H    | 1:6:A:LYS:HB2   | 7        | 0.58          |
| (1,751) | 1:33:A:GLN:HE21 | 1:8:A:PRO:HG3   | 16       | 0.58          |
| (1,720) | 2:84:B:TYR:HE1  | 1:23:A:TYR:HE1  | 10       | 0.58          |
| (1,720) | 2:84:B:TYR:HE1  | 1:23:A:TYR:HE2  | 10       | 0.58          |
| (1,720) | 2:84:B:TYR:HE2  | 1:23:A:TYR:HE1  | 10       | 0.58          |
| (1,720) | 2:84:B:TYR:HE2  | 1:23:A:TYR:HE2  | 10       | 0.58          |
| (1,605) | 1:33:A:GLN:HE22 | 1:24:A:TYR:HB3  | 19       | 0.58          |
| (1,544) | 1:11:A:TRP:HD1  | 1:7:A:LEU:HB2   | 20       | 0.58          |
| (1,483) | 1:24:A:TYR:HD1  | 1:37:A:PRO:HB2  | 16       | 0.58          |
| (1,483) | 1:24:A:TYR:HD2  | 1:37:A:PRO:HB2  | 16       | 0.58          |
| (1,480) | 1:33:A:GLN:HE21 | 1:35:A:GLU:HG2  | 7        | 0.58          |
| (1,468) | 2:85:B:SEP:H    | 1:14:A:ARG:HB3  | 16       | 0.58          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,465) | 1:23:A:TYR:HE1  | 2:86:B:PRO:HB3 | 8        | 0.58          |
| (1,465) | 1:23:A:TYR:HE2  | 2:86:B:PRO:HB3 | 8        | 0.58          |
| (1,465) | 1:23:A:TYR:HE1  | 2:86:B:PRO:HB3 | 12       | 0.58          |
| (1,465) | 1:23:A:TYR:HE2  | 2:86:B:PRO:HB3 | 12       | 0.58          |
| (1,465) | 1:23:A:TYR:HE1  | 2:86:B:PRO:HB3 | 24       | 0.58          |
| (1,465) | 1:23:A:TYR:HE2  | 2:86:B:PRO:HB3 | 24       | 0.58          |
| (1,370) | 1:22:A:VAL:H    | 1:16:A:SER:HB2 | 13       | 0.58          |
| (1,217) | 1:16:A:SER:HB2  | 1:21:A:ARG:HG2 | 25       | 0.58          |
| (1,192) | 1:9:A:PRO:HD3   | 1:8:A:PRO:HG3  | 24       | 0.58          |
| (1,87)  | 1:23:A:TYR:HE1  | 1:16:A:SER:HB3 | 1        | 0.58          |
| (1,87)  | 1:23:A:TYR:HE2  | 1:16:A:SER:HB3 | 1        | 0.58          |
| (1,836) | 2:88:B:PRO:HA   | 1:17:A:ARG:HG2 | 15       | 0.57          |
| (1,761) | 1:23:A:TYR:HE1  | 1:21:A:ARG:HB2 | 4        | 0.57          |
| (1,761) | 1:23:A:TYR:HE2  | 1:21:A:ARG:HB2 | 4        | 0.57          |
| (1,761) | 1:23:A:TYR:HE1  | 1:21:A:ARG:HB2 | 21       | 0.57          |
| (1,761) | 1:23:A:TYR:HE2  | 1:21:A:ARG:HB2 | 21       | 0.57          |
| (1,751) | 1:33:A:GLN:HE21 | 1:8:A:PRO:HG3  | 6        | 0.57          |
| (1,736) | 1:33:A:GLN:H    | 1:7:A:LEU:HD21 | 1        | 0.57          |
| (1,736) | 1:33:A:GLN:H    | 1:7:A:LEU:HD22 | 1        | 0.57          |
| (1,736) | 1:33:A:GLN:H    | 1:7:A:LEU:HD23 | 1        | 0.57          |
| (1,720) | 2:84:B:TYR:HE1  | 1:23:A:TYR:HE1 | 24       | 0.57          |
| (1,720) | 2:84:B:TYR:HE1  | 1:23:A:TYR:HE2 | 24       | 0.57          |
| (1,720) | 2:84:B:TYR:HE2  | 1:23:A:TYR:HE1 | 24       | 0.57          |
| (1,720) | 2:84:B:TYR:HE2  | 1:23:A:TYR:HE2 | 24       | 0.57          |
| (1,696) | 2:85:B:SEP:HB3  | 2:84:B:TYR:HB3 | 2        | 0.57          |
| (1,683) | 2:83:B:PRO:HD2  | 2:84:B:TYR:HB3 | 21       | 0.57          |
| (1,676) | 1:8:A:PRO:HD3   | 1:7:A:LEU:HD11 | 16       | 0.57          |
| (1,676) | 1:8:A:PRO:HD3   | 1:7:A:LEU:HD12 | 16       | 0.57          |
| (1,676) | 1:8:A:PRO:HD3   | 1:7:A:LEU:HD13 | 16       | 0.57          |
| (1,674) | 2:86:B:PRO:HD3  | 1:14:A:ARG:HD2 | 16       | 0.57          |
| (1,516) | 1:11:A:TRP:HH2  | 1:37:A:PRO:HD2 | 8        | 0.57          |
| (1,483) | 1:24:A:TYR:HD1  | 1:37:A:PRO:HB2 | 18       | 0.57          |
| (1,483) | 1:24:A:TYR:HD2  | 1:37:A:PRO:HB2 | 18       | 0.57          |
| (1,468) | 2:85:B:SEP:H    | 1:14:A:ARG:HB3 | 23       | 0.57          |
| (1,465) | 1:23:A:TYR:HE1  | 2:86:B:PRO:HB3 | 13       | 0.57          |
| (1,465) | 1:23:A:TYR:HE2  | 2:86:B:PRO:HB3 | 13       | 0.57          |
| (1,465) | 1:23:A:TYR:HE1  | 2:86:B:PRO:HB3 | 25       | 0.57          |
| (1,465) | 1:23:A:TYR:HE2  | 2:86:B:PRO:HB3 | 25       | 0.57          |
| (1,872) | 2:89:B:GLU:HB2  | 1:16:A:SER:HB3 | 10       | 0.56          |
| (1,841) | 1:5:A:GLU:HA    | 1:6:A:LYS:HB3  | 4        | 0.56          |
| (1,841) | 1:5:A:GLU:HA    | 1:6:A:LYS:HB3  | 18       | 0.56          |
| (1,836) | 2:88:B:PRO:HA   | 1:17:A:ARG:HG2 | 2        | 0.56          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,836) | 2:88:B:PRO:HA   | 1:17:A:ARG:HG2 | 7        | 0.56          |
| (1,762) | 1:23:A:TYR:HE1  | 1:17:A:ARG:HG3 | 17       | 0.56          |
| (1,762) | 1:23:A:TYR:HE2  | 1:17:A:ARG:HG3 | 17       | 0.56          |
| (1,762) | 1:23:A:TYR:HE1  | 1:17:A:ARG:HG3 | 18       | 0.56          |
| (1,762) | 1:23:A:TYR:HE2  | 1:17:A:ARG:HG3 | 18       | 0.56          |
| (1,666) | 1:37:A:PRO:HD3  | 1:36:A:ARG:HG3 | 17       | 0.56          |
| (1,604) | 1:33:A:GLN:HE22 | 1:35:A:GLU:HG2 | 15       | 0.56          |
| (1,465) | 1:23:A:TYR:HE1  | 2:86:B:PRO:HB3 | 11       | 0.56          |
| (1,465) | 1:23:A:TYR:HE2  | 2:86:B:PRO:HB3 | 11       | 0.56          |
| (1,87)  | 1:23:A:TYR:HE1  | 1:16:A:SER:HB3 | 11       | 0.56          |
| (1,87)  | 1:23:A:TYR:HE2  | 1:16:A:SER:HB3 | 11       | 0.56          |
| (1,75)  | 1:37:A:PRO:HD3  | 1:36:A:ARG:HD2 | 11       | 0.56          |
| (1,2)   | 1:13:A:LYS:H    | 1:12:A:GLU:HG2 | 20       | 0.56          |
| (1,879) | 2:88:B:PRO:HD2  | 1:17:A:ARG:HD2 | 16       | 0.55          |
| (1,876) | 1:27:A:HIS:HD2  | 1:11:A:TRP:H   | 13       | 0.55          |
| (1,808) | 1:11:A:TRP:HE3  | 1:37:A:PRO:HD2 | 18       | 0.55          |
| (1,779) | 1:11:A:TRP:HZ3  | 1:7:A:LEU:HD11 | 25       | 0.55          |
| (1,779) | 1:11:A:TRP:HZ3  | 1:7:A:LEU:HD12 | 25       | 0.55          |
| (1,779) | 1:11:A:TRP:HZ3  | 1:7:A:LEU:HD13 | 25       | 0.55          |
| (1,674) | 2:86:B:PRO:HD3  | 1:14:A:ARG:HD2 | 11       | 0.55          |
| (1,553) | 1:34:A:TRP:HH2  | 2:86:B:PRO:HB2 | 11       | 0.55          |
| (1,553) | 1:34:A:TRP:HH2  | 2:86:B:PRO:HB2 | 25       | 0.55          |
| (1,465) | 1:23:A:TYR:HE1  | 2:86:B:PRO:HB3 | 14       | 0.55          |
| (1,465) | 1:23:A:TYR:HE2  | 2:86:B:PRO:HB3 | 14       | 0.55          |
| (1,465) | 1:23:A:TYR:HE1  | 2:86:B:PRO:HB3 | 22       | 0.55          |
| (1,465) | 1:23:A:TYR:HE2  | 2:86:B:PRO:HB3 | 22       | 0.55          |
| (1,254) | 1:11:A:TRP:HE1  | 1:37:A:PRO:HD3 | 13       | 0.55          |
| (1,254) | 1:11:A:TRP:HE1  | 1:37:A:PRO:HD3 | 23       | 0.55          |
| (1,876) | 1:27:A:HIS:HD2  | 1:11:A:TRP:H   | 1        | 0.54          |
| (1,841) | 1:5:A:GLU:HA    | 1:6:A:LYS:HB3  | 1        | 0.54          |
| (1,837) | 1:21:A:ARG:HA   | 2:88:B:PRO:HB3 | 3        | 0.54          |
| (1,836) | 2:88:B:PRO:HA   | 1:17:A:ARG:HG2 | 3        | 0.54          |
| (1,683) | 2:83:B:PRO:HD2  | 2:84:B:TYR:HB3 | 11       | 0.54          |
| (1,633) | 1:18:A:SER:HB2  | 1:17:A:ARG:HB3 | 5        | 0.54          |
| (1,553) | 1:34:A:TRP:HH2  | 2:86:B:PRO:HB2 | 9        | 0.54          |
| (1,516) | 1:11:A:TRP:HH2  | 1:37:A:PRO:HD2 | 11       | 0.54          |
| (1,483) | 1:24:A:TYR:HD1  | 1:37:A:PRO:HB2 | 17       | 0.54          |
| (1,483) | 1:24:A:TYR:HD2  | 1:37:A:PRO:HB2 | 17       | 0.54          |
| (1,465) | 1:23:A:TYR:HE1  | 2:86:B:PRO:HB3 | 4        | 0.54          |
| (1,465) | 1:23:A:TYR:HE2  | 2:86:B:PRO:HB3 | 4        | 0.54          |
| (1,465) | 1:23:A:TYR:HE1  | 2:86:B:PRO:HB3 | 16       | 0.54          |
| (1,465) | 1:23:A:TYR:HE2  | 2:86:B:PRO:HB3 | 16       | 0.54          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,465) | 1:23:A:TYR:HE1  | 2:86:B:PRO:HB3  | 23       | 0.54          |
| (1,465) | 1:23:A:TYR:HE2  | 2:86:B:PRO:HB3  | 23       | 0.54          |
| (1,407) | 1:35:A:GLU:H    | 1:33:A:GLN:HE22 | 23       | 0.54          |
| (1,343) | 1:25:A:PHE:H    | 1:14:A:ARG:HB3  | 14       | 0.54          |
| (1,217) | 1:16:A:SER:HB2  | 1:21:A:ARG:HG2  | 4        | 0.54          |
| (1,87)  | 1:23:A:TYR:HE1  | 1:16:A:SER:HB3  | 4        | 0.54          |
| (1,87)  | 1:23:A:TYR:HE2  | 1:16:A:SER:HB3  | 4        | 0.54          |
| (1,87)  | 1:23:A:TYR:HE1  | 1:16:A:SER:HB3  | 14       | 0.54          |
| (1,87)  | 1:23:A:TYR:HE2  | 1:16:A:SER:HB3  | 14       | 0.54          |
| (1,12)  | 1:21:A:ARG:H    | 1:16:A:SER:HB2  | 22       | 0.54          |
| (1,12)  | 1:21:A:ARG:H    | 1:16:A:SER:HB2  | 23       | 0.54          |
| (1,2)   | 1:13:A:LYS:H    | 1:12:A:GLU:HG2  | 8        | 0.54          |
| (1,2)   | 1:13:A:LYS:H    | 1:12:A:GLU:HG2  | 14       | 0.54          |
| (1,859) | 1:13:A:LYS:HB3  | 1:7:A:LEU:HD11  | 13       | 0.53          |
| (1,859) | 1:13:A:LYS:HB3  | 1:7:A:LEU:HD12  | 13       | 0.53          |
| (1,859) | 1:13:A:LYS:HB3  | 1:7:A:LEU:HD13  | 13       | 0.53          |
| (1,844) | 1:25:A:PHE:HB3  | 1:14:A:ARG:HB3  | 19       | 0.53          |
| (1,779) | 1:11:A:TRP:HZ3  | 1:7:A:LEU:HD11  | 13       | 0.53          |
| (1,779) | 1:11:A:TRP:HZ3  | 1:7:A:LEU:HD12  | 13       | 0.53          |
| (1,779) | 1:11:A:TRP:HZ3  | 1:7:A:LEU:HD13  | 13       | 0.53          |
| (1,697) | 2:85:B:SEP:HB3  | 1:17:A:ARG:HA   | 11       | 0.53          |
| (1,697) | 2:85:B:SEP:HB3  | 1:17:A:ARG:HA   | 25       | 0.53          |
| (1,604) | 1:33:A:GLN:HE22 | 1:35:A:GLU:HG2  | 13       | 0.53          |
| (1,483) | 1:24:A:TYR:HD1  | 1:37:A:PRO:HB2  | 6        | 0.53          |
| (1,483) | 1:24:A:TYR:HD2  | 1:37:A:PRO:HB2  | 6        | 0.53          |
| (1,465) | 1:23:A:TYR:HE1  | 2:86:B:PRO:HB3  | 1        | 0.53          |
| (1,465) | 1:23:A:TYR:HE2  | 2:86:B:PRO:HB3  | 1        | 0.53          |
| (1,254) | 1:11:A:TRP:HE1  | 1:37:A:PRO:HD3  | 12       | 0.53          |
| (1,75)  | 1:37:A:PRO:HD3  | 1:36:A:ARG:HD2  | 18       | 0.53          |
| (1,12)  | 1:21:A:ARG:H    | 1:16:A:SER:HB2  | 13       | 0.53          |
| (1,876) | 1:27:A:HIS:HD2  | 1:11:A:TRP:H    | 7        | 0.52          |
| (1,849) | 1:14:A:ARG:HB3  | 1:15:A:MET:HG3  | 7        | 0.52          |
| (1,841) | 1:5:A:GLU:HA    | 1:6:A:LYS:HB3   | 5        | 0.52          |
| (1,825) | 2:87:B:PHE:HE1  | 2:81:B:GLY:HA2  | 7        | 0.52          |
| (1,825) | 2:87:B:PHE:HE2  | 2:81:B:GLY:HA2  | 7        | 0.52          |
| (1,820) | 1:21:A:ARG:HB3  | 1:19:A:SER:HA   | 10       | 0.52          |
| (1,697) | 2:85:B:SEP:HB3  | 1:17:A:ARG:HA   | 16       | 0.52          |
| (1,683) | 2:83:B:PRO:HD2  | 2:84:B:TYR:HB3  | 14       | 0.52          |
| (1,553) | 1:34:A:TRP:HH2  | 2:86:B:PRO:HB2  | 14       | 0.52          |
| (1,553) | 1:34:A:TRP:HH2  | 2:86:B:PRO:HB2  | 18       | 0.52          |
| (1,544) | 1:11:A:TRP:HD1  | 1:7:A:LEU:HB2   | 17       | 0.52          |
| (1,544) | 1:11:A:TRP:HD1  | 1:7:A:LEU:HB2   | 23       | 0.52          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,516) | 1:11:A:TRP:HH2  | 1:37:A:PRO:HD2  | 6        | 0.52          |
| (1,501) | 1:24:A:TYR:HE1  | 1:33:A:GLN:HG2  | 19       | 0.52          |
| (1,501) | 1:24:A:TYR:HE2  | 1:33:A:GLN:HG2  | 19       | 0.52          |
| (1,499) | 1:25:A:PHE:HE1  | 1:12:A:GLU:HG2  | 10       | 0.52          |
| (1,499) | 1:25:A:PHE:HE2  | 1:12:A:GLU:HG2  | 10       | 0.52          |
| (1,487) | 1:25:A:PHE:HD1  | 1:14:A:ARG:HB3  | 5        | 0.52          |
| (1,487) | 1:25:A:PHE:HD2  | 1:14:A:ARG:HB3  | 5        | 0.52          |
| (1,479) | 1:33:A:GLN:HE21 | 1:35:A:GLU:HB2  | 25       | 0.52          |
| (1,465) | 1:23:A:TYR:HE1  | 2:86:B:PRO:HB3  | 20       | 0.52          |
| (1,465) | 1:23:A:TYR:HE2  | 2:86:B:PRO:HB3  | 20       | 0.52          |
| (1,407) | 1:35:A:GLU:H    | 1:33:A:GLN:HE22 | 8        | 0.52          |
| (1,370) | 1:22:A:VAL:H    | 1:16:A:SER:HB2  | 24       | 0.52          |
| (1,254) | 1:11:A:TRP:HE1  | 1:37:A:PRO:HD3  | 4        | 0.52          |
| (1,87)  | 1:23:A:TYR:HE1  | 1:16:A:SER:HB3  | 12       | 0.52          |
| (1,87)  | 1:23:A:TYR:HE2  | 1:16:A:SER:HB3  | 12       | 0.52          |
| (1,75)  | 1:37:A:PRO:HD3  | 1:36:A:ARG:HD2  | 22       | 0.52          |
| (1,849) | 1:14:A:ARG:HB3  | 1:15:A:MET:HG3  | 19       | 0.51          |
| (1,841) | 1:5:A:GLU:HA    | 1:6:A:LYS:HB3   | 15       | 0.51          |
| (1,836) | 2:88:B:PRO:HA   | 1:17:A:ARG:HG2  | 12       | 0.51          |
| (1,707) | 1:17:A:ARG:HD3  | 2:88:B:PRO:HD3  | 20       | 0.51          |
| (1,682) | 1:23:A:TYR:HB3  | 1:16:A:SER:HB3  | 17       | 0.51          |
| (1,606) | 1:34:A:TRP:HD1  | 2:89:B:GLU:HG2  | 1        | 0.51          |
| (1,553) | 1:34:A:TRP:HH2  | 2:86:B:PRO:HB2  | 16       | 0.51          |
| (1,553) | 1:34:A:TRP:HH2  | 2:86:B:PRO:HB2  | 23       | 0.51          |
| (1,544) | 1:11:A:TRP:HD1  | 1:7:A:LEU:HB2   | 4        | 0.51          |
| (1,479) | 1:33:A:GLN:HE21 | 1:35:A:GLU:HB2  | 6        | 0.51          |
| (1,465) | 1:23:A:TYR:HE1  | 2:86:B:PRO:HB3  | 21       | 0.51          |
| (1,465) | 1:23:A:TYR:HE2  | 2:86:B:PRO:HB3  | 21       | 0.51          |
| (1,407) | 1:35:A:GLU:H    | 1:33:A:GLN:HE22 | 15       | 0.51          |
| (1,407) | 1:35:A:GLU:H    | 1:33:A:GLN:HE22 | 18       | 0.51          |
| (1,217) | 1:16:A:SER:HB2  | 1:21:A:ARG:HG2  | 12       | 0.51          |
| (1,180) | 1:7:A:LEU:H     | 1:6:A:LYS:HE3   | 14       | 0.51          |
| (1,876) | 1:27:A:HIS:HD2  | 1:11:A:TRP:H    | 16       | 0.5           |
| (1,872) | 2:89:B:GLU:HB2  | 1:16:A:SER:HB3  | 20       | 0.5           |
| (1,841) | 1:5:A:GLU:HA    | 1:6:A:LYS:HB3   | 25       | 0.5           |
| (1,837) | 1:21:A:ARG:HA   | 2:88:B:PRO:HB3  | 4        | 0.5           |
| (1,783) | 1:34:A:TRP:HZ3  | 2:85:B:SEP:HB2  | 12       | 0.5           |
| (1,696) | 2:85:B:SEP:HB3  | 2:84:B:TYR:HB3  | 15       | 0.5           |
| (1,682) | 1:23:A:TYR:HB3  | 1:16:A:SER:HB3  | 11       | 0.5           |
| (1,639) | 2:84:B:TYR:HD1  | 1:14:A:ARG:HG2  | 3        | 0.5           |
| (1,639) | 2:84:B:TYR:HD2  | 1:14:A:ARG:HG2  | 3        | 0.5           |
| (1,606) | 1:34:A:TRP:HD1  | 2:89:B:GLU:HG2  | 5        | 0.5           |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,578) | 1:34:A:TRP:HH2  | 1:21:A:ARG:HD3  | 24       | 0.5           |
| (1,562) | 1:34:A:TRP:HZ2  | 1:16:A:SER:HB3  | 20       | 0.5           |
| (1,516) | 1:11:A:TRP:HH2  | 1:37:A:PRO:HD2  | 23       | 0.5           |
| (1,365) | 1:34:A:TRP:H    | 1:35:A:GLU:HB2  | 21       | 0.5           |
| (1,362) | 1:7:A:LEU:H     | 1:36:A:ARG:HG3  | 17       | 0.5           |
| (1,343) | 1:25:A:PHE:H    | 1:14:A:ARG:HB3  | 22       | 0.5           |
| (1,343) | 1:25:A:PHE:H    | 1:14:A:ARG:HB3  | 24       | 0.5           |
| (1,296) | 1:26:A:ASN:HD22 | 1:10:A:GLY:HA2  | 18       | 0.5           |
| (1,254) | 1:11:A:TRP:HE1  | 1:37:A:PRO:HD3  | 14       | 0.5           |
| (1,87)  | 1:23:A:TYR:HE1  | 1:16:A:SER:HB3  | 6        | 0.5           |
| (1,87)  | 1:23:A:TYR:HE2  | 1:16:A:SER:HB3  | 6        | 0.5           |
| (1,876) | 1:27:A:HIS:HD2  | 1:11:A:TRP:H    | 4        | 0.49          |
| (1,876) | 1:27:A:HIS:HD2  | 1:11:A:TRP:H    | 10       | 0.49          |
| (1,876) | 1:27:A:HIS:HD2  | 1:11:A:TRP:H    | 19       | 0.49          |
| (1,875) | 2:84:B:TYR:HD1  | 1:30:A:ASN:HD22 | 5        | 0.49          |
| (1,875) | 2:84:B:TYR:HD2  | 1:30:A:ASN:HD22 | 5        | 0.49          |
| (1,866) | 1:11:A:TRP:HB3  | 1:7:A:LEU:HD21  | 10       | 0.49          |
| (1,866) | 1:11:A:TRP:HB3  | 1:7:A:LEU:HD22  | 10       | 0.49          |
| (1,866) | 1:11:A:TRP:HB3  | 1:7:A:LEU:HD23  | 10       | 0.49          |
| (1,836) | 2:88:B:PRO:HA   | 1:17:A:ARG:HG2  | 22       | 0.49          |
| (1,696) | 2:85:B:SEP:HB3  | 2:84:B:TYR:HB3  | 9        | 0.49          |
| (1,674) | 2:86:B:PRO:HD3  | 1:14:A:ARG:HD2  | 7        | 0.49          |
| (1,633) | 1:18:A:SER:HB2  | 1:17:A:ARG:HB3  | 23       | 0.49          |
| (1,553) | 1:34:A:TRP:HH2  | 2:86:B:PRO:HB2  | 1        | 0.49          |
| (1,553) | 1:34:A:TRP:HH2  | 2:86:B:PRO:HB2  | 6        | 0.49          |
| (1,553) | 1:34:A:TRP:HH2  | 2:86:B:PRO:HB2  | 20       | 0.49          |
| (1,463) | 1:23:A:TYR:HE1  | 1:14:A:ARG:HD2  | 8        | 0.49          |
| (1,463) | 1:23:A:TYR:HE2  | 1:14:A:ARG:HD2  | 8        | 0.49          |
| (1,407) | 1:35:A:GLU:H    | 1:33:A:GLN:HE22 | 10       | 0.49          |
| (1,296) | 1:26:A:ASN:HD22 | 1:10:A:GLY:HA2  | 10       | 0.49          |
| (1,254) | 1:11:A:TRP:HE1  | 1:37:A:PRO:HD3  | 15       | 0.49          |
| (1,137) | 2:85:B:SEP:HB2  | 1:17:A:ARG:HD3  | 16       | 0.49          |
| (1,102) | 1:23:A:TYR:HE1  | 1:25:A:PHE:HB3  | 24       | 0.49          |
| (1,102) | 1:23:A:TYR:HE2  | 1:25:A:PHE:HB3  | 24       | 0.49          |
| (1,876) | 1:27:A:HIS:HD2  | 1:11:A:TRP:H    | 9        | 0.48          |
| (1,841) | 1:5:A:GLU:HA    | 1:6:A:LYS:HB3   | 24       | 0.48          |
| (1,820) | 1:21:A:ARG:HB3  | 1:19:A:SER:HA   | 20       | 0.48          |
| (1,779) | 1:11:A:TRP:HZ3  | 1:7:A:LEU:HD11  | 10       | 0.48          |
| (1,779) | 1:11:A:TRP:HZ3  | 1:7:A:LEU:HD12  | 10       | 0.48          |
| (1,779) | 1:11:A:TRP:HZ3  | 1:7:A:LEU:HD13  | 10       | 0.48          |
| (1,762) | 1:23:A:TYR:HE1  | 1:17:A:ARG:HG3  | 21       | 0.48          |
| (1,762) | 1:23:A:TYR:HE2  | 1:17:A:ARG:HG3  | 21       | 0.48          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,749) | 1:34:A:TRP:HE1  | 2:88:B:PRO:HB2  | 2        | 0.48          |
| (1,697) | 2:85:B:SEP:HB3  | 1:17:A:ARG:HA   | 8        | 0.48          |
| (1,553) | 1:34:A:TRP:HH2  | 2:86:B:PRO:HB2  | 8        | 0.48          |
| (1,553) | 1:34:A:TRP:HH2  | 2:86:B:PRO:HB2  | 19       | 0.48          |
| (1,516) | 1:11:A:TRP:HH2  | 1:37:A:PRO:HD2  | 22       | 0.48          |
| (1,501) | 1:24:A:TYR:HE1  | 1:33:A:GLN:HG2  | 2        | 0.48          |
| (1,501) | 1:24:A:TYR:HE2  | 1:33:A:GLN:HG2  | 2        | 0.48          |
| (1,487) | 1:25:A:PHE:HD1  | 1:14:A:ARG:HB3  | 16       | 0.48          |
| (1,487) | 1:25:A:PHE:HD2  | 1:14:A:ARG:HB3  | 16       | 0.48          |
| (1,487) | 1:25:A:PHE:HD1  | 1:14:A:ARG:HB3  | 22       | 0.48          |
| (1,487) | 1:25:A:PHE:HD2  | 1:14:A:ARG:HB3  | 22       | 0.48          |
| (1,487) | 1:25:A:PHE:HD1  | 1:14:A:ARG:HB3  | 24       | 0.48          |
| (1,487) | 1:25:A:PHE:HD2  | 1:14:A:ARG:HB3  | 24       | 0.48          |
| (1,407) | 1:35:A:GLU:H    | 1:33:A:GLN:HE22 | 4        | 0.48          |
| (1,296) | 1:26:A:ASN:HD22 | 1:10:A:GLY:HA2  | 17       | 0.48          |
| (1,254) | 1:11:A:TRP:HE1  | 1:37:A:PRO:HD3  | 8        | 0.48          |
| (1,876) | 1:27:A:HIS:HD2  | 1:11:A:TRP:H    | 2        | 0.47          |
| (1,876) | 1:27:A:HIS:HD2  | 1:11:A:TRP:H    | 5        | 0.47          |
| (1,832) | 1:11:A:TRP:HZ2  | 1:37:A:PRO:HD2  | 14       | 0.47          |
| (1,777) | 1:24:A:TYR:HE1  | 1:7:A:LEU:HA    | 14       | 0.47          |
| (1,777) | 1:24:A:TYR:HE2  | 1:7:A:LEU:HA    | 14       | 0.47          |
| (1,697) | 2:85:B:SEP:HB3  | 1:17:A:ARG:HA   | 15       | 0.47          |
| (1,696) | 2:85:B:SEP:HB3  | 2:84:B:TYR:HB3  | 3        | 0.47          |
| (1,553) | 1:34:A:TRP:HH2  | 2:86:B:PRO:HB2  | 4        | 0.47          |
| (1,553) | 1:34:A:TRP:HH2  | 2:86:B:PRO:HB2  | 21       | 0.47          |
| (1,553) | 1:34:A:TRP:HH2  | 2:86:B:PRO:HB2  | 24       | 0.47          |
| (1,544) | 1:11:A:TRP:HD1  | 1:7:A:LEU:HB2   | 18       | 0.47          |
| (1,516) | 1:11:A:TRP:HH2  | 1:37:A:PRO:HD2  | 13       | 0.47          |
| (1,501) | 1:24:A:TYR:HE1  | 1:33:A:GLN:HG2  | 3        | 0.47          |
| (1,501) | 1:24:A:TYR:HE2  | 1:33:A:GLN:HG2  | 3        | 0.47          |
| (1,494) | 1:25:A:PHE:HD1  | 2:83:B:PRO:HG2  | 1        | 0.47          |
| (1,494) | 1:25:A:PHE:HD2  | 2:83:B:PRO:HG2  | 1        | 0.47          |
| (1,487) | 1:25:A:PHE:HD1  | 1:14:A:ARG:HB3  | 1        | 0.47          |
| (1,487) | 1:25:A:PHE:HD2  | 1:14:A:ARG:HB3  | 1        | 0.47          |
| (1,487) | 1:25:A:PHE:HD1  | 1:14:A:ARG:HB3  | 9        | 0.47          |
| (1,487) | 1:25:A:PHE:HD2  | 1:14:A:ARG:HB3  | 9        | 0.47          |
| (1,487) | 1:25:A:PHE:HD1  | 1:14:A:ARG:HB3  | 14       | 0.47          |
| (1,487) | 1:25:A:PHE:HD2  | 1:14:A:ARG:HB3  | 14       | 0.47          |
| (1,468) | 2:85:B:SEP:H    | 1:14:A:ARG:HB3  | 3        | 0.47          |
| (1,468) | 2:85:B:SEP:H    | 1:14:A:ARG:HB3  | 22       | 0.47          |
| (1,407) | 1:35:A:GLU:H    | 1:33:A:GLN:HE22 | 1        | 0.47          |
| (1,342) | 1:25:A:PHE:H    | 1:14:A:ARG:HG2  | 21       | 0.47          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,322) | 1:17:A:ARG:HD3  | 2:81:B:GLY:HA2  | 10       | 0.47          |
| (1,75)  | 1:37:A:PRO:HD3  | 1:36:A:ARG:HD2  | 12       | 0.47          |
| (1,12)  | 1:21:A:ARG:H    | 1:16:A:SER:HB2  | 6        | 0.47          |
| (1,876) | 1:27:A:HIS:HD2  | 1:11:A:TRP:H    | 15       | 0.46          |
| (1,876) | 1:27:A:HIS:HD2  | 1:11:A:TRP:H    | 22       | 0.46          |
| (1,836) | 2:88:B:PRO:HA   | 1:17:A:ARG:HG2  | 13       | 0.46          |
| (1,808) | 1:11:A:TRP:HE3  | 1:37:A:PRO:HD2  | 1        | 0.46          |
| (1,807) | 1:25:A:PHE:HZ   | 2:83:B:PRO:HB3  | 8        | 0.46          |
| (1,720) | 2:84:B:TYR:HE1  | 1:23:A:TYR:HE1  | 12       | 0.46          |
| (1,720) | 2:84:B:TYR:HE1  | 1:23:A:TYR:HE2  | 12       | 0.46          |
| (1,720) | 2:84:B:TYR:HE2  | 1:23:A:TYR:HE1  | 12       | 0.46          |
| (1,720) | 2:84:B:TYR:HE2  | 1:23:A:TYR:HE2  | 12       | 0.46          |
| (1,720) | 2:84:B:TYR:HE1  | 1:23:A:TYR:HE1  | 15       | 0.46          |
| (1,720) | 2:84:B:TYR:HE1  | 1:23:A:TYR:HE2  | 15       | 0.46          |
| (1,720) | 2:84:B:TYR:HE2  | 1:23:A:TYR:HE1  | 15       | 0.46          |
| (1,720) | 2:84:B:TYR:HE2  | 1:23:A:TYR:HE2  | 15       | 0.46          |
| (1,697) | 2:85:B:SEP:HB3  | 1:17:A:ARG:HA   | 23       | 0.46          |
| (1,683) | 2:83:B:PRO:HD2  | 2:84:B:TYR:HB3  | 13       | 0.46          |
| (1,622) | 1:33:A:GLN:HG2  | 1:24:A:TYR:HB3  | 19       | 0.46          |
| (1,553) | 1:34:A:TRP:HH2  | 2:86:B:PRO:HB2  | 22       | 0.46          |
| (1,544) | 1:11:A:TRP:HD1  | 1:7:A:LEU:HB2   | 7        | 0.46          |
| (1,516) | 1:11:A:TRP:HH2  | 1:37:A:PRO:HD2  | 15       | 0.46          |
| (1,494) | 1:25:A:PHE:HD1  | 2:83:B:PRO:HG2  | 8        | 0.46          |
| (1,494) | 1:25:A:PHE:HD2  | 2:83:B:PRO:HG2  | 8        | 0.46          |
| (1,407) | 1:35:A:GLU:H    | 1:33:A:GLN:HE22 | 5        | 0.46          |
| (1,365) | 1:34:A:TRP:H    | 1:35:A:GLU:HB2  | 1        | 0.46          |
| (1,343) | 1:25:A:PHE:H    | 1:14:A:ARG:HB3  | 3        | 0.46          |
| (1,254) | 1:11:A:TRP:HE1  | 1:37:A:PRO:HD3  | 5        | 0.46          |
| (1,180) | 1:7:A:LEU:H     | 1:6:A:LYS:HE3   | 4        | 0.46          |
| (1,879) | 2:88:B:PRO:HD2  | 1:17:A:ARG:HD2  | 19       | 0.45          |
| (1,876) | 1:27:A:HIS:HD2  | 1:11:A:TRP:H    | 11       | 0.45          |
| (1,849) | 1:14:A:ARG:HB3  | 1:15:A:MET:HG3  | 8        | 0.45          |
| (1,832) | 1:11:A:TRP:HZ2  | 1:37:A:PRO:HD2  | 25       | 0.45          |
| (1,823) | 1:25:A:PHE:HZ   | 1:14:A:ARG:HD2  | 21       | 0.45          |
| (1,822) | 1:25:A:PHE:HZ   | 1:14:A:ARG:HD2  | 21       | 0.45          |
| (1,808) | 1:11:A:TRP:HE3  | 1:37:A:PRO:HD2  | 4        | 0.45          |
| (1,779) | 1:11:A:TRP:HZ3  | 1:7:A:LEU:HD11  | 15       | 0.45          |
| (1,779) | 1:11:A:TRP:HZ3  | 1:7:A:LEU:HD12  | 15       | 0.45          |
| (1,779) | 1:11:A:TRP:HZ3  | 1:7:A:LEU:HD13  | 15       | 0.45          |
| (1,752) | 1:33:A:GLN:HE21 | 1:37:A:PRO:HD3  | 19       | 0.45          |
| (1,749) | 1:34:A:TRP:HE1  | 2:88:B:PRO:HB2  | 12       | 0.45          |
| (1,749) | 1:34:A:TRP:HE1  | 2:88:B:PRO:HB2  | 22       | 0.45          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,710) | 1:34:A:TRP:HB3 | 2:86:B:PRO:HD2  | 17       | 0.45          |
| (1,689) | 1:14:A:ARG:HD2 | 2:84:B:TYR:HA   | 20       | 0.45          |
| (1,553) | 1:34:A:TRP:HH2 | 2:86:B:PRO:HB2  | 13       | 0.45          |
| (1,553) | 1:34:A:TRP:HH2 | 2:86:B:PRO:HB2  | 15       | 0.45          |
| (1,544) | 1:11:A:TRP:HD1 | 1:7:A:LEU:HB2   | 9        | 0.45          |
| (1,487) | 1:25:A:PHE:HD1 | 1:14:A:ARG:HB3  | 17       | 0.45          |
| (1,487) | 1:25:A:PHE:HD2 | 1:14:A:ARG:HB3  | 17       | 0.45          |
| (1,370) | 1:22:A:VAL:H   | 1:16:A:SER:HB2  | 18       | 0.45          |
| (1,87)  | 1:23:A:TYR:HE1 | 1:16:A:SER:HB3  | 17       | 0.45          |
| (1,87)  | 1:23:A:TYR:HE2 | 1:16:A:SER:HB3  | 17       | 0.45          |
| (1,75)  | 1:37:A:PRO:HD3 | 1:36:A:ARG:HD2  | 21       | 0.45          |
| (1,24)  | 1:13:A:LYS:HE2 | 1:22:A:VAL:HG11 | 1        | 0.45          |
| (1,24)  | 1:13:A:LYS:HE2 | 1:22:A:VAL:HG12 | 1        | 0.45          |
| (1,24)  | 1:13:A:LYS:HE2 | 1:22:A:VAL:HG13 | 1        | 0.45          |
| (1,12)  | 1:21:A:ARG:H   | 1:16:A:SER:HB2  | 14       | 0.45          |
| (1,2)   | 1:13:A:LYS:H   | 1:12:A:GLU:HG2  | 23       | 0.45          |
| (1,841) | 1:5:A:GLU:HA   | 1:6:A:LYS:HB3   | 10       | 0.44          |
| (1,770) | 1:25:A:PHE:HE1 | 1:14:A:ARG:HD2  | 22       | 0.44          |
| (1,770) | 1:25:A:PHE:HE2 | 1:14:A:ARG:HD2  | 22       | 0.44          |
| (1,720) | 2:84:B:TYR:HE1 | 1:23:A:TYR:HE1  | 19       | 0.44          |
| (1,720) | 2:84:B:TYR:HE1 | 1:23:A:TYR:HE2  | 19       | 0.44          |
| (1,720) | 2:84:B:TYR:HE2 | 1:23:A:TYR:HE1  | 19       | 0.44          |
| (1,720) | 2:84:B:TYR:HE2 | 1:23:A:TYR:HE2  | 19       | 0.44          |
| (1,696) | 2:85:B:SEP:HB3 | 2:84:B:TYR:HB3  | 10       | 0.44          |
| (1,639) | 2:84:B:TYR:HD1 | 1:14:A:ARG:HG2  | 19       | 0.44          |
| (1,639) | 2:84:B:TYR:HD2 | 1:14:A:ARG:HG2  | 19       | 0.44          |
| (1,553) | 1:34:A:TRP:HH2 | 2:86:B:PRO:HB2  | 2        | 0.44          |
| (1,544) | 1:11:A:TRP:HD1 | 1:7:A:LEU:HB2   | 8        | 0.44          |
| (1,544) | 1:11:A:TRP:HD1 | 1:7:A:LEU:HB2   | 10       | 0.44          |
| (1,494) | 1:25:A:PHE:HD1 | 2:83:B:PRO:HG2  | 7        | 0.44          |
| (1,494) | 1:25:A:PHE:HD2 | 2:83:B:PRO:HG2  | 7        | 0.44          |
| (1,487) | 1:25:A:PHE:HD1 | 1:14:A:ARG:HB3  | 23       | 0.44          |
| (1,487) | 1:25:A:PHE:HD2 | 1:14:A:ARG:HB3  | 23       | 0.44          |
| (1,365) | 1:34:A:TRP:H   | 1:35:A:GLU:HB2  | 20       | 0.44          |
| (1,343) | 1:25:A:PHE:H   | 1:14:A:ARG:HB3  | 23       | 0.44          |
| (1,322) | 1:17:A:ARG:HD3 | 2:81:B:GLY:HA2  | 8        | 0.44          |
| (1,866) | 1:11:A:TRP:HB3 | 1:7:A:LEU:HD21  | 25       | 0.43          |
| (1,866) | 1:11:A:TRP:HB3 | 1:7:A:LEU:HD22  | 25       | 0.43          |
| (1,866) | 1:11:A:TRP:HB3 | 1:7:A:LEU:HD23  | 25       | 0.43          |
| (1,808) | 1:11:A:TRP:HE3 | 1:37:A:PRO:HD2  | 14       | 0.43          |
| (1,762) | 1:23:A:TYR:HE1 | 1:17:A:ARG:HG3  | 16       | 0.43          |
| (1,762) | 1:23:A:TYR:HE2 | 1:17:A:ARG:HG3  | 16       | 0.43          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,720) | 2:84:B:TYR:HE1 | 1:23:A:TYR:HE1  | 8        | 0.43          |
| (1,720) | 2:84:B:TYR:HE1 | 1:23:A:TYR:HE2  | 8        | 0.43          |
| (1,720) | 2:84:B:TYR:HE2 | 1:23:A:TYR:HE1  | 8        | 0.43          |
| (1,720) | 2:84:B:TYR:HE2 | 1:23:A:TYR:HE2  | 8        | 0.43          |
| (1,720) | 2:84:B:TYR:HE1 | 1:23:A:TYR:HE1  | 11       | 0.43          |
| (1,720) | 2:84:B:TYR:HE1 | 1:23:A:TYR:HE2  | 11       | 0.43          |
| (1,720) | 2:84:B:TYR:HE2 | 1:23:A:TYR:HE1  | 11       | 0.43          |
| (1,720) | 2:84:B:TYR:HE2 | 1:23:A:TYR:HE2  | 11       | 0.43          |
| (1,704) | 1:16:A:SER:HB3 | 1:17:A:ARG:HA   | 19       | 0.43          |
| (1,696) | 2:85:B:SEP:HB3 | 2:84:B:TYR:HB3  | 1        | 0.43          |
| (1,696) | 2:85:B:SEP:HB3 | 2:84:B:TYR:HB3  | 19       | 0.43          |
| (1,639) | 2:84:B:TYR:HD1 | 1:14:A:ARG:HG2  | 16       | 0.43          |
| (1,639) | 2:84:B:TYR:HD2 | 1:14:A:ARG:HG2  | 16       | 0.43          |
| (1,562) | 1:34:A:TRP:HZ2 | 1:16:A:SER:HB3  | 15       | 0.43          |
| (1,553) | 1:34:A:TRP:HH2 | 2:86:B:PRO:HB2  | 5        | 0.43          |
| (1,516) | 1:11:A:TRP:HH2 | 1:37:A:PRO:HD2  | 5        | 0.43          |
| (1,494) | 1:25:A:PHE:HD1 | 2:83:B:PRO:HG2  | 16       | 0.43          |
| (1,494) | 1:25:A:PHE:HD2 | 2:83:B:PRO:HG2  | 16       | 0.43          |
| (1,494) | 1:25:A:PHE:HD1 | 2:83:B:PRO:HG2  | 25       | 0.43          |
| (1,494) | 1:25:A:PHE:HD2 | 2:83:B:PRO:HG2  | 25       | 0.43          |
| (1,487) | 1:25:A:PHE:HD1 | 1:14:A:ARG:HB3  | 15       | 0.43          |
| (1,487) | 1:25:A:PHE:HD2 | 1:14:A:ARG:HB3  | 15       | 0.43          |
| (1,407) | 1:35:A:GLU:H   | 1:33:A:GLN:HE22 | 14       | 0.43          |
| (1,365) | 1:34:A:TRP:H   | 1:35:A:GLU:HB2  | 4        | 0.43          |
| (1,876) | 1:27:A:HIS:HD2 | 1:11:A:TRP:H    | 12       | 0.42          |
| (1,866) | 1:11:A:TRP:HB3 | 1:7:A:LEU:HD21  | 22       | 0.42          |
| (1,866) | 1:11:A:TRP:HB3 | 1:7:A:LEU:HD22  | 22       | 0.42          |
| (1,866) | 1:11:A:TRP:HB3 | 1:7:A:LEU:HD23  | 22       | 0.42          |
| (1,832) | 1:11:A:TRP:HZ2 | 1:37:A:PRO:HD2  | 4        | 0.42          |
| (1,820) | 1:21:A:ARG:HB3 | 1:19:A:SER:HA   | 24       | 0.42          |
| (1,770) | 1:25:A:PHE:HE1 | 1:14:A:ARG:HD2  | 4        | 0.42          |
| (1,770) | 1:25:A:PHE:HE2 | 1:14:A:ARG:HD2  | 4        | 0.42          |
| (1,762) | 1:23:A:TYR:HE1 | 1:17:A:ARG:HG3  | 4        | 0.42          |
| (1,762) | 1:23:A:TYR:HE2 | 1:17:A:ARG:HG3  | 4        | 0.42          |
| (1,749) | 1:34:A:TRP:HE1 | 2:88:B:PRO:HB2  | 1        | 0.42          |
| (1,749) | 1:34:A:TRP:HE1 | 2:88:B:PRO:HB2  | 20       | 0.42          |
| (1,749) | 1:34:A:TRP:HE1 | 2:88:B:PRO:HB2  | 24       | 0.42          |
| (1,720) | 2:84:B:TYR:HE1 | 1:23:A:TYR:HE1  | 23       | 0.42          |
| (1,720) | 2:84:B:TYR:HE1 | 1:23:A:TYR:HE2  | 23       | 0.42          |
| (1,720) | 2:84:B:TYR:HE2 | 1:23:A:TYR:HE1  | 23       | 0.42          |
| (1,720) | 2:84:B:TYR:HE2 | 1:23:A:TYR:HE2  | 23       | 0.42          |
| (1,704) | 1:16:A:SER:HB3 | 1:17:A:ARG:HA   | 18       | 0.42          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,643) | 2:85:B:SEP:HB2  | 1:17:A:ARG:HG2 | 5        | 0.42          |
| (1,633) | 1:18:A:SER:HB2  | 1:17:A:ARG:HB3 | 8        | 0.42          |
| (1,553) | 1:34:A:TRP:HH2  | 2:86:B:PRO:HB2 | 7        | 0.42          |
| (1,494) | 1:25:A:PHE:HD1  | 2:83:B:PRO:HG2 | 11       | 0.42          |
| (1,494) | 1:25:A:PHE:HD2  | 2:83:B:PRO:HG2 | 11       | 0.42          |
| (1,494) | 1:25:A:PHE:HD1  | 2:83:B:PRO:HG2 | 20       | 0.42          |
| (1,494) | 1:25:A:PHE:HD2  | 2:83:B:PRO:HG2 | 20       | 0.42          |
| (1,494) | 1:25:A:PHE:HD1  | 2:83:B:PRO:HG2 | 23       | 0.42          |
| (1,494) | 1:25:A:PHE:HD2  | 2:83:B:PRO:HG2 | 23       | 0.42          |
| (1,463) | 1:23:A:TYR:HE1  | 1:14:A:ARG:HD2 | 20       | 0.42          |
| (1,463) | 1:23:A:TYR:HE2  | 1:14:A:ARG:HD2 | 20       | 0.42          |
| (1,192) | 1:9:A:PRO:HD3   | 1:8:A:PRO:HG3  | 14       | 0.42          |
| (1,75)  | 1:37:A:PRO:HD3  | 1:36:A:ARG:HD2 | 2        | 0.42          |
| (1,876) | 1:27:A:HIS:HD2  | 1:11:A:TRP:H   | 6        | 0.41          |
| (1,815) | 1:7:A:LEU:HD11  | 1:8:A:PRO:HA   | 9        | 0.41          |
| (1,815) | 1:7:A:LEU:HD12  | 1:8:A:PRO:HA   | 9        | 0.41          |
| (1,815) | 1:7:A:LEU:HD13  | 1:8:A:PRO:HA   | 9        | 0.41          |
| (1,808) | 1:11:A:TRP:HE3  | 1:37:A:PRO:HD2 | 17       | 0.41          |
| (1,779) | 1:11:A:TRP:HZ3  | 1:7:A:LEU:HD11 | 4        | 0.41          |
| (1,779) | 1:11:A:TRP:HZ3  | 1:7:A:LEU:HD12 | 4        | 0.41          |
| (1,779) | 1:11:A:TRP:HZ3  | 1:7:A:LEU:HD13 | 4        | 0.41          |
| (1,779) | 1:11:A:TRP:HZ3  | 1:7:A:LEU:HD11 | 17       | 0.41          |
| (1,779) | 1:11:A:TRP:HZ3  | 1:7:A:LEU:HD12 | 17       | 0.41          |
| (1,779) | 1:11:A:TRP:HZ3  | 1:7:A:LEU:HD13 | 17       | 0.41          |
| (1,751) | 1:33:A:GLN:HE21 | 1:8:A:PRO:HG3  | 9        | 0.41          |
| (1,749) | 1:34:A:TRP:HE1  | 2:88:B:PRO:HB2 | 6        | 0.41          |
| (1,696) | 2:85:B:SEP:HB3  | 2:84:B:TYR:HB3 | 12       | 0.41          |
| (1,639) | 2:84:B:TYR:HD1  | 1:14:A:ARG:HG2 | 4        | 0.41          |
| (1,639) | 2:84:B:TYR:HD2  | 1:14:A:ARG:HG2 | 4        | 0.41          |
| (1,639) | 2:84:B:TYR:HD1  | 1:14:A:ARG:HG2 | 6        | 0.41          |
| (1,639) | 2:84:B:TYR:HD2  | 1:14:A:ARG:HG2 | 6        | 0.41          |
| (1,633) | 1:18:A:SER:HB2  | 1:17:A:ARG:HB3 | 9        | 0.41          |
| (1,633) | 1:18:A:SER:HB2  | 1:17:A:ARG:HB3 | 14       | 0.41          |
| (1,516) | 1:11:A:TRP:HH2  | 1:37:A:PRO:HD2 | 2        | 0.41          |
| (1,516) | 1:11:A:TRP:HH2  | 1:37:A:PRO:HD2 | 21       | 0.41          |
| (1,494) | 1:25:A:PHE:HD1  | 2:83:B:PRO:HG2 | 3        | 0.41          |
| (1,494) | 1:25:A:PHE:HD2  | 2:83:B:PRO:HG2 | 3        | 0.41          |
| (1,494) | 1:25:A:PHE:HD1  | 2:83:B:PRO:HG2 | 6        | 0.41          |
| (1,494) | 1:25:A:PHE:HD2  | 2:83:B:PRO:HG2 | 6        | 0.41          |
| (1,494) | 1:25:A:PHE:HD1  | 2:83:B:PRO:HG2 | 10       | 0.41          |
| (1,494) | 1:25:A:PHE:HD2  | 2:83:B:PRO:HG2 | 10       | 0.41          |
| (1,494) | 1:25:A:PHE:HD1  | 2:83:B:PRO:HG2 | 19       | 0.41          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,494) | 1:25:A:PHE:HD2  | 2:83:B:PRO:HG2 | 19       | 0.41          |
| (1,463) | 1:23:A:TYR:HE1  | 1:14:A:ARG:HD2 | 21       | 0.41          |
| (1,463) | 1:23:A:TYR:HE2  | 1:14:A:ARG:HD2 | 21       | 0.41          |
| (1,296) | 1:26:A:ASN:HD22 | 1:10:A:GLY:HA2 | 23       | 0.41          |
| (1,181) | 1:7:A:LEU:H     | 1:6:A:LYS:HD2  | 3        | 0.41          |
| (1,167) | 2:84:B:TYR:HD1  | 2:85:B:SEP:HB2 | 20       | 0.41          |
| (1,167) | 2:84:B:TYR:HD2  | 2:85:B:SEP:HB2 | 20       | 0.41          |
| (1,879) | 2:88:B:PRO:HD2  | 1:17:A:ARG:HD2 | 21       | 0.4           |
| (1,866) | 1:11:A:TRP:HB3  | 1:7:A:LEU:HD21 | 11       | 0.4           |
| (1,866) | 1:11:A:TRP:HB3  | 1:7:A:LEU:HD22 | 11       | 0.4           |
| (1,866) | 1:11:A:TRP:HB3  | 1:7:A:LEU:HD23 | 11       | 0.4           |
| (1,836) | 2:88:B:PRO:HA   | 1:17:A:ARG:HG2 | 1        | 0.4           |
| (1,808) | 1:11:A:TRP:HE3  | 1:37:A:PRO:HD2 | 3        | 0.4           |
| (1,756) | 1:41:A:SER:H    | 1:6:A:LYS:HB2  | 3        | 0.4           |
| (1,749) | 1:34:A:TRP:HE1  | 2:88:B:PRO:HB2 | 7        | 0.4           |
| (1,749) | 1:34:A:TRP:HE1  | 2:88:B:PRO:HB2 | 11       | 0.4           |
| (1,725) | 2:84:B:TYR:HB3  | 1:14:A:ARG:HD2 | 21       | 0.4           |
| (1,720) | 2:84:B:TYR:HE1  | 1:23:A:TYR:HE1 | 7        | 0.4           |
| (1,720) | 2:84:B:TYR:HE1  | 1:23:A:TYR:HE2 | 7        | 0.4           |
| (1,720) | 2:84:B:TYR:HE2  | 1:23:A:TYR:HE1 | 7        | 0.4           |
| (1,720) | 2:84:B:TYR:HE2  | 1:23:A:TYR:HE2 | 7        | 0.4           |
| (1,720) | 2:84:B:TYR:HE1  | 1:23:A:TYR:HE1 | 22       | 0.4           |
| (1,720) | 2:84:B:TYR:HE1  | 1:23:A:TYR:HE2 | 22       | 0.4           |
| (1,720) | 2:84:B:TYR:HE2  | 1:23:A:TYR:HE1 | 22       | 0.4           |
| (1,720) | 2:84:B:TYR:HE2  | 1:23:A:TYR:HE2 | 22       | 0.4           |
| (1,714) | 1:13:A:LYS:H    | 1:24:A:TYR:HE1 | 20       | 0.4           |
| (1,714) | 1:13:A:LYS:H    | 1:24:A:TYR:HE2 | 20       | 0.4           |
| (1,710) | 1:34:A:TRP:HB3  | 2:86:B:PRO:HD2 | 11       | 0.4           |
| (1,697) | 2:85:B:SEP:HB3  | 1:17:A:ARG:HA  | 5        | 0.4           |
| (1,639) | 2:84:B:TYR:HD1  | 1:14:A:ARG:HG2 | 14       | 0.4           |
| (1,639) | 2:84:B:TYR:HD2  | 1:14:A:ARG:HG2 | 14       | 0.4           |
| (1,562) | 1:34:A:TRP:HZ2  | 1:16:A:SER:HB3 | 7        | 0.4           |
| (1,553) | 1:34:A:TRP:HH2  | 2:86:B:PRO:HB2 | 12       | 0.4           |
| (1,501) | 1:24:A:TYR:HE1  | 1:33:A:GLN:HG2 | 22       | 0.4           |
| (1,501) | 1:24:A:TYR:HE2  | 1:33:A:GLN:HG2 | 22       | 0.4           |
| (1,493) | 1:24:A:TYR:HE1  | 1:7:A:LEU:HB3  | 14       | 0.4           |
| (1,493) | 1:24:A:TYR:HE2  | 1:7:A:LEU:HB3  | 14       | 0.4           |
| (1,468) | 2:85:B:SEP:H    | 1:14:A:ARG:HB3 | 6        | 0.4           |
| (1,433) | 1:11:A:TRP:HZ3  | 1:37:A:PRO:HG2 | 7        | 0.4           |
| (1,365) | 1:34:A:TRP:H    | 1:35:A:GLU:HB2 | 14       | 0.4           |
| (1,254) | 1:11:A:TRP:HE1  | 1:37:A:PRO:HD3 | 1        | 0.4           |
| (1,129) | 1:7:A:LEU:HB2   | 1:8:A:PRO:HD3  | 11       | 0.4           |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,879) | 2:88:B:PRO:HD2 | 1:17:A:ARG:HD2 | 7        | 0.39          |
| (1,866) | 1:11:A:TRP:HB3 | 1:7:A:LEU:HD21 | 15       | 0.39          |
| (1,866) | 1:11:A:TRP:HB3 | 1:7:A:LEU:HD22 | 15       | 0.39          |
| (1,866) | 1:11:A:TRP:HB3 | 1:7:A:LEU:HD23 | 15       | 0.39          |
| (1,815) | 1:7:A:LEU:HD11 | 1:8:A:PRO:HA   | 1        | 0.39          |
| (1,815) | 1:7:A:LEU:HD12 | 1:8:A:PRO:HA   | 1        | 0.39          |
| (1,815) | 1:7:A:LEU:HD13 | 1:8:A:PRO:HA   | 1        | 0.39          |
| (1,779) | 1:11:A:TRP:HZ3 | 1:7:A:LEU:HD11 | 18       | 0.39          |
| (1,779) | 1:11:A:TRP:HZ3 | 1:7:A:LEU:HD12 | 18       | 0.39          |
| (1,779) | 1:11:A:TRP:HZ3 | 1:7:A:LEU:HD13 | 18       | 0.39          |
| (1,777) | 1:24:A:TYR:HE1 | 1:7:A:LEU:HA   | 15       | 0.39          |
| (1,777) | 1:24:A:TYR:HE2 | 1:7:A:LEU:HA   | 15       | 0.39          |
| (1,770) | 1:25:A:PHE:HE1 | 1:14:A:ARG:HD2 | 5        | 0.39          |
| (1,770) | 1:25:A:PHE:HE2 | 1:14:A:ARG:HD2 | 5        | 0.39          |
| (1,770) | 1:25:A:PHE:HE1 | 1:14:A:ARG:HD2 | 14       | 0.39          |
| (1,770) | 1:25:A:PHE:HE2 | 1:14:A:ARG:HD2 | 14       | 0.39          |
| (1,749) | 1:34:A:TRP:HE1 | 2:88:B:PRO:HB2 | 10       | 0.39          |
| (1,749) | 1:34:A:TRP:HE1 | 2:88:B:PRO:HB2 | 17       | 0.39          |
| (1,710) | 1:34:A:TRP:HB3 | 2:86:B:PRO:HD2 | 12       | 0.39          |
| (1,696) | 2:85:B:SEP:HB3 | 2:84:B:TYR:HB3 | 16       | 0.39          |
| (1,639) | 2:84:B:TYR:HD1 | 1:14:A:ARG:HG2 | 15       | 0.39          |
| (1,639) | 2:84:B:TYR:HD2 | 1:14:A:ARG:HG2 | 15       | 0.39          |
| (1,553) | 1:34:A:TRP:HH2 | 2:86:B:PRO:HB2 | 10       | 0.39          |
| (1,494) | 1:25:A:PHE:HD1 | 2:83:B:PRO:HG2 | 2        | 0.39          |
| (1,494) | 1:25:A:PHE:HD2 | 2:83:B:PRO:HG2 | 2        | 0.39          |
| (1,494) | 1:25:A:PHE:HD1 | 2:83:B:PRO:HG2 | 22       | 0.39          |
| (1,494) | 1:25:A:PHE:HD2 | 2:83:B:PRO:HG2 | 22       | 0.39          |
| (1,370) | 1:22:A:VAL:H   | 1:16:A:SER:HB2 | 19       | 0.39          |
| (1,12)  | 1:21:A:ARG:H   | 1:16:A:SER:HB2 | 21       | 0.39          |
| (1,879) | 2:88:B:PRO:HD2 | 1:17:A:ARG:HD2 | 18       | 0.38          |
| (1,876) | 1:27:A:HIS:HD2 | 1:11:A:TRP:H   | 14       | 0.38          |
| (1,851) | 1:7:A:LEU:HD11 | 1:37:A:PRO:HD3 | 7        | 0.38          |
| (1,851) | 1:7:A:LEU:HD12 | 1:37:A:PRO:HD3 | 7        | 0.38          |
| (1,851) | 1:7:A:LEU:HD13 | 1:37:A:PRO:HD3 | 7        | 0.38          |
| (1,815) | 1:7:A:LEU:HD11 | 1:8:A:PRO:HA   | 7        | 0.38          |
| (1,815) | 1:7:A:LEU:HD12 | 1:8:A:PRO:HA   | 7        | 0.38          |
| (1,815) | 1:7:A:LEU:HD13 | 1:8:A:PRO:HA   | 7        | 0.38          |
| (1,808) | 1:11:A:TRP:HE3 | 1:37:A:PRO:HD2 | 12       | 0.38          |
| (1,783) | 1:34:A:TRP:HZ3 | 2:85:B:SEP:HB2 | 24       | 0.38          |
| (1,779) | 1:11:A:TRP:HZ3 | 1:7:A:LEU:HD11 | 22       | 0.38          |
| (1,779) | 1:11:A:TRP:HZ3 | 1:7:A:LEU:HD12 | 22       | 0.38          |
| (1,779) | 1:11:A:TRP:HZ3 | 1:7:A:LEU:HD13 | 22       | 0.38          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,770) | 1:25:A:PHE:HE1  | 1:14:A:ARG:HD2 | 1        | 0.38          |
| (1,770) | 1:25:A:PHE:HE2  | 1:14:A:ARG:HD2 | 1        | 0.38          |
| (1,770) | 1:25:A:PHE:HE1  | 1:14:A:ARG:HD2 | 24       | 0.38          |
| (1,770) | 1:25:A:PHE:HE2  | 1:14:A:ARG:HD2 | 24       | 0.38          |
| (1,720) | 2:84:B:TYR:HE1  | 1:23:A:TYR:HE1 | 21       | 0.38          |
| (1,720) | 2:84:B:TYR:HE1  | 1:23:A:TYR:HE2 | 21       | 0.38          |
| (1,720) | 2:84:B:TYR:HE2  | 1:23:A:TYR:HE1 | 21       | 0.38          |
| (1,720) | 2:84:B:TYR:HE2  | 1:23:A:TYR:HE2 | 21       | 0.38          |
| (1,714) | 1:13:A:LYS:H    | 1:24:A:TYR:HE1 | 5        | 0.38          |
| (1,714) | 1:13:A:LYS:H    | 1:24:A:TYR:HE2 | 5        | 0.38          |
| (1,710) | 1:34:A:TRP:HB3  | 2:86:B:PRO:HD2 | 20       | 0.38          |
| (1,697) | 2:85:B:SEP:HB3  | 1:17:A:ARG:HA  | 6        | 0.38          |
| (1,682) | 1:23:A:TYR:HB3  | 1:16:A:SER:HB3 | 10       | 0.38          |
| (1,622) | 1:33:A:GLN:HG2  | 1:24:A:TYR:HB3 | 3        | 0.38          |
| (1,619) | 2:84:B:TYR:HB2  | 2:83:B:PRO:HG3 | 17       | 0.38          |
| (1,605) | 1:33:A:GLN:HE22 | 1:24:A:TYR:HB3 | 21       | 0.38          |
| (1,578) | 1:34:A:TRP:HH2  | 1:21:A:ARG:HD3 | 1        | 0.38          |
| (1,578) | 1:34:A:TRP:HH2  | 1:21:A:ARG:HD3 | 11       | 0.38          |
| (1,468) | 2:85:B:SEP:H    | 1:14:A:ARG:HB3 | 18       | 0.38          |
| (1,254) | 1:11:A:TRP:HE1  | 1:37:A:PRO:HD3 | 9        | 0.38          |
| (1,227) | 1:34:A:TRP:HE3  | 1:21:A:ARG:HB2 | 6        | 0.38          |
| (1,227) | 1:34:A:TRP:HE3  | 1:21:A:ARG:HB2 | 7        | 0.38          |
| (1,192) | 1:9:A:PRO:HD3   | 1:8:A:PRO:HG3  | 6        | 0.38          |
| (1,114) | 2:87:B:PHE:H    | 2:88:B:PRO:HD2 | 8        | 0.38          |
| (1,102) | 1:23:A:TYR:HE1  | 1:25:A:PHE:HB3 | 10       | 0.38          |
| (1,102) | 1:23:A:TYR:HE2  | 1:25:A:PHE:HB3 | 10       | 0.38          |
| (1,102) | 1:23:A:TYR:HE1  | 1:25:A:PHE:HB3 | 19       | 0.38          |
| (1,102) | 1:23:A:TYR:HE2  | 1:25:A:PHE:HB3 | 19       | 0.38          |
| (1,75)  | 1:37:A:PRO:HD3  | 1:36:A:ARG:HD2 | 5        | 0.38          |
| (1,26)  | 1:22:A:VAL:H    | 1:21:A:ARG:HG3 | 3        | 0.38          |
| (1,866) | 1:11:A:TRP:HB3  | 1:7:A:LEU:HD21 | 14       | 0.37          |
| (1,866) | 1:11:A:TRP:HB3  | 1:7:A:LEU:HD22 | 14       | 0.37          |
| (1,866) | 1:11:A:TRP:HB3  | 1:7:A:LEU:HD23 | 14       | 0.37          |
| (1,815) | 1:7:A:LEU:HD11  | 1:8:A:PRO:HA   | 20       | 0.37          |
| (1,815) | 1:7:A:LEU:HD12  | 1:8:A:PRO:HA   | 20       | 0.37          |
| (1,815) | 1:7:A:LEU:HD13  | 1:8:A:PRO:HA   | 20       | 0.37          |
| (1,783) | 1:34:A:TRP:HZ3  | 2:85:B:SEP:HB2 | 10       | 0.37          |
| (1,779) | 1:11:A:TRP:HZ3  | 1:7:A:LEU:HD11 | 2        | 0.37          |
| (1,779) | 1:11:A:TRP:HZ3  | 1:7:A:LEU:HD12 | 2        | 0.37          |
| (1,779) | 1:11:A:TRP:HZ3  | 1:7:A:LEU:HD13 | 2        | 0.37          |
| (1,770) | 1:25:A:PHE:HE1  | 1:14:A:ARG:HD2 | 9        | 0.37          |
| (1,770) | 1:25:A:PHE:HE2  | 1:14:A:ARG:HD2 | 9        | 0.37          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,770) | 1:25:A:PHE:HE1  | 1:14:A:ARG:HD2  | 17       | 0.37          |
| (1,770) | 1:25:A:PHE:HE2  | 1:14:A:ARG:HD2  | 17       | 0.37          |
| (1,752) | 1:33:A:GLN:HE21 | 1:37:A:PRO:HD3  | 3        | 0.37          |
| (1,749) | 1:34:A:TRP:HE1  | 2:88:B:PRO:HB2  | 15       | 0.37          |
| (1,749) | 1:34:A:TRP:HE1  | 2:88:B:PRO:HB2  | 16       | 0.37          |
| (1,749) | 1:34:A:TRP:HE1  | 2:88:B:PRO:HB2  | 21       | 0.37          |
| (1,714) | 1:13:A:LYS:H    | 1:24:A:TYR:HE1  | 17       | 0.37          |
| (1,714) | 1:13:A:LYS:H    | 1:24:A:TYR:HE2  | 17       | 0.37          |
| (1,710) | 1:34:A:TRP:HB3  | 2:86:B:PRO:HD2  | 10       | 0.37          |
| (1,710) | 1:34:A:TRP:HB3  | 2:86:B:PRO:HD2  | 21       | 0.37          |
| (1,710) | 1:34:A:TRP:HB3  | 2:86:B:PRO:HD2  | 24       | 0.37          |
| (1,704) | 1:16:A:SER:HB3  | 1:17:A:ARG:HA   | 3        | 0.37          |
| (1,676) | 1:8:A:PRO:HD3   | 1:7:A:LEU:HD11  | 7        | 0.37          |
| (1,676) | 1:8:A:PRO:HD3   | 1:7:A:LEU:HD12  | 7        | 0.37          |
| (1,676) | 1:8:A:PRO:HD3   | 1:7:A:LEU:HD13  | 7        | 0.37          |
| (1,639) | 2:84:B:TYR:HD1  | 1:14:A:ARG:HG2  | 7        | 0.37          |
| (1,639) | 2:84:B:TYR:HD2  | 1:14:A:ARG:HG2  | 7        | 0.37          |
| (1,639) | 2:84:B:TYR:HD1  | 1:14:A:ARG:HG2  | 25       | 0.37          |
| (1,639) | 2:84:B:TYR:HD2  | 1:14:A:ARG:HG2  | 25       | 0.37          |
| (1,605) | 1:33:A:GLN:HE22 | 1:24:A:TYR:HB3  | 6        | 0.37          |
| (1,553) | 1:34:A:TRP:HH2  | 2:86:B:PRO:HB2  | 17       | 0.37          |
| (1,544) | 1:11:A:TRP:HD1  | 1:7:A:LEU:HB2   | 19       | 0.37          |
| (1,518) | 1:11:A:TRP:HZ3  | 1:11:A:TRP:HB2  | 10       | 0.37          |
| (1,494) | 1:25:A:PHE:HD1  | 2:83:B:PRO:HG2  | 18       | 0.37          |
| (1,494) | 1:25:A:PHE:HD2  | 2:83:B:PRO:HG2  | 18       | 0.37          |
| (1,407) | 1:35:A:GLU:H    | 1:33:A:GLN:HE22 | 13       | 0.37          |
| (1,407) | 1:35:A:GLU:H    | 1:33:A:GLN:HE22 | 25       | 0.37          |
| (1,227) | 1:34:A:TRP:HE3  | 1:21:A:ARG:HB2  | 1        | 0.37          |
| (1,227) | 1:34:A:TRP:HE3  | 1:21:A:ARG:HB2  | 8        | 0.37          |
| (1,114) | 2:87:B:PHE:H    | 2:88:B:PRO:HD2  | 16       | 0.37          |
| (1,87)  | 1:23:A:TYR:HE1  | 1:16:A:SER:HB3  | 9        | 0.37          |
| (1,87)  | 1:23:A:TYR:HE2  | 1:16:A:SER:HB3  | 9        | 0.37          |
| (1,849) | 1:14:A:ARG:HB3  | 1:15:A:MET:HG3  | 18       | 0.36          |
| (1,815) | 1:7:A:LEU:HD11  | 1:8:A:PRO:HA    | 5        | 0.36          |
| (1,815) | 1:7:A:LEU:HD12  | 1:8:A:PRO:HA    | 5        | 0.36          |
| (1,815) | 1:7:A:LEU:HD13  | 1:8:A:PRO:HA    | 5        | 0.36          |
| (1,815) | 1:7:A:LEU:HD11  | 1:8:A:PRO:HA    | 6        | 0.36          |
| (1,815) | 1:7:A:LEU:HD12  | 1:8:A:PRO:HA    | 6        | 0.36          |
| (1,815) | 1:7:A:LEU:HD13  | 1:8:A:PRO:HA    | 6        | 0.36          |
| (1,815) | 1:7:A:LEU:HD11  | 1:8:A:PRO:HA    | 12       | 0.36          |
| (1,815) | 1:7:A:LEU:HD12  | 1:8:A:PRO:HA    | 12       | 0.36          |
| (1,815) | 1:7:A:LEU:HD13  | 1:8:A:PRO:HA    | 12       | 0.36          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,751) | 1:33:A:GLN:HE21 | 1:8:A:PRO:HG3  | 5        | 0.36          |
| (1,751) | 1:33:A:GLN:HE21 | 1:8:A:PRO:HG3  | 23       | 0.36          |
| (1,749) | 1:34:A:TRP:HE1  | 2:88:B:PRO:HB2 | 4        | 0.36          |
| (1,749) | 1:34:A:TRP:HE1  | 2:88:B:PRO:HB2 | 23       | 0.36          |
| (1,720) | 2:84:B:TYR:HE1  | 1:23:A:TYR:HE1 | 9        | 0.36          |
| (1,720) | 2:84:B:TYR:HE1  | 1:23:A:TYR:HE2 | 9        | 0.36          |
| (1,720) | 2:84:B:TYR:HE2  | 1:23:A:TYR:HE1 | 9        | 0.36          |
| (1,720) | 2:84:B:TYR:HE2  | 1:23:A:TYR:HE2 | 9        | 0.36          |
| (1,720) | 2:84:B:TYR:HE1  | 1:23:A:TYR:HE1 | 13       | 0.36          |
| (1,720) | 2:84:B:TYR:HE1  | 1:23:A:TYR:HE2 | 13       | 0.36          |
| (1,720) | 2:84:B:TYR:HE2  | 1:23:A:TYR:HE1 | 13       | 0.36          |
| (1,720) | 2:84:B:TYR:HE2  | 1:23:A:TYR:HE2 | 13       | 0.36          |
| (1,710) | 1:34:A:TRP:HB3  | 2:86:B:PRO:HD2 | 1        | 0.36          |
| (1,683) | 2:83:B:PRO:HD2  | 2:84:B:TYR:HB3 | 17       | 0.36          |
| (1,674) | 2:86:B:PRO:HD3  | 1:14:A:ARG:HD2 | 14       | 0.36          |
| (1,553) | 1:34:A:TRP:HH2  | 2:86:B:PRO:HB2 | 3        | 0.36          |
| (1,518) | 1:11:A:TRP:HZ3  | 1:11:A:TRP:HB2 | 17       | 0.36          |
| (1,518) | 1:11:A:TRP:HZ3  | 1:11:A:TRP:HB2 | 22       | 0.36          |
| (1,494) | 1:25:A:PHE:HD1  | 2:83:B:PRO:HG2 | 9        | 0.36          |
| (1,494) | 1:25:A:PHE:HD2  | 2:83:B:PRO:HG2 | 9        | 0.36          |
| (1,494) | 1:25:A:PHE:HD1  | 2:83:B:PRO:HG2 | 12       | 0.36          |
| (1,494) | 1:25:A:PHE:HD2  | 2:83:B:PRO:HG2 | 12       | 0.36          |
| (1,494) | 1:25:A:PHE:HD1  | 2:83:B:PRO:HG2 | 14       | 0.36          |
| (1,494) | 1:25:A:PHE:HD2  | 2:83:B:PRO:HG2 | 14       | 0.36          |
| (1,494) | 1:25:A:PHE:HD1  | 2:83:B:PRO:HG2 | 15       | 0.36          |
| (1,494) | 1:25:A:PHE:HD2  | 2:83:B:PRO:HG2 | 15       | 0.36          |
| (1,493) | 1:24:A:TYR:HE1  | 1:7:A:LEU:HB3  | 13       | 0.36          |
| (1,493) | 1:24:A:TYR:HE2  | 1:7:A:LEU:HB3  | 13       | 0.36          |
| (1,468) | 2:85:B:SEP:H    | 1:14:A:ARG:HB3 | 5        | 0.36          |
| (1,468) | 2:85:B:SEP:H    | 1:14:A:ARG:HB3 | 14       | 0.36          |
| (1,370) | 1:22:A:VAL:H    | 1:16:A:SER:HB2 | 3        | 0.36          |
| (1,296) | 1:26:A:ASN:HD22 | 1:10:A:GLY:HA2 | 21       | 0.36          |
| (1,281) | 1:16:A:SER:H    | 2:85:B:SEP:HB2 | 17       | 0.36          |
| (1,227) | 1:34:A:TRP:HE3  | 1:21:A:ARG:HB2 | 5        | 0.36          |
| (1,227) | 1:34:A:TRP:HE3  | 1:21:A:ARG:HB2 | 9        | 0.36          |
| (1,114) | 2:87:B:PHE:H    | 2:88:B:PRO:HD2 | 7        | 0.36          |
| (1,75)  | 1:37:A:PRO:HD3  | 1:36:A:ARG:HD2 | 23       | 0.36          |
| (1,12)  | 1:21:A:ARG:H    | 1:16:A:SER:HB2 | 2        | 0.36          |
| (1,832) | 1:11:A:TRP:HZ2  | 1:37:A:PRO:HD2 | 16       | 0.35          |
| (1,815) | 1:7:A:LEU:HD11  | 1:8:A:PRO:HA   | 8        | 0.35          |
| (1,815) | 1:7:A:LEU:HD12  | 1:8:A:PRO:HA   | 8        | 0.35          |
| (1,815) | 1:7:A:LEU:HD13  | 1:8:A:PRO:HA   | 8        | 0.35          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,770) | 1:25:A:PHE:HE1  | 1:14:A:ARG:HD2 | 11       | 0.35          |
| (1,770) | 1:25:A:PHE:HE2  | 1:14:A:ARG:HD2 | 11       | 0.35          |
| (1,769) | 1:25:A:PHE:HE1  | 2:83:B:PRO:HB3 | 8        | 0.35          |
| (1,769) | 1:25:A:PHE:HE2  | 2:83:B:PRO:HB3 | 8        | 0.35          |
| (1,761) | 1:23:A:TYR:HE1  | 1:21:A:ARG:HB2 | 25       | 0.35          |
| (1,761) | 1:23:A:TYR:HE2  | 1:21:A:ARG:HB2 | 25       | 0.35          |
| (1,754) | 1:11:A:TRP:HE3  | 1:13:A:LYS:HB3 | 4        | 0.35          |
| (1,754) | 1:11:A:TRP:HE3  | 1:13:A:LYS:HB3 | 11       | 0.35          |
| (1,754) | 1:11:A:TRP:HE3  | 1:13:A:LYS:HB3 | 16       | 0.35          |
| (1,720) | 2:84:B:TYR:HE1  | 1:23:A:TYR:HE1 | 14       | 0.35          |
| (1,720) | 2:84:B:TYR:HE1  | 1:23:A:TYR:HE2 | 14       | 0.35          |
| (1,720) | 2:84:B:TYR:HE2  | 1:23:A:TYR:HE1 | 14       | 0.35          |
| (1,720) | 2:84:B:TYR:HE2  | 1:23:A:TYR:HE2 | 14       | 0.35          |
| (1,710) | 1:34:A:TRP:HB3  | 2:86:B:PRO:HD2 | 2        | 0.35          |
| (1,710) | 1:34:A:TRP:HB3  | 2:86:B:PRO:HD2 | 7        | 0.35          |
| (1,704) | 1:16:A:SER:HB3  | 1:17:A:ARG:HA  | 24       | 0.35          |
| (1,697) | 2:85:B:SEP:HB3  | 1:17:A:ARG:HA  | 20       | 0.35          |
| (1,697) | 2:85:B:SEP:HB3  | 1:17:A:ARG:HA  | 21       | 0.35          |
| (1,697) | 2:85:B:SEP:HB3  | 1:17:A:ARG:HA  | 22       | 0.35          |
| (1,658) | 1:17:A:ARG:HD3  | 2:88:B:PRO:HD3 | 23       | 0.35          |
| (1,578) | 1:34:A:TRP:HH2  | 1:21:A:ARG:HD3 | 21       | 0.35          |
| (1,518) | 1:11:A:TRP:HZ3  | 1:11:A:TRP:HB2 | 2        | 0.35          |
| (1,518) | 1:11:A:TRP:HZ3  | 1:11:A:TRP:HB2 | 12       | 0.35          |
| (1,518) | 1:11:A:TRP:HZ3  | 1:11:A:TRP:HB2 | 13       | 0.35          |
| (1,494) | 1:25:A:PHE:HD1  | 2:83:B:PRO:HG2 | 4        | 0.35          |
| (1,494) | 1:25:A:PHE:HD2  | 2:83:B:PRO:HG2 | 4        | 0.35          |
| (1,487) | 1:25:A:PHE:HD1  | 1:14:A:ARG:HB3 | 18       | 0.35          |
| (1,487) | 1:25:A:PHE:HD2  | 1:14:A:ARG:HB3 | 18       | 0.35          |
| (1,343) | 1:25:A:PHE:H    | 1:14:A:ARG:HB3 | 15       | 0.35          |
| (1,296) | 1:26:A:ASN:HD22 | 1:10:A:GLY:HA2 | 24       | 0.35          |
| (1,247) | 1:24:A:TYR:HE1  | 1:36:A:ARG:HD2 | 5        | 0.35          |
| (1,247) | 1:24:A:TYR:HE2  | 1:36:A:ARG:HD2 | 5        | 0.35          |
| (1,114) | 2:87:B:PHE:H    | 2:88:B:PRO:HD2 | 25       | 0.35          |
| (1,832) | 1:11:A:TRP:HZ2  | 1:37:A:PRO:HD2 | 1        | 0.34          |
| (1,815) | 1:7:A:LEU:HD11  | 1:8:A:PRO:HA   | 24       | 0.34          |
| (1,815) | 1:7:A:LEU:HD12  | 1:8:A:PRO:HA   | 24       | 0.34          |
| (1,815) | 1:7:A:LEU:HD13  | 1:8:A:PRO:HA   | 24       | 0.34          |
| (1,808) | 1:11:A:TRP:HE3  | 1:37:A:PRO:HD2 | 8        | 0.34          |
| (1,762) | 1:23:A:TYR:HE1  | 1:17:A:ARG:HG3 | 10       | 0.34          |
| (1,762) | 1:23:A:TYR:HE2  | 1:17:A:ARG:HG3 | 10       | 0.34          |
| (1,752) | 1:33:A:GLN:HE21 | 1:37:A:PRO:HD3 | 2        | 0.34          |
| (1,749) | 1:34:A:TRP:HE1  | 2:88:B:PRO:HB2 | 3        | 0.34          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,722) | 2:90:B:GLY:HA2  | 1:21:A:ARG:HG3 | 22       | 0.34          |
| (1,710) | 1:34:A:TRP:HB3  | 2:86:B:PRO:HD2 | 6        | 0.34          |
| (1,710) | 1:34:A:TRP:HB3  | 2:86:B:PRO:HD2 | 22       | 0.34          |
| (1,674) | 2:86:B:PRO:HD3  | 1:14:A:ARG:HD2 | 15       | 0.34          |
| (1,605) | 1:33:A:GLN:HE22 | 1:24:A:TYR:HB3 | 23       | 0.34          |
| (1,544) | 1:11:A:TRP:HD1  | 1:7:A:LEU:HB2  | 16       | 0.34          |
| (1,518) | 1:11:A:TRP:HZ3  | 1:11:A:TRP:HB2 | 4        | 0.34          |
| (1,518) | 1:11:A:TRP:HZ3  | 1:11:A:TRP:HB2 | 8        | 0.34          |
| (1,518) | 1:11:A:TRP:HZ3  | 1:11:A:TRP:HB2 | 15       | 0.34          |
| (1,227) | 1:34:A:TRP:HE3  | 1:21:A:ARG:HB2 | 17       | 0.34          |
| (1,129) | 1:7:A:LEU:HB2   | 1:8:A:PRO:HD3  | 14       | 0.34          |
| (1,114) | 2:87:B:PHE:H    | 2:88:B:PRO:HD2 | 1        | 0.34          |
| (1,114) | 2:87:B:PHE:H    | 2:88:B:PRO:HD2 | 9        | 0.34          |
| (1,114) | 2:87:B:PHE:H    | 2:88:B:PRO:HD2 | 13       | 0.34          |
| (1,114) | 2:87:B:PHE:H    | 2:88:B:PRO:HD2 | 14       | 0.34          |
| (1,114) | 2:87:B:PHE:H    | 2:88:B:PRO:HD2 | 22       | 0.34          |
| (1,866) | 1:11:A:TRP:HB3  | 1:7:A:LEU:HD21 | 4        | 0.33          |
| (1,866) | 1:11:A:TRP:HB3  | 1:7:A:LEU:HD22 | 4        | 0.33          |
| (1,866) | 1:11:A:TRP:HB3  | 1:7:A:LEU:HD23 | 4        | 0.33          |
| (1,849) | 1:14:A:ARG:HB3  | 1:15:A:MET:HG3 | 13       | 0.33          |
| (1,832) | 1:11:A:TRP:HZ2  | 1:37:A:PRO:HD2 | 20       | 0.33          |
| (1,808) | 1:11:A:TRP:HE3  | 1:37:A:PRO:HD2 | 10       | 0.33          |
| (1,770) | 1:25:A:PHE:HE1  | 1:14:A:ARG:HD2 | 16       | 0.33          |
| (1,770) | 1:25:A:PHE:HE2  | 1:14:A:ARG:HD2 | 16       | 0.33          |
| (1,754) | 1:11:A:TRP:HE3  | 1:13:A:LYS:HB3 | 10       | 0.33          |
| (1,754) | 1:11:A:TRP:HE3  | 1:13:A:LYS:HB3 | 12       | 0.33          |
| (1,754) | 1:11:A:TRP:HE3  | 1:13:A:LYS:HB3 | 21       | 0.33          |
| (1,749) | 1:34:A:TRP:HE1  | 2:88:B:PRO:HB2 | 19       | 0.33          |
| (1,749) | 1:34:A:TRP:HE1  | 2:88:B:PRO:HB2 | 25       | 0.33          |
| (1,710) | 1:34:A:TRP:HB3  | 2:86:B:PRO:HD2 | 5        | 0.33          |
| (1,710) | 1:34:A:TRP:HB3  | 2:86:B:PRO:HD2 | 15       | 0.33          |
| (1,710) | 1:34:A:TRP:HB3  | 2:86:B:PRO:HD2 | 18       | 0.33          |
| (1,643) | 2:85:B:SEP:HB2  | 1:17:A:ARG:HG2 | 23       | 0.33          |
| (1,605) | 1:33:A:GLN:HE22 | 1:24:A:TYR:HB3 | 24       | 0.33          |
| (1,604) | 1:33:A:GLN:HE22 | 1:35:A:GLU:HG2 | 7        | 0.33          |
| (1,544) | 1:11:A:TRP:HD1  | 1:7:A:LEU:HB2  | 6        | 0.33          |
| (1,544) | 1:11:A:TRP:HD1  | 1:7:A:LEU:HB2  | 12       | 0.33          |
| (1,544) | 1:11:A:TRP:HD1  | 1:7:A:LEU:HB2  | 22       | 0.33          |
| (1,544) | 1:11:A:TRP:HD1  | 1:7:A:LEU:HB2  | 24       | 0.33          |
| (1,518) | 1:11:A:TRP:HZ3  | 1:11:A:TRP:HB2 | 1        | 0.33          |
| (1,518) | 1:11:A:TRP:HZ3  | 1:11:A:TRP:HB2 | 7        | 0.33          |
| (1,518) | 1:11:A:TRP:HZ3  | 1:11:A:TRP:HB2 | 11       | 0.33          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,518) | 1:11:A:TRP:HZ3  | 1:11:A:TRP:HB2 | 19       | 0.33          |
| (1,494) | 1:25:A:PHE:HD1  | 2:83:B:PRO:HG2 | 21       | 0.33          |
| (1,494) | 1:25:A:PHE:HD2  | 2:83:B:PRO:HG2 | 21       | 0.33          |
| (1,494) | 1:25:A:PHE:HD1  | 2:83:B:PRO:HG2 | 24       | 0.33          |
| (1,494) | 1:25:A:PHE:HD2  | 2:83:B:PRO:HG2 | 24       | 0.33          |
| (1,493) | 1:24:A:TYR:HE1  | 1:7:A:LEU:HB3  | 11       | 0.33          |
| (1,493) | 1:24:A:TYR:HE2  | 1:7:A:LEU:HB3  | 11       | 0.33          |
| (1,247) | 1:24:A:TYR:HE1  | 1:36:A:ARG:HD2 | 20       | 0.33          |
| (1,247) | 1:24:A:TYR:HE2  | 1:36:A:ARG:HD2 | 20       | 0.33          |
| (1,227) | 1:34:A:TRP:HE3  | 1:21:A:ARG:HB2 | 2        | 0.33          |
| (1,227) | 1:34:A:TRP:HE3  | 1:21:A:ARG:HB2 | 12       | 0.33          |
| (1,217) | 1:16:A:SER:HB2  | 1:21:A:ARG:HG2 | 9        | 0.33          |
| (1,137) | 2:85:B:SEP:HB2  | 1:17:A:ARG:HD3 | 7        | 0.33          |
| (1,118) | 1:24:A:TYR:HA   | 1:13:A:LYS:HG3 | 10       | 0.33          |
| (1,114) | 2:87:B:PHE:H    | 2:88:B:PRO:HD2 | 2        | 0.33          |
| (1,114) | 2:87:B:PHE:H    | 2:88:B:PRO:HD2 | 5        | 0.33          |
| (1,114) | 2:87:B:PHE:H    | 2:88:B:PRO:HD2 | 6        | 0.33          |
| (1,114) | 2:87:B:PHE:H    | 2:88:B:PRO:HD2 | 15       | 0.33          |
| (1,114) | 2:87:B:PHE:H    | 2:88:B:PRO:HD2 | 17       | 0.33          |
| (1,114) | 2:87:B:PHE:H    | 2:88:B:PRO:HD2 | 19       | 0.33          |
| (1,114) | 2:87:B:PHE:H    | 2:88:B:PRO:HD2 | 23       | 0.33          |
| (1,114) | 2:87:B:PHE:H    | 2:88:B:PRO:HD2 | 24       | 0.33          |
| (1,88)  | 1:33:A:GLN:HE21 | 1:37:A:PRO:HA  | 10       | 0.33          |
| (1,87)  | 1:23:A:TYR:HE1  | 1:16:A:SER:HB3 | 3        | 0.33          |
| (1,87)  | 1:23:A:TYR:HE2  | 1:16:A:SER:HB3 | 3        | 0.33          |
| (1,879) | 2:88:B:PRO:HD2  | 1:17:A:ARG:HD2 | 1        | 0.32          |
| (1,866) | 1:11:A:TRP:HB3  | 1:7:A:LEU:HD21 | 17       | 0.32          |
| (1,866) | 1:11:A:TRP:HB3  | 1:7:A:LEU:HD22 | 17       | 0.32          |
| (1,866) | 1:11:A:TRP:HB3  | 1:7:A:LEU:HD23 | 17       | 0.32          |
| (1,815) | 1:7:A:LEU:HD11  | 1:8:A:PRO:HA   | 3        | 0.32          |
| (1,815) | 1:7:A:LEU:HD12  | 1:8:A:PRO:HA   | 3        | 0.32          |
| (1,815) | 1:7:A:LEU:HD13  | 1:8:A:PRO:HA   | 3        | 0.32          |
| (1,808) | 1:11:A:TRP:HE3  | 1:37:A:PRO:HD2 | 24       | 0.32          |
| (1,777) | 1:24:A:TYR:HE1  | 1:7:A:LEU:HA   | 11       | 0.32          |
| (1,777) | 1:24:A:TYR:HE2  | 1:7:A:LEU:HA   | 11       | 0.32          |
| (1,770) | 1:25:A:PHE:HE1  | 1:14:A:ARG:HD2 | 23       | 0.32          |
| (1,770) | 1:25:A:PHE:HE2  | 1:14:A:ARG:HD2 | 23       | 0.32          |
| (1,749) | 1:34:A:TRP:HE1  | 2:88:B:PRO:HB2 | 13       | 0.32          |
| (1,710) | 1:34:A:TRP:HB3  | 2:86:B:PRO:HD2 | 3        | 0.32          |
| (1,710) | 1:34:A:TRP:HB3  | 2:86:B:PRO:HD2 | 4        | 0.32          |
| (1,710) | 1:34:A:TRP:HB3  | 2:86:B:PRO:HD2 | 16       | 0.32          |
| (1,710) | 1:34:A:TRP:HB3  | 2:86:B:PRO:HD2 | 25       | 0.32          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,704) | 1:16:A:SER:HB3  | 1:17:A:ARG:HA  | 13       | 0.32          |
| (1,697) | 2:85:B:SEP:HB3  | 1:17:A:ARG:HA  | 18       | 0.32          |
| (1,697) | 2:85:B:SEP:HB3  | 1:17:A:ARG:HA  | 19       | 0.32          |
| (1,518) | 1:11:A:TRP:HZ3  | 1:11:A:TRP:HB2 | 3        | 0.32          |
| (1,518) | 1:11:A:TRP:HZ3  | 1:11:A:TRP:HB2 | 14       | 0.32          |
| (1,518) | 1:11:A:TRP:HZ3  | 1:11:A:TRP:HB2 | 18       | 0.32          |
| (1,518) | 1:11:A:TRP:HZ3  | 1:11:A:TRP:HB2 | 20       | 0.32          |
| (1,518) | 1:11:A:TRP:HZ3  | 1:11:A:TRP:HB2 | 21       | 0.32          |
| (1,494) | 1:25:A:PHE:HD1  | 2:83:B:PRO:HG2 | 5        | 0.32          |
| (1,494) | 1:25:A:PHE:HD2  | 2:83:B:PRO:HG2 | 5        | 0.32          |
| (1,493) | 1:24:A:TYR:HE1  | 1:7:A:LEU:HB3  | 15       | 0.32          |
| (1,493) | 1:24:A:TYR:HE2  | 1:7:A:LEU:HB3  | 15       | 0.32          |
| (1,487) | 1:25:A:PHE:HD1  | 1:14:A:ARG:HB3 | 3        | 0.32          |
| (1,487) | 1:25:A:PHE:HD2  | 1:14:A:ARG:HB3 | 3        | 0.32          |
| (1,227) | 1:34:A:TRP:HE3  | 1:21:A:ARG:HB2 | 4        | 0.32          |
| (1,227) | 1:34:A:TRP:HE3  | 1:21:A:ARG:HB2 | 16       | 0.32          |
| (1,114) | 2:87:B:PHE:H    | 2:88:B:PRO:HD2 | 4        | 0.32          |
| (1,114) | 2:87:B:PHE:H    | 2:88:B:PRO:HD2 | 12       | 0.32          |
| (1,114) | 2:87:B:PHE:H    | 2:88:B:PRO:HD2 | 20       | 0.32          |
| (1,75)  | 1:37:A:PRO:HD3  | 1:36:A:ARG:HD2 | 3        | 0.32          |
| (1,866) | 1:11:A:TRP:HB3  | 1:7:A:LEU:HD21 | 13       | 0.31          |
| (1,866) | 1:11:A:TRP:HB3  | 1:7:A:LEU:HD22 | 13       | 0.31          |
| (1,866) | 1:11:A:TRP:HB3  | 1:7:A:LEU:HD23 | 13       | 0.31          |
| (1,864) | 1:7:A:LEU:HD11  | 1:11:A:TRP:HB3 | 19       | 0.31          |
| (1,864) | 1:7:A:LEU:HD12  | 1:11:A:TRP:HB3 | 19       | 0.31          |
| (1,864) | 1:7:A:LEU:HD13  | 1:11:A:TRP:HB3 | 19       | 0.31          |
| (1,832) | 1:11:A:TRP:HZ2  | 1:37:A:PRO:HD2 | 24       | 0.31          |
| (1,815) | 1:7:A:LEU:HD11  | 1:8:A:PRO:HA   | 16       | 0.31          |
| (1,815) | 1:7:A:LEU:HD12  | 1:8:A:PRO:HA   | 16       | 0.31          |
| (1,815) | 1:7:A:LEU:HD13  | 1:8:A:PRO:HA   | 16       | 0.31          |
| (1,807) | 1:25:A:PHE:HZ   | 2:83:B:PRO:HB3 | 6        | 0.31          |
| (1,790) | 1:25:A:PHE:HZ   | 1:27:A:HIS:HB2 | 1        | 0.31          |
| (1,710) | 1:34:A:TRP:HB3  | 2:86:B:PRO:HD2 | 14       | 0.31          |
| (1,710) | 1:34:A:TRP:HB3  | 2:86:B:PRO:HD2 | 23       | 0.31          |
| (1,639) | 2:84:B:TYR:HD1  | 1:14:A:ARG:HG2 | 12       | 0.31          |
| (1,639) | 2:84:B:TYR:HD2  | 1:14:A:ARG:HG2 | 12       | 0.31          |
| (1,554) | 1:27:A:HIS:HD2  | 1:12:A:GLU:HG2 | 4        | 0.31          |
| (1,518) | 1:11:A:TRP:HZ3  | 1:11:A:TRP:HB2 | 6        | 0.31          |
| (1,518) | 1:11:A:TRP:HZ3  | 1:11:A:TRP:HB2 | 16       | 0.31          |
| (1,518) | 1:11:A:TRP:HZ3  | 1:11:A:TRP:HB2 | 25       | 0.31          |
| (1,479) | 1:33:A:GLN:HE21 | 1:35:A:GLU:HB2 | 24       | 0.31          |
| (1,296) | 1:26:A:ASN:HD22 | 1:10:A:GLY:HA2 | 22       | 0.31          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,247) | 1:24:A:TYR:HE1 | 1:36:A:ARG:HD2 | 9        | 0.31          |
| (1,247) | 1:24:A:TYR:HE2 | 1:36:A:ARG:HD2 | 9        | 0.31          |
| (1,167) | 2:84:B:TYR:HD1 | 2:85:B:SEP:HB2 | 4        | 0.31          |
| (1,167) | 2:84:B:TYR:HD2 | 2:85:B:SEP:HB2 | 4        | 0.31          |
| (1,114) | 2:87:B:PHE:H   | 2:88:B:PRO:HD2 | 10       | 0.31          |
| (1,114) | 2:87:B:PHE:H   | 2:88:B:PRO:HD2 | 21       | 0.31          |
| (1,849) | 1:14:A:ARG:HB3 | 1:15:A:MET:HG3 | 25       | 0.3           |
| (1,762) | 1:23:A:TYR:HE1 | 1:17:A:ARG:HG3 | 6        | 0.3           |
| (1,762) | 1:23:A:TYR:HE2 | 1:17:A:ARG:HG3 | 6        | 0.3           |
| (1,749) | 1:34:A:TRP:HE1 | 2:88:B:PRO:HB2 | 5        | 0.3           |
| (1,714) | 1:13:A:LYS:H   | 1:24:A:TYR:HE1 | 8        | 0.3           |
| (1,714) | 1:13:A:LYS:H   | 1:24:A:TYR:HE2 | 8        | 0.3           |
| (1,710) | 1:34:A:TRP:HB3 | 2:86:B:PRO:HD2 | 13       | 0.3           |
| (1,697) | 2:85:B:SEP:HB3 | 1:17:A:ARG:HA  | 1        | 0.3           |
| (1,697) | 2:85:B:SEP:HB3 | 1:17:A:ARG:HA  | 7        | 0.3           |
| (1,697) | 2:85:B:SEP:HB3 | 1:17:A:ARG:HA  | 12       | 0.3           |
| (1,676) | 1:8:A:PRO:HD3  | 1:7:A:LEU:HD11 | 12       | 0.3           |
| (1,676) | 1:8:A:PRO:HD3  | 1:7:A:LEU:HD12 | 12       | 0.3           |
| (1,676) | 1:8:A:PRO:HD3  | 1:7:A:LEU:HD13 | 12       | 0.3           |
| (1,674) | 2:86:B:PRO:HD3 | 1:14:A:ARG:HD2 | 12       | 0.3           |
| (1,518) | 1:11:A:TRP:HZ3 | 1:11:A:TRP:HB2 | 5        | 0.3           |
| (1,506) | 1:25:A:PHE:HE1 | 1:32:A:SER:HB3 | 17       | 0.3           |
| (1,506) | 1:25:A:PHE:HE2 | 1:32:A:SER:HB3 | 17       | 0.3           |
| (1,494) | 1:25:A:PHE:HD1 | 2:83:B:PRO:HG2 | 13       | 0.3           |
| (1,494) | 1:25:A:PHE:HD2 | 2:83:B:PRO:HG2 | 13       | 0.3           |
| (1,493) | 1:24:A:TYR:HE1 | 1:7:A:LEU:HB3  | 18       | 0.3           |
| (1,493) | 1:24:A:TYR:HE2 | 1:7:A:LEU:HB3  | 18       | 0.3           |
| (1,483) | 1:24:A:TYR:HD1 | 1:37:A:PRO:HB2 | 9        | 0.3           |
| (1,483) | 1:24:A:TYR:HD2 | 1:37:A:PRO:HB2 | 9        | 0.3           |
| (1,483) | 1:24:A:TYR:HD1 | 1:37:A:PRO:HB2 | 12       | 0.3           |
| (1,483) | 1:24:A:TYR:HD2 | 1:37:A:PRO:HB2 | 12       | 0.3           |
| (1,227) | 1:34:A:TRP:HE3 | 1:21:A:ARG:HB2 | 24       | 0.3           |
| (1,114) | 2:87:B:PHE:H   | 2:88:B:PRO:HD2 | 3        | 0.3           |
| (1,102) | 1:23:A:TYR:HE1 | 1:25:A:PHE:HB3 | 6        | 0.3           |
| (1,102) | 1:23:A:TYR:HE2 | 1:25:A:PHE:HB3 | 6        | 0.3           |
| (1,851) | 1:7:A:LEU:HD11 | 1:37:A:PRO:HD3 | 9        | 0.29          |
| (1,851) | 1:7:A:LEU:HD12 | 1:37:A:PRO:HD3 | 9        | 0.29          |
| (1,851) | 1:7:A:LEU:HD13 | 1:37:A:PRO:HD3 | 9        | 0.29          |
| (1,820) | 1:21:A:ARG:HB3 | 1:19:A:SER:HA  | 8        | 0.29          |
| (1,808) | 1:11:A:TRP:HE3 | 1:37:A:PRO:HD2 | 20       | 0.29          |
| (1,783) | 1:34:A:TRP:HZ3 | 2:85:B:SEP:HB2 | 15       | 0.29          |
| (1,761) | 1:23:A:TYR:HE1 | 1:21:A:ARG:HB2 | 9        | 0.29          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,761) | 1:23:A:TYR:HE2  | 1:21:A:ARG:HB2 | 9        | 0.29          |
| (1,754) | 1:11:A:TRP:HE3  | 1:13:A:LYS:HB3 | 13       | 0.29          |
| (1,754) | 1:11:A:TRP:HE3  | 1:13:A:LYS:HB3 | 14       | 0.29          |
| (1,720) | 2:84:B:TYR:HE1  | 1:23:A:TYR:HE1 | 1        | 0.29          |
| (1,720) | 2:84:B:TYR:HE1  | 1:23:A:TYR:HE2 | 1        | 0.29          |
| (1,720) | 2:84:B:TYR:HE2  | 1:23:A:TYR:HE1 | 1        | 0.29          |
| (1,720) | 2:84:B:TYR:HE2  | 1:23:A:TYR:HE2 | 1        | 0.29          |
| (1,682) | 1:23:A:TYR:HB3  | 1:16:A:SER:HB3 | 21       | 0.29          |
| (1,633) | 1:18:A:SER:HB2  | 1:17:A:ARG:HB3 | 12       | 0.29          |
| (1,605) | 1:33:A:GLN:HE22 | 1:24:A:TYR:HB3 | 3        | 0.29          |
| (1,554) | 1:27:A:HIS:HD2  | 1:12:A:GLU:HG2 | 11       | 0.29          |
| (1,554) | 1:27:A:HIS:HD2  | 1:12:A:GLU:HG2 | 12       | 0.29          |
| (1,506) | 1:25:A:PHE:HE1  | 1:32:A:SER:HB3 | 8        | 0.29          |
| (1,506) | 1:25:A:PHE:HE2  | 1:32:A:SER:HB3 | 8        | 0.29          |
| (1,493) | 1:24:A:TYR:HE1  | 1:7:A:LEU:HB3  | 4        | 0.29          |
| (1,493) | 1:24:A:TYR:HE2  | 1:7:A:LEU:HB3  | 4        | 0.29          |
| (1,343) | 1:25:A:PHE:H    | 1:14:A:ARG:HB3 | 18       | 0.29          |
| (1,254) | 1:11:A:TRP:HE1  | 1:37:A:PRO:HD3 | 16       | 0.29          |
| (1,227) | 1:34:A:TRP:HE3  | 1:21:A:ARG:HB2 | 14       | 0.29          |
| (1,129) | 1:7:A:LEU:HB2   | 1:8:A:PRO:HD3  | 24       | 0.29          |
| (1,87)  | 1:23:A:TYR:HE1  | 1:16:A:SER:HB3 | 16       | 0.29          |
| (1,87)  | 1:23:A:TYR:HE2  | 1:16:A:SER:HB3 | 16       | 0.29          |
| (1,87)  | 1:23:A:TYR:HE1  | 1:16:A:SER:HB3 | 25       | 0.29          |
| (1,87)  | 1:23:A:TYR:HE2  | 1:16:A:SER:HB3 | 25       | 0.29          |
| (1,75)  | 1:37:A:PRO:HD3  | 1:36:A:ARG:HD2 | 14       | 0.29          |
| (1,26)  | 1:22:A:VAL:H    | 1:21:A:ARG:HG3 | 25       | 0.29          |
| (1,876) | 1:27:A:HIS:HD2  | 1:11:A:TRP:H   | 8        | 0.28          |
| (1,851) | 1:7:A:LEU:HD11  | 1:37:A:PRO:HD3 | 1        | 0.28          |
| (1,851) | 1:7:A:LEU:HD12  | 1:37:A:PRO:HD3 | 1        | 0.28          |
| (1,851) | 1:7:A:LEU:HD13  | 1:37:A:PRO:HD3 | 1        | 0.28          |
| (1,851) | 1:7:A:LEU:HD11  | 1:37:A:PRO:HD3 | 5        | 0.28          |
| (1,851) | 1:7:A:LEU:HD12  | 1:37:A:PRO:HD3 | 5        | 0.28          |
| (1,851) | 1:7:A:LEU:HD13  | 1:37:A:PRO:HD3 | 5        | 0.28          |
| (1,832) | 1:11:A:TRP:HZ2  | 1:37:A:PRO:HD2 | 10       | 0.28          |
| (1,815) | 1:7:A:LEU:HD11  | 1:8:A:PRO:HA   | 23       | 0.28          |
| (1,815) | 1:7:A:LEU:HD12  | 1:8:A:PRO:HA   | 23       | 0.28          |
| (1,815) | 1:7:A:LEU:HD13  | 1:8:A:PRO:HA   | 23       | 0.28          |
| (1,777) | 1:24:A:TYR:HE1  | 1:7:A:LEU:HA   | 8        | 0.28          |
| (1,777) | 1:24:A:TYR:HE2  | 1:7:A:LEU:HA   | 8        | 0.28          |
| (1,777) | 1:24:A:TYR:HE1  | 1:7:A:LEU:HA   | 10       | 0.28          |
| (1,777) | 1:24:A:TYR:HE2  | 1:7:A:LEU:HA   | 10       | 0.28          |
| (1,760) | 2:85:B:SEP:H    | 1:34:A:TRP:HZ2 | 24       | 0.28          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,749) | 1:34:A:TRP:HE1  | 2:88:B:PRO:HB2  | 9        | 0.28          |
| (1,720) | 2:84:B:TYR:HE1  | 1:23:A:TYR:HE1  | 4        | 0.28          |
| (1,720) | 2:84:B:TYR:HE1  | 1:23:A:TYR:HE2  | 4        | 0.28          |
| (1,720) | 2:84:B:TYR:HE2  | 1:23:A:TYR:HE1  | 4        | 0.28          |
| (1,720) | 2:84:B:TYR:HE2  | 1:23:A:TYR:HE2  | 4        | 0.28          |
| (1,718) | 1:24:A:TYR:HE1  | 1:37:A:PRO:HD2  | 20       | 0.28          |
| (1,718) | 1:24:A:TYR:HE2  | 1:37:A:PRO:HD2  | 20       | 0.28          |
| (1,718) | 1:24:A:TYR:HE1  | 1:37:A:PRO:HD2  | 24       | 0.28          |
| (1,718) | 1:24:A:TYR:HE2  | 1:37:A:PRO:HD2  | 24       | 0.28          |
| (1,714) | 1:13:A:LYS:H    | 1:24:A:TYR:HE1  | 10       | 0.28          |
| (1,714) | 1:13:A:LYS:H    | 1:24:A:TYR:HE2  | 10       | 0.28          |
| (1,710) | 1:34:A:TRP:HB3  | 2:86:B:PRO:HD2  | 9        | 0.28          |
| (1,710) | 1:34:A:TRP:HB3  | 2:86:B:PRO:HD2  | 19       | 0.28          |
| (1,697) | 2:85:B:SEP:HB3  | 1:17:A:ARG:HA   | 14       | 0.28          |
| (1,633) | 1:18:A:SER:HB2  | 1:17:A:ARG:HB3  | 4        | 0.28          |
| (1,605) | 1:33:A:GLN:HE22 | 1:24:A:TYR:HB3  | 16       | 0.28          |
| (1,544) | 1:11:A:TRP:HD1  | 1:7:A:LEU:HB2   | 15       | 0.28          |
| (1,518) | 1:11:A:TRP:HZ3  | 1:11:A:TRP:HB2  | 23       | 0.28          |
| (1,506) | 1:25:A:PHE:HE1  | 1:32:A:SER:HB3  | 13       | 0.28          |
| (1,506) | 1:25:A:PHE:HE2  | 1:32:A:SER:HB3  | 13       | 0.28          |
| (1,493) | 1:24:A:TYR:HE1  | 1:7:A:LEU:HB3   | 10       | 0.28          |
| (1,493) | 1:24:A:TYR:HE2  | 1:7:A:LEU:HB3   | 10       | 0.28          |
| (1,487) | 1:25:A:PHE:HD1  | 1:14:A:ARG:HB3  | 6        | 0.28          |
| (1,487) | 1:25:A:PHE:HD2  | 1:14:A:ARG:HB3  | 6        | 0.28          |
| (1,483) | 1:24:A:TYR:HD1  | 1:37:A:PRO:HB2  | 14       | 0.28          |
| (1,483) | 1:24:A:TYR:HD2  | 1:37:A:PRO:HB2  | 14       | 0.28          |
| (1,483) | 1:24:A:TYR:HD1  | 1:37:A:PRO:HB2  | 23       | 0.28          |
| (1,483) | 1:24:A:TYR:HD2  | 1:37:A:PRO:HB2  | 23       | 0.28          |
| (1,407) | 1:35:A:GLU:H    | 1:33:A:GLN:HE22 | 12       | 0.28          |
| (1,407) | 1:35:A:GLU:H    | 1:33:A:GLN:HE22 | 21       | 0.28          |
| (1,227) | 1:34:A:TRP:HE3  | 1:21:A:ARG:HB2  | 20       | 0.28          |
| (1,227) | 1:34:A:TRP:HE3  | 1:21:A:ARG:HB2  | 22       | 0.28          |
| (1,227) | 1:34:A:TRP:HE3  | 1:21:A:ARG:HB2  | 23       | 0.28          |
| (1,220) | 1:18:A:SER:HA   | 1:17:A:ARG:HD2  | 21       | 0.28          |
| (1,217) | 1:16:A:SER:HB2  | 1:21:A:ARG:HG2  | 3        | 0.28          |
| (1,114) | 2:87:B:PHE:H    | 2:88:B:PRO:HD2  | 18       | 0.28          |
| (1,75)  | 1:37:A:PRO:HD3  | 1:36:A:ARG:HD2  | 10       | 0.28          |
| (1,861) | 1:37:A:PRO:HD2  | 1:7:A:LEU:HD21  | 6        | 0.27          |
| (1,861) | 1:37:A:PRO:HD2  | 1:7:A:LEU:HD22  | 6        | 0.27          |
| (1,861) | 1:37:A:PRO:HD2  | 1:7:A:LEU:HD23  | 6        | 0.27          |
| (1,842) | 1:37:A:PRO:HD2  | 1:7:A:LEU:HD21  | 6        | 0.27          |
| (1,842) | 1:37:A:PRO:HD2  | 1:7:A:LEU:HD22  | 6        | 0.27          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,842) | 1:37:A:PRO:HD2 | 1:7:A:LEU:HD23 | 6        | 0.27          |
| (1,832) | 1:11:A:TRP:HZ2 | 1:37:A:PRO:HD2 | 17       | 0.27          |
| (1,808) | 1:11:A:TRP:HE3 | 1:37:A:PRO:HD2 | 25       | 0.27          |
| (1,776) | 1:24:A:TYR:HD1 | 1:7:A:LEU:HA   | 13       | 0.27          |
| (1,776) | 1:24:A:TYR:HD2 | 1:7:A:LEU:HA   | 13       | 0.27          |
| (1,770) | 1:25:A:PHE:HE1 | 1:14:A:ARG:HD2 | 2        | 0.27          |
| (1,770) | 1:25:A:PHE:HE2 | 1:14:A:ARG:HD2 | 2        | 0.27          |
| (1,760) | 2:85:B:SEP:H   | 1:34:A:TRP:HZ2 | 3        | 0.27          |
| (1,760) | 2:85:B:SEP:H   | 1:34:A:TRP:HZ2 | 13       | 0.27          |
| (1,754) | 1:11:A:TRP:HE3 | 1:13:A:LYS:HB3 | 5        | 0.27          |
| (1,754) | 1:11:A:TRP:HE3 | 1:13:A:LYS:HB3 | 6        | 0.27          |
| (1,715) | 1:16:A:SER:H   | 1:15:A:MET:HE1 | 10       | 0.27          |
| (1,715) | 1:16:A:SER:H   | 1:15:A:MET:HE2 | 10       | 0.27          |
| (1,715) | 1:16:A:SER:H   | 1:15:A:MET:HE3 | 10       | 0.27          |
| (1,714) | 1:13:A:LYS:H   | 1:24:A:TYR:HE1 | 22       | 0.27          |
| (1,714) | 1:13:A:LYS:H   | 1:24:A:TYR:HE2 | 22       | 0.27          |
| (1,676) | 1:8:A:PRO:HD3  | 1:7:A:LEU:HD11 | 20       | 0.27          |
| (1,676) | 1:8:A:PRO:HD3  | 1:7:A:LEU:HD12 | 20       | 0.27          |
| (1,676) | 1:8:A:PRO:HD3  | 1:7:A:LEU:HD13 | 20       | 0.27          |
| (1,639) | 2:84:B:TYR:HD1 | 1:14:A:ARG:HG2 | 11       | 0.27          |
| (1,639) | 2:84:B:TYR:HD2 | 1:14:A:ARG:HG2 | 11       | 0.27          |
| (1,544) | 1:11:A:TRP:HD1 | 1:7:A:LEU:HB2  | 5        | 0.27          |
| (1,518) | 1:11:A:TRP:HZ3 | 1:11:A:TRP:HB2 | 9        | 0.27          |
| (1,518) | 1:11:A:TRP:HZ3 | 1:11:A:TRP:HB2 | 24       | 0.27          |
| (1,506) | 1:25:A:PHE:HE1 | 1:32:A:SER:HB3 | 2        | 0.27          |
| (1,506) | 1:25:A:PHE:HE2 | 1:32:A:SER:HB3 | 2        | 0.27          |
| (1,506) | 1:25:A:PHE:HE1 | 1:32:A:SER:HB3 | 14       | 0.27          |
| (1,506) | 1:25:A:PHE:HE2 | 1:32:A:SER:HB3 | 14       | 0.27          |
| (1,433) | 1:11:A:TRP:HZ3 | 1:37:A:PRO:HG2 | 22       | 0.27          |
| (1,384) | 1:34:A:TRP:HE3 | 1:21:A:ARG:HG2 | 4        | 0.27          |
| (1,254) | 1:11:A:TRP:HE1 | 1:37:A:PRO:HD3 | 6        | 0.27          |
| (1,227) | 1:34:A:TRP:HE3 | 1:21:A:ARG:HB2 | 19       | 0.27          |
| (1,227) | 1:34:A:TRP:HE3 | 1:21:A:ARG:HB2 | 21       | 0.27          |
| (1,222) | 1:17:A:ARG:HA  | 1:17:A:ARG:HG2 | 16       | 0.27          |
| (1,193) | 1:9:A:PRO:HD3  | 1:8:A:PRO:HG2  | 15       | 0.27          |
| (1,87)  | 1:23:A:TYR:HE1 | 1:16:A:SER:HB3 | 21       | 0.27          |
| (1,87)  | 1:23:A:TYR:HE2 | 1:16:A:SER:HB3 | 21       | 0.27          |
| (1,75)  | 1:37:A:PRO:HD3 | 1:36:A:ARG:HD2 | 8        | 0.27          |
| (1,879) | 2:88:B:PRO:HD2 | 1:17:A:ARG:HD2 | 11       | 0.26          |
| (1,851) | 1:7:A:LEU:HD11 | 1:37:A:PRO:HD3 | 23       | 0.26          |
| (1,851) | 1:7:A:LEU:HD12 | 1:37:A:PRO:HD3 | 23       | 0.26          |
| (1,851) | 1:7:A:LEU:HD13 | 1:37:A:PRO:HD3 | 23       | 0.26          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,849) | 1:14:A:ARG:HB3 | 1:15:A:MET:HG3  | 12       | 0.26          |
| (1,832) | 1:11:A:TRP:HZ2 | 1:37:A:PRO:HD2  | 6        | 0.26          |
| (1,832) | 1:11:A:TRP:HZ2 | 1:37:A:PRO:HD2  | 7        | 0.26          |
| (1,832) | 1:11:A:TRP:HZ2 | 1:37:A:PRO:HD2  | 13       | 0.26          |
| (1,832) | 1:11:A:TRP:HZ2 | 1:37:A:PRO:HD2  | 18       | 0.26          |
| (1,823) | 1:25:A:PHE:HZ  | 1:14:A:ARG:HD2  | 8        | 0.26          |
| (1,822) | 1:25:A:PHE:HZ  | 1:14:A:ARG:HD2  | 8        | 0.26          |
| (1,808) | 1:11:A:TRP:HE3 | 1:37:A:PRO:HD2  | 16       | 0.26          |
| (1,770) | 1:25:A:PHE:HE1 | 1:14:A:ARG:HD2  | 13       | 0.26          |
| (1,770) | 1:25:A:PHE:HE2 | 1:14:A:ARG:HD2  | 13       | 0.26          |
| (1,770) | 1:25:A:PHE:HE1 | 1:14:A:ARG:HD2  | 15       | 0.26          |
| (1,770) | 1:25:A:PHE:HE2 | 1:14:A:ARG:HD2  | 15       | 0.26          |
| (1,754) | 1:11:A:TRP:HE3 | 1:13:A:LYS:HB3  | 7        | 0.26          |
| (1,754) | 1:11:A:TRP:HE3 | 1:13:A:LYS:HB3  | 9        | 0.26          |
| (1,754) | 1:11:A:TRP:HE3 | 1:13:A:LYS:HB3  | 23       | 0.26          |
| (1,754) | 1:11:A:TRP:HE3 | 1:13:A:LYS:HB3  | 24       | 0.26          |
| (1,749) | 1:34:A:TRP:HE1 | 2:88:B:PRO:HB2  | 14       | 0.26          |
| (1,718) | 1:24:A:TYR:HE1 | 1:37:A:PRO:HD2  | 25       | 0.26          |
| (1,718) | 1:24:A:TYR:HE2 | 1:37:A:PRO:HD2  | 25       | 0.26          |
| (1,714) | 1:13:A:LYS:H   | 1:24:A:TYR:HE1  | 11       | 0.26          |
| (1,714) | 1:13:A:LYS:H   | 1:24:A:TYR:HE2  | 11       | 0.26          |
| (1,674) | 2:86:B:PRO:HD3 | 1:14:A:ARG:HD2  | 5        | 0.26          |
| (1,652) | 1:8:A:PRO:HD2  | 1:9:A:PRO:HA    | 11       | 0.26          |
| (1,578) | 1:34:A:TRP:HH2 | 1:21:A:ARG:HD3  | 6        | 0.26          |
| (1,506) | 1:25:A:PHE:HE1 | 1:32:A:SER:HB3  | 7        | 0.26          |
| (1,506) | 1:25:A:PHE:HE2 | 1:32:A:SER:HB3  | 7        | 0.26          |
| (1,506) | 1:25:A:PHE:HE1 | 1:32:A:SER:HB3  | 21       | 0.26          |
| (1,506) | 1:25:A:PHE:HE2 | 1:32:A:SER:HB3  | 21       | 0.26          |
| (1,483) | 1:24:A:TYR:HD1 | 1:37:A:PRO:HB2  | 8        | 0.26          |
| (1,483) | 1:24:A:TYR:HD2 | 1:37:A:PRO:HB2  | 8        | 0.26          |
| (1,483) | 1:24:A:TYR:HD1 | 1:37:A:PRO:HB2  | 21       | 0.26          |
| (1,483) | 1:24:A:TYR:HD2 | 1:37:A:PRO:HB2  | 21       | 0.26          |
| (1,407) | 1:35:A:GLU:H   | 1:33:A:GLN:HE22 | 24       | 0.26          |
| (1,220) | 1:18:A:SER:HA  | 1:17:A:ARG:HD2  | 18       | 0.26          |
| (1,220) | 1:18:A:SER:HA  | 1:17:A:ARG:HD2  | 19       | 0.26          |
| (1,193) | 1:9:A:PRO:HD3  | 1:8:A:PRO:HG2   | 3        | 0.26          |
| (1,193) | 1:9:A:PRO:HD3  | 1:8:A:PRO:HG2   | 18       | 0.26          |
| (1,180) | 1:7:A:LEU:H    | 1:6:A:LYS:HE3   | 10       | 0.26          |
| (1,145) | 1:27:A:HIS:HE1 | 1:25:A:PHE:HD1  | 23       | 0.26          |
| (1,145) | 1:27:A:HIS:HE1 | 1:25:A:PHE:HD2  | 23       | 0.26          |
| (1,102) | 1:23:A:TYR:HE1 | 1:25:A:PHE:HB3  | 15       | 0.26          |
| (1,102) | 1:23:A:TYR:HE2 | 1:25:A:PHE:HB3  | 15       | 0.26          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,883) | 2:87:B:PHE:H   | 2:86:B:PRO:HA  | 11       | 0.25          |
| (1,881) | 2:89:B:GLU:HB2 | 2:90:B:GLY:HA2 | 14       | 0.25          |
| (1,832) | 1:11:A:TRP:HZ2 | 1:37:A:PRO:HD2 | 11       | 0.25          |
| (1,808) | 1:11:A:TRP:HE3 | 1:37:A:PRO:HD2 | 5        | 0.25          |
| (1,770) | 1:25:A:PHE:HE1 | 1:14:A:ARG:HD2 | 25       | 0.25          |
| (1,770) | 1:25:A:PHE:HE2 | 1:14:A:ARG:HD2 | 25       | 0.25          |
| (1,760) | 2:85:B:SEP:H   | 1:34:A:TRP:HZ2 | 5        | 0.25          |
| (1,760) | 2:85:B:SEP:H   | 1:34:A:TRP:HZ2 | 15       | 0.25          |
| (1,754) | 1:11:A:TRP:HE3 | 1:13:A:LYS:HB3 | 3        | 0.25          |
| (1,754) | 1:11:A:TRP:HE3 | 1:13:A:LYS:HB3 | 25       | 0.25          |
| (1,718) | 1:24:A:TYR:HE1 | 1:37:A:PRO:HD2 | 4        | 0.25          |
| (1,718) | 1:24:A:TYR:HE2 | 1:37:A:PRO:HD2 | 4        | 0.25          |
| (1,718) | 1:24:A:TYR:HE1 | 1:37:A:PRO:HD2 | 9        | 0.25          |
| (1,718) | 1:24:A:TYR:HE2 | 1:37:A:PRO:HD2 | 9        | 0.25          |
| (1,718) | 1:24:A:TYR:HE1 | 1:37:A:PRO:HD2 | 16       | 0.25          |
| (1,718) | 1:24:A:TYR:HE2 | 1:37:A:PRO:HD2 | 16       | 0.25          |
| (1,714) | 1:13:A:LYS:H   | 1:24:A:TYR:HE1 | 3        | 0.25          |
| (1,714) | 1:13:A:LYS:H   | 1:24:A:TYR:HE2 | 3        | 0.25          |
| (1,696) | 2:85:B:SEP:HB3 | 2:84:B:TYR:HB3 | 23       | 0.25          |
| (1,674) | 2:86:B:PRO:HD3 | 1:14:A:ARG:HD2 | 9        | 0.25          |
| (1,384) | 1:34:A:TRP:HE3 | 1:21:A:ARG:HG2 | 9        | 0.25          |
| (1,384) | 1:34:A:TRP:HE3 | 1:21:A:ARG:HG2 | 25       | 0.25          |
| (1,247) | 1:24:A:TYR:HE1 | 1:36:A:ARG:HD2 | 2        | 0.25          |
| (1,247) | 1:24:A:TYR:HE2 | 1:36:A:ARG:HD2 | 2        | 0.25          |
| (1,227) | 1:34:A:TRP:HE3 | 1:21:A:ARG:HB2 | 13       | 0.25          |
| (1,227) | 1:34:A:TRP:HE3 | 1:21:A:ARG:HB2 | 15       | 0.25          |
| (1,94)  | 1:34:A:TRP:HZ3 | 1:21:A:ARG:HG2 | 3        | 0.25          |
| (1,879) | 2:88:B:PRO:HD2 | 1:17:A:ARG:HD2 | 2        | 0.24          |
| (1,861) | 1:37:A:PRO:HD2 | 1:7:A:LEU:HD21 | 12       | 0.24          |
| (1,861) | 1:37:A:PRO:HD2 | 1:7:A:LEU:HD22 | 12       | 0.24          |
| (1,861) | 1:37:A:PRO:HD2 | 1:7:A:LEU:HD23 | 12       | 0.24          |
| (1,842) | 1:37:A:PRO:HD2 | 1:7:A:LEU:HD21 | 12       | 0.24          |
| (1,842) | 1:37:A:PRO:HD2 | 1:7:A:LEU:HD22 | 12       | 0.24          |
| (1,842) | 1:37:A:PRO:HD2 | 1:7:A:LEU:HD23 | 12       | 0.24          |
| (1,825) | 2:87:B:PHE:HE1 | 2:81:B:GLY:HA2 | 2        | 0.24          |
| (1,825) | 2:87:B:PHE:HE2 | 2:81:B:GLY:HA2 | 2        | 0.24          |
| (1,820) | 1:21:A:ARG:HB3 | 1:19:A:SER:HA  | 1        | 0.24          |
| (1,808) | 1:11:A:TRP:HE3 | 1:37:A:PRO:HD2 | 11       | 0.24          |
| (1,754) | 1:11:A:TRP:HE3 | 1:13:A:LYS:HB3 | 20       | 0.24          |
| (1,749) | 1:34:A:TRP:HE1 | 2:88:B:PRO:HB2 | 18       | 0.24          |
| (1,736) | 1:33:A:GLN:H   | 1:7:A:LEU:HD21 | 21       | 0.24          |
| (1,736) | 1:33:A:GLN:H   | 1:7:A:LEU:HD22 | 21       | 0.24          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,736) | 1:33:A:GLN:H   | 1:7:A:LEU:HD23  | 21       | 0.24          |
| (1,722) | 2:90:B:GLY:HA2 | 1:21:A:ARG:HG3  | 15       | 0.24          |
| (1,718) | 1:24:A:TYR:HE1 | 1:37:A:PRO:HD2  | 1        | 0.24          |
| (1,718) | 1:24:A:TYR:HE2 | 1:37:A:PRO:HD2  | 1        | 0.24          |
| (1,718) | 1:24:A:TYR:HE1 | 1:37:A:PRO:HD2  | 14       | 0.24          |
| (1,718) | 1:24:A:TYR:HE2 | 1:37:A:PRO:HD2  | 14       | 0.24          |
| (1,697) | 2:85:B:SEP:HB3 | 1:17:A:ARG:HA   | 24       | 0.24          |
| (1,676) | 1:8:A:PRO:HD3  | 1:7:A:LEU:HD11  | 3        | 0.24          |
| (1,676) | 1:8:A:PRO:HD3  | 1:7:A:LEU:HD12  | 3        | 0.24          |
| (1,676) | 1:8:A:PRO:HD3  | 1:7:A:LEU:HD13  | 3        | 0.24          |
| (1,506) | 1:25:A:PHE:HE1 | 1:32:A:SER:HB3  | 18       | 0.24          |
| (1,506) | 1:25:A:PHE:HE2 | 1:32:A:SER:HB3  | 18       | 0.24          |
| (1,506) | 1:25:A:PHE:HE1 | 1:32:A:SER:HB3  | 25       | 0.24          |
| (1,506) | 1:25:A:PHE:HE2 | 1:32:A:SER:HB3  | 25       | 0.24          |
| (1,493) | 1:24:A:TYR:HE1 | 1:7:A:LEU:HB3   | 17       | 0.24          |
| (1,493) | 1:24:A:TYR:HE2 | 1:7:A:LEU:HB3   | 17       | 0.24          |
| (1,468) | 2:85:B:SEP:H   | 1:14:A:ARG:HB3  | 24       | 0.24          |
| (1,430) | 1:24:A:TYR:HE1 | 1:37:A:PRO:HG2  | 16       | 0.24          |
| (1,430) | 1:24:A:TYR:HE2 | 1:37:A:PRO:HG2  | 16       | 0.24          |
| (1,407) | 1:35:A:GLU:H   | 1:33:A:GLN:HE22 | 20       | 0.24          |
| (1,21)  | 1:16:A:SER:H   | 1:15:A:MET:HG2  | 16       | 0.24          |
| (1,884) | 2:87:B:PHE:HD1 | 1:34:A:TRP:HB3  | 18       | 0.23          |
| (1,884) | 2:87:B:PHE:HD2 | 1:34:A:TRP:HB3  | 18       | 0.23          |
| (1,875) | 2:84:B:TYR:HD1 | 1:30:A:ASN:HD22 | 2        | 0.23          |
| (1,875) | 2:84:B:TYR:HD2 | 1:30:A:ASN:HD22 | 2        | 0.23          |
| (1,866) | 1:11:A:TRP:HB3 | 1:7:A:LEU:HD21  | 18       | 0.23          |
| (1,866) | 1:11:A:TRP:HB3 | 1:7:A:LEU:HD22  | 18       | 0.23          |
| (1,866) | 1:11:A:TRP:HB3 | 1:7:A:LEU:HD23  | 18       | 0.23          |
| (1,851) | 1:7:A:LEU:HD11 | 1:37:A:PRO:HD3  | 6        | 0.23          |
| (1,851) | 1:7:A:LEU:HD12 | 1:37:A:PRO:HD3  | 6        | 0.23          |
| (1,851) | 1:7:A:LEU:HD13 | 1:37:A:PRO:HD3  | 6        | 0.23          |
| (1,832) | 1:11:A:TRP:HZ2 | 1:37:A:PRO:HD2  | 12       | 0.23          |
| (1,825) | 2:87:B:PHE:HE1 | 2:81:B:GLY:HA2  | 21       | 0.23          |
| (1,825) | 2:87:B:PHE:HE2 | 2:81:B:GLY:HA2  | 21       | 0.23          |
| (1,808) | 1:11:A:TRP:HE3 | 1:37:A:PRO:HD2  | 2        | 0.23          |
| (1,760) | 2:85:B:SEP:H   | 1:34:A:TRP:HZ2  | 7        | 0.23          |
| (1,760) | 2:85:B:SEP:H   | 1:34:A:TRP:HZ2  | 10       | 0.23          |
| (1,754) | 1:11:A:TRP:HE3 | 1:13:A:LYS:HB3  | 1        | 0.23          |
| (1,736) | 1:33:A:GLN:H   | 1:7:A:LEU:HD21  | 13       | 0.23          |
| (1,736) | 1:33:A:GLN:H   | 1:7:A:LEU:HD22  | 13       | 0.23          |
| (1,736) | 1:33:A:GLN:H   | 1:7:A:LEU:HD23  | 13       | 0.23          |
| (1,718) | 1:24:A:TYR:HE1 | 1:37:A:PRO:HD2  | 15       | 0.23          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,718) | 1:24:A:TYR:HE2  | 1:37:A:PRO:HD2  | 15       | 0.23          |
| (1,676) | 1:8:A:PRO:HD3   | 1:7:A:LEU:HD11  | 1        | 0.23          |
| (1,676) | 1:8:A:PRO:HD3   | 1:7:A:LEU:HD12  | 1        | 0.23          |
| (1,676) | 1:8:A:PRO:HD3   | 1:7:A:LEU:HD13  | 1        | 0.23          |
| (1,674) | 2:86:B:PRO:HD3  | 1:14:A:ARG:HD2  | 22       | 0.23          |
| (1,639) | 2:84:B:TYR:HD1  | 1:14:A:ARG:HG2  | 13       | 0.23          |
| (1,639) | 2:84:B:TYR:HD2  | 1:14:A:ARG:HG2  | 13       | 0.23          |
| (1,544) | 1:11:A:TRP:HD1  | 1:7:A:LEU:HB2   | 25       | 0.23          |
| (1,506) | 1:25:A:PHE:HE1  | 1:32:A:SER:HB3  | 6        | 0.23          |
| (1,506) | 1:25:A:PHE:HE2  | 1:32:A:SER:HB3  | 6        | 0.23          |
| (1,506) | 1:25:A:PHE:HE1  | 1:32:A:SER:HB3  | 19       | 0.23          |
| (1,506) | 1:25:A:PHE:HE2  | 1:32:A:SER:HB3  | 19       | 0.23          |
| (1,493) | 1:24:A:TYR:HE1  | 1:7:A:LEU:HB3   | 22       | 0.23          |
| (1,493) | 1:24:A:TYR:HE2  | 1:7:A:LEU:HB3   | 22       | 0.23          |
| (1,480) | 1:33:A:GLN:HE21 | 1:35:A:GLU:HG2  | 13       | 0.23          |
| (1,343) | 1:25:A:PHE:H    | 1:14:A:ARG:HB3  | 6        | 0.23          |
| (1,254) | 1:11:A:TRP:HE1  | 1:37:A:PRO:HD3  | 18       | 0.23          |
| (1,227) | 1:34:A:TRP:HE3  | 1:21:A:ARG:HB2  | 25       | 0.23          |
| (1,129) | 1:7:A:LEU:HB2   | 1:8:A:PRO:HD3   | 5        | 0.23          |
| (1,94)  | 1:34:A:TRP:HZ3  | 1:21:A:ARG:HG2  | 11       | 0.23          |
| (1,75)  | 1:37:A:PRO:HD3  | 1:36:A:ARG:HD2  | 6        | 0.23          |
| (1,75)  | 1:37:A:PRO:HD3  | 1:36:A:ARG:HD2  | 15       | 0.23          |
| (1,861) | 1:37:A:PRO:HD2  | 1:7:A:LEU:HD21  | 5        | 0.22          |
| (1,861) | 1:37:A:PRO:HD2  | 1:7:A:LEU:HD22  | 5        | 0.22          |
| (1,861) | 1:37:A:PRO:HD2  | 1:7:A:LEU:HD23  | 5        | 0.22          |
| (1,857) | 1:28:A:ILE:HG13 | 1:31:A:ALA:HB1  | 18       | 0.22          |
| (1,857) | 1:28:A:ILE:HG13 | 1:31:A:ALA:HB2  | 18       | 0.22          |
| (1,857) | 1:28:A:ILE:HG13 | 1:31:A:ALA:HB3  | 18       | 0.22          |
| (1,856) | 1:7:A:LEU:HD11  | 1:36:A:ARG:HG3  | 13       | 0.22          |
| (1,856) | 1:7:A:LEU:HD12  | 1:36:A:ARG:HG3  | 13       | 0.22          |
| (1,856) | 1:7:A:LEU:HD13  | 1:36:A:ARG:HG3  | 13       | 0.22          |
| (1,842) | 1:37:A:PRO:HD2  | 1:7:A:LEU:HD21  | 5        | 0.22          |
| (1,842) | 1:37:A:PRO:HD2  | 1:7:A:LEU:HD22  | 5        | 0.22          |
| (1,842) | 1:37:A:PRO:HD2  | 1:7:A:LEU:HD23  | 5        | 0.22          |
| (1,832) | 1:11:A:TRP:HZ2  | 1:37:A:PRO:HD2  | 15       | 0.22          |
| (1,828) | 1:11:A:TRP:HZ2  | 1:29:A:THR:HG21 | 8        | 0.22          |
| (1,828) | 1:11:A:TRP:HZ2  | 1:29:A:THR:HG22 | 8        | 0.22          |
| (1,828) | 1:11:A:TRP:HZ2  | 1:29:A:THR:HG23 | 8        | 0.22          |
| (1,770) | 1:25:A:PHE:HE1  | 1:14:A:ARG:HD2  | 3        | 0.22          |
| (1,770) | 1:25:A:PHE:HE2  | 1:14:A:ARG:HD2  | 3        | 0.22          |
| (1,760) | 2:85:B:SEP:H    | 1:34:A:TRP:HZ2  | 12       | 0.22          |
| (1,754) | 1:11:A:TRP:HE3  | 1:13:A:LYS:HB3  | 17       | 0.22          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,718) | 1:24:A:TYR:HE1  | 1:37:A:PRO:HD2 | 12       | 0.22          |
| (1,718) | 1:24:A:TYR:HE2  | 1:37:A:PRO:HD2 | 12       | 0.22          |
| (1,718) | 1:24:A:TYR:HE1  | 1:37:A:PRO:HD2 | 23       | 0.22          |
| (1,718) | 1:24:A:TYR:HE2  | 1:37:A:PRO:HD2 | 23       | 0.22          |
| (1,715) | 1:16:A:SER:H    | 1:15:A:MET:HE1 | 16       | 0.22          |
| (1,715) | 1:16:A:SER:H    | 1:15:A:MET:HE2 | 16       | 0.22          |
| (1,715) | 1:16:A:SER:H    | 1:15:A:MET:HE3 | 16       | 0.22          |
| (1,697) | 2:85:B:SEP:HB3  | 1:17:A:ARG:HA  | 4        | 0.22          |
| (1,682) | 1:23:A:TYR:HB3  | 1:16:A:SER:HB3 | 6        | 0.22          |
| (1,652) | 1:8:A:PRO:HD2   | 1:9:A:PRO:HA   | 14       | 0.22          |
| (1,506) | 1:25:A:PHE:HE1  | 1:32:A:SER:HB3 | 15       | 0.22          |
| (1,506) | 1:25:A:PHE:HE2  | 1:32:A:SER:HB3 | 15       | 0.22          |
| (1,499) | 1:25:A:PHE:HE1  | 1:12:A:GLU:HG2 | 17       | 0.22          |
| (1,499) | 1:25:A:PHE:HE2  | 1:12:A:GLU:HG2 | 17       | 0.22          |
| (1,493) | 1:24:A:TYR:HE1  | 1:7:A:LEU:HB3  | 25       | 0.22          |
| (1,493) | 1:24:A:TYR:HE2  | 1:7:A:LEU:HB3  | 25       | 0.22          |
| (1,222) | 1:17:A:ARG:HA   | 1:17:A:ARG:HG2 | 1        | 0.22          |
| (1,222) | 1:17:A:ARG:HA   | 1:17:A:ARG:HG2 | 22       | 0.22          |
| (1,220) | 1:18:A:SER:HA   | 1:17:A:ARG:HD2 | 6        | 0.22          |
| (1,193) | 1:9:A:PRO:HD3   | 1:8:A:PRO:HG2  | 22       | 0.22          |
| (1,129) | 1:7:A:LEU:HB2   | 1:8:A:PRO:HD3  | 23       | 0.22          |
| (1,129) | 1:7:A:LEU:HB2   | 1:8:A:PRO:HD3  | 25       | 0.22          |
| (1,94)  | 1:34:A:TRP:HZ3  | 1:21:A:ARG:HG2 | 25       | 0.22          |
| (1,88)  | 1:33:A:GLN:HE21 | 1:37:A:PRO:HA  | 18       | 0.22          |
| (1,75)  | 1:37:A:PRO:HD3  | 1:36:A:ARG:HD2 | 13       | 0.22          |
| (1,12)  | 1:21:A:ARG:H    | 1:16:A:SER:HB2 | 18       | 0.22          |
| (1,884) | 2:87:B:PHE:HD1  | 1:34:A:TRP:HB3 | 19       | 0.21          |
| (1,884) | 2:87:B:PHE:HD2  | 1:34:A:TRP:HB3 | 19       | 0.21          |
| (1,881) | 2:89:B:GLU:HB2  | 2:90:B:GLY:HA2 | 3        | 0.21          |
| (1,881) | 2:89:B:GLU:HB2  | 2:90:B:GLY:HA2 | 15       | 0.21          |
| (1,866) | 1:11:A:TRP:HB3  | 1:7:A:LEU:HD21 | 2        | 0.21          |
| (1,866) | 1:11:A:TRP:HB3  | 1:7:A:LEU:HD22 | 2        | 0.21          |
| (1,866) | 1:11:A:TRP:HB3  | 1:7:A:LEU:HD23 | 2        | 0.21          |
| (1,861) | 1:37:A:PRO:HD2  | 1:7:A:LEU:HD21 | 8        | 0.21          |
| (1,861) | 1:37:A:PRO:HD2  | 1:7:A:LEU:HD22 | 8        | 0.21          |
| (1,861) | 1:37:A:PRO:HD2  | 1:7:A:LEU:HD23 | 8        | 0.21          |
| (1,861) | 1:37:A:PRO:HD2  | 1:7:A:LEU:HD21 | 21       | 0.21          |
| (1,861) | 1:37:A:PRO:HD2  | 1:7:A:LEU:HD22 | 21       | 0.21          |
| (1,861) | 1:37:A:PRO:HD2  | 1:7:A:LEU:HD23 | 21       | 0.21          |
| (1,861) | 1:37:A:PRO:HD2  | 1:7:A:LEU:HD21 | 23       | 0.21          |
| (1,861) | 1:37:A:PRO:HD2  | 1:7:A:LEU:HD22 | 23       | 0.21          |
| (1,861) | 1:37:A:PRO:HD2  | 1:7:A:LEU:HD23 | 23       | 0.21          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,842) | 1:37:A:PRO:HD2  | 1:7:A:LEU:HD21 | 8        | 0.21          |
| (1,842) | 1:37:A:PRO:HD2  | 1:7:A:LEU:HD22 | 8        | 0.21          |
| (1,842) | 1:37:A:PRO:HD2  | 1:7:A:LEU:HD23 | 8        | 0.21          |
| (1,842) | 1:37:A:PRO:HD2  | 1:7:A:LEU:HD21 | 21       | 0.21          |
| (1,842) | 1:37:A:PRO:HD2  | 1:7:A:LEU:HD22 | 21       | 0.21          |
| (1,842) | 1:37:A:PRO:HD2  | 1:7:A:LEU:HD23 | 21       | 0.21          |
| (1,842) | 1:37:A:PRO:HD2  | 1:7:A:LEU:HD21 | 23       | 0.21          |
| (1,842) | 1:37:A:PRO:HD2  | 1:7:A:LEU:HD22 | 23       | 0.21          |
| (1,842) | 1:37:A:PRO:HD2  | 1:7:A:LEU:HD23 | 23       | 0.21          |
| (1,832) | 1:11:A:TRP:HZ2  | 1:37:A:PRO:HD2 | 8        | 0.21          |
| (1,832) | 1:11:A:TRP:HZ2  | 1:37:A:PRO:HD2 | 21       | 0.21          |
| (1,832) | 1:11:A:TRP:HZ2  | 1:37:A:PRO:HD2 | 23       | 0.21          |
| (1,808) | 1:11:A:TRP:HE3  | 1:37:A:PRO:HD2 | 23       | 0.21          |
| (1,790) | 1:25:A:PHE:HZ   | 1:27:A:HIS:HB2 | 16       | 0.21          |
| (1,777) | 1:24:A:TYR:HE1  | 1:7:A:LEU:HA   | 6        | 0.21          |
| (1,777) | 1:24:A:TYR:HE2  | 1:7:A:LEU:HA   | 6        | 0.21          |
| (1,762) | 1:23:A:TYR:HE1  | 1:17:A:ARG:HG3 | 15       | 0.21          |
| (1,762) | 1:23:A:TYR:HE2  | 1:17:A:ARG:HG3 | 15       | 0.21          |
| (1,760) | 2:85:B:SEP:H    | 1:34:A:TRP:HZ2 | 4        | 0.21          |
| (1,760) | 2:85:B:SEP:H    | 1:34:A:TRP:HZ2 | 20       | 0.21          |
| (1,754) | 1:11:A:TRP:HE3  | 1:13:A:LYS:HB3 | 2        | 0.21          |
| (1,754) | 1:11:A:TRP:HE3  | 1:13:A:LYS:HB3 | 18       | 0.21          |
| (1,752) | 1:33:A:GLN:HE21 | 1:37:A:PRO:HD3 | 22       | 0.21          |
| (1,725) | 2:84:B:TYR:HB3  | 1:14:A:ARG:HD2 | 6        | 0.21          |
| (1,720) | 2:84:B:TYR:HE1  | 1:23:A:TYR:HE1 | 5        | 0.21          |
| (1,720) | 2:84:B:TYR:HE1  | 1:23:A:TYR:HE2 | 5        | 0.21          |
| (1,720) | 2:84:B:TYR:HE2  | 1:23:A:TYR:HE1 | 5        | 0.21          |
| (1,720) | 2:84:B:TYR:HE2  | 1:23:A:TYR:HE2 | 5        | 0.21          |
| (1,718) | 1:24:A:TYR:HE1  | 1:37:A:PRO:HD2 | 18       | 0.21          |
| (1,718) | 1:24:A:TYR:HE2  | 1:37:A:PRO:HD2 | 18       | 0.21          |
| (1,718) | 1:24:A:TYR:HE1  | 1:37:A:PRO:HD2 | 21       | 0.21          |
| (1,718) | 1:24:A:TYR:HE2  | 1:37:A:PRO:HD2 | 21       | 0.21          |
| (1,676) | 1:8:A:PRO:HD3   | 1:7:A:LEU:HD11 | 21       | 0.21          |
| (1,676) | 1:8:A:PRO:HD3   | 1:7:A:LEU:HD12 | 21       | 0.21          |
| (1,676) | 1:8:A:PRO:HD3   | 1:7:A:LEU:HD13 | 21       | 0.21          |
| (1,658) | 1:17:A:ARG:HD3  | 2:88:B:PRO:HD3 | 20       | 0.21          |
| (1,652) | 1:8:A:PRO:HD2   | 1:9:A:PRO:HA   | 9        | 0.21          |
| (1,622) | 1:33:A:GLN:HG2  | 1:24:A:TYR:HB3 | 8        | 0.21          |
| (1,480) | 1:33:A:GLN:HE21 | 1:35:A:GLU:HG2 | 19       | 0.21          |
| (1,468) | 2:85:B:SEP:H    | 1:14:A:ARG:HB3 | 9        | 0.21          |
| (1,379) | 1:40:A:ASN:H    | 1:9:A:PRO:HD3  | 22       | 0.21          |
| (1,291) | 1:25:A:PHE:HE1  | 1:32:A:SER:HB2 | 1        | 0.21          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,291) | 1:25:A:PHE:HE2  | 1:32:A:SER:HB2 | 1        | 0.21          |
| (1,291) | 1:25:A:PHE:HE1  | 1:32:A:SER:HB2 | 3        | 0.21          |
| (1,291) | 1:25:A:PHE:HE2  | 1:32:A:SER:HB2 | 3        | 0.21          |
| (1,291) | 1:25:A:PHE:HE1  | 1:32:A:SER:HB2 | 16       | 0.21          |
| (1,291) | 1:25:A:PHE:HE2  | 1:32:A:SER:HB2 | 16       | 0.21          |
| (1,227) | 1:34:A:TRP:HE3  | 1:21:A:ARG:HB2 | 10       | 0.21          |
| (1,220) | 1:18:A:SER:HA   | 1:17:A:ARG:HD2 | 9        | 0.21          |
| (1,94)  | 1:34:A:TRP:HZ3  | 1:21:A:ARG:HG2 | 4        | 0.21          |
| (1,87)  | 1:23:A:TYR:HE1  | 1:16:A:SER:HB3 | 7        | 0.21          |
| (1,87)  | 1:23:A:TYR:HE2  | 1:16:A:SER:HB3 | 7        | 0.21          |
| (1,26)  | 1:22:A:VAL:H    | 1:21:A:ARG:HG3 | 4        | 0.21          |
| (1,12)  | 1:21:A:ARG:H    | 1:16:A:SER:HB2 | 17       | 0.21          |
| (1,876) | 1:27:A:HIS:HD2  | 1:11:A:TRP:H   | 23       | 0.2           |
| (1,851) | 1:7:A:LEU:HD11  | 1:37:A:PRO:HD3 | 24       | 0.2           |
| (1,851) | 1:7:A:LEU:HD12  | 1:37:A:PRO:HD3 | 24       | 0.2           |
| (1,851) | 1:7:A:LEU:HD13  | 1:37:A:PRO:HD3 | 24       | 0.2           |
| (1,832) | 1:11:A:TRP:HZ2  | 1:37:A:PRO:HD2 | 9        | 0.2           |
| (1,807) | 1:25:A:PHE:HZ   | 2:83:B:PRO:HB3 | 7        | 0.2           |
| (1,777) | 1:24:A:TYR:HE1  | 1:7:A:LEU:HA   | 4        | 0.2           |
| (1,777) | 1:24:A:TYR:HE2  | 1:7:A:LEU:HA   | 4        | 0.2           |
| (1,769) | 1:25:A:PHE:HE1  | 2:83:B:PRO:HB3 | 25       | 0.2           |
| (1,769) | 1:25:A:PHE:HE2  | 2:83:B:PRO:HB3 | 25       | 0.2           |
| (1,752) | 1:33:A:GLN:HE21 | 1:37:A:PRO:HD3 | 7        | 0.2           |
| (1,714) | 1:13:A:LYS:H    | 1:24:A:TYR:HE1 | 16       | 0.2           |
| (1,714) | 1:13:A:LYS:H    | 1:24:A:TYR:HE2 | 16       | 0.2           |
| (1,707) | 1:17:A:ARG:HD3  | 2:88:B:PRO:HD3 | 5        | 0.2           |
| (1,697) | 2:85:B:SEP:HB3  | 1:17:A:ARG:HA  | 3        | 0.2           |
| (1,683) | 2:83:B:PRO:HD2  | 2:84:B:TYR:HB3 | 7        | 0.2           |
| (1,652) | 1:8:A:PRO:HD2   | 1:9:A:PRO:HA   | 5        | 0.2           |
| (1,652) | 1:8:A:PRO:HD2   | 1:9:A:PRO:HA   | 13       | 0.2           |
| (1,639) | 2:84:B:TYR:HD1  | 1:14:A:ARG:HG2 | 8        | 0.2           |
| (1,639) | 2:84:B:TYR:HD2  | 1:14:A:ARG:HG2 | 8        | 0.2           |
| (1,605) | 1:33:A:GLN:HE22 | 1:24:A:TYR:HB3 | 2        | 0.2           |
| (1,547) | 1:11:A:TRP:HD1  | 1:7:A:LEU:HD11 | 25       | 0.2           |
| (1,547) | 1:11:A:TRP:HD1  | 1:7:A:LEU:HD12 | 25       | 0.2           |
| (1,547) | 1:11:A:TRP:HD1  | 1:7:A:LEU:HD13 | 25       | 0.2           |
| (1,499) | 1:25:A:PHE:HE1  | 1:12:A:GLU:HG2 | 22       | 0.2           |
| (1,499) | 1:25:A:PHE:HE2  | 1:12:A:GLU:HG2 | 22       | 0.2           |
| (1,437) | 1:11:A:TRP:HD1  | 1:37:A:PRO:HG3 | 24       | 0.2           |
| (1,362) | 1:7:A:LEU:H     | 1:36:A:ARG:HG3 | 24       | 0.2           |
| (1,291) | 1:25:A:PHE:HE1  | 1:32:A:SER:HB2 | 11       | 0.2           |
| (1,291) | 1:25:A:PHE:HE2  | 1:32:A:SER:HB2 | 11       | 0.2           |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,247) | 1:24:A:TYR:HE1 | 1:36:A:ARG:HD2  | 19       | 0.2           |
| (1,247) | 1:24:A:TYR:HE2 | 1:36:A:ARG:HD2  | 19       | 0.2           |
| (1,222) | 1:17:A:ARG:HA  | 1:17:A:ARG:HG2  | 15       | 0.2           |
| (1,87)  | 1:23:A:TYR:HE1 | 1:16:A:SER:HB3  | 15       | 0.2           |
| (1,87)  | 1:23:A:TYR:HE2 | 1:16:A:SER:HB3  | 15       | 0.2           |
| (1,24)  | 1:13:A:LYS:HE2 | 1:22:A:VAL:HG11 | 9        | 0.2           |
| (1,24)  | 1:13:A:LYS:HE2 | 1:22:A:VAL:HG12 | 9        | 0.2           |
| (1,24)  | 1:13:A:LYS:HE2 | 1:22:A:VAL:HG13 | 9        | 0.2           |
| (1,884) | 2:87:B:PHE:HD1 | 1:34:A:TRP:HB3  | 5        | 0.19          |
| (1,884) | 2:87:B:PHE:HD2 | 1:34:A:TRP:HB3  | 5        | 0.19          |
| (1,884) | 2:87:B:PHE:HD1 | 1:34:A:TRP:HB3  | 9        | 0.19          |
| (1,884) | 2:87:B:PHE:HD2 | 1:34:A:TRP:HB3  | 9        | 0.19          |
| (1,884) | 2:87:B:PHE:HD1 | 1:34:A:TRP:HB3  | 10       | 0.19          |
| (1,884) | 2:87:B:PHE:HD2 | 1:34:A:TRP:HB3  | 10       | 0.19          |
| (1,884) | 2:87:B:PHE:HD1 | 1:34:A:TRP:HB3  | 14       | 0.19          |
| (1,884) | 2:87:B:PHE:HD2 | 1:34:A:TRP:HB3  | 14       | 0.19          |
| (1,884) | 2:87:B:PHE:HD1 | 1:34:A:TRP:HB3  | 21       | 0.19          |
| (1,884) | 2:87:B:PHE:HD2 | 1:34:A:TRP:HB3  | 21       | 0.19          |
| (1,884) | 2:87:B:PHE:HD1 | 1:34:A:TRP:HB3  | 23       | 0.19          |
| (1,884) | 2:87:B:PHE:HD2 | 1:34:A:TRP:HB3  | 23       | 0.19          |
| (1,881) | 2:89:B:GLU:HB2 | 2:90:B:GLY:HA2  | 2        | 0.19          |
| (1,861) | 1:37:A:PRO:HD2 | 1:7:A:LEU:HD21  | 16       | 0.19          |
| (1,861) | 1:37:A:PRO:HD2 | 1:7:A:LEU:HD22  | 16       | 0.19          |
| (1,861) | 1:37:A:PRO:HD2 | 1:7:A:LEU:HD23  | 16       | 0.19          |
| (1,856) | 1:7:A:LEU:HD11 | 1:36:A:ARG:HG3  | 10       | 0.19          |
| (1,856) | 1:7:A:LEU:HD12 | 1:36:A:ARG:HG3  | 10       | 0.19          |
| (1,856) | 1:7:A:LEU:HD13 | 1:36:A:ARG:HG3  | 10       | 0.19          |
| (1,842) | 1:37:A:PRO:HD2 | 1:7:A:LEU:HD21  | 16       | 0.19          |
| (1,842) | 1:37:A:PRO:HD2 | 1:7:A:LEU:HD22  | 16       | 0.19          |
| (1,842) | 1:37:A:PRO:HD2 | 1:7:A:LEU:HD23  | 16       | 0.19          |
| (1,825) | 2:87:B:PHE:HE1 | 2:81:B:GLY:HA2  | 14       | 0.19          |
| (1,825) | 2:87:B:PHE:HE2 | 2:81:B:GLY:HA2  | 14       | 0.19          |
| (1,815) | 1:7:A:LEU:HD11 | 1:8:A:PRO:HA    | 21       | 0.19          |
| (1,815) | 1:7:A:LEU:HD12 | 1:8:A:PRO:HA    | 21       | 0.19          |
| (1,815) | 1:7:A:LEU:HD13 | 1:8:A:PRO:HA    | 21       | 0.19          |
| (1,783) | 1:34:A:TRP:HZ3 | 2:85:B:SEP:HB2  | 7        | 0.19          |
| (1,777) | 1:24:A:TYR:HE1 | 1:7:A:LEU:HA    | 12       | 0.19          |
| (1,777) | 1:24:A:TYR:HE2 | 1:7:A:LEU:HA    | 12       | 0.19          |
| (1,762) | 1:23:A:TYR:HE1 | 1:17:A:ARG:HG3  | 7        | 0.19          |
| (1,762) | 1:23:A:TYR:HE2 | 1:17:A:ARG:HG3  | 7        | 0.19          |
| (1,760) | 2:85:B:SEP:H   | 1:34:A:TRP:HZ2  | 1        | 0.19          |
| (1,760) | 2:85:B:SEP:H   | 1:34:A:TRP:HZ2  | 25       | 0.19          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,714) | 1:13:A:LYS:H    | 1:24:A:TYR:HE1  | 12       | 0.19          |
| (1,714) | 1:13:A:LYS:H    | 1:24:A:TYR:HE2  | 12       | 0.19          |
| (1,710) | 1:34:A:TRP:HB3  | 2:86:B:PRO:HD2  | 8        | 0.19          |
| (1,652) | 1:8:A:PRO:HD2   | 1:9:A:PRO:HA    | 2        | 0.19          |
| (1,652) | 1:8:A:PRO:HD2   | 1:9:A:PRO:HA    | 25       | 0.19          |
| (1,644) | 2:85:B:SEP:HB2  | 1:17:A:ARG:HD2  | 17       | 0.19          |
| (1,643) | 2:85:B:SEP:HB2  | 1:17:A:ARG:HG2  | 9        | 0.19          |
| (1,578) | 1:34:A:TRP:HH2  | 1:21:A:ARG:HD3  | 18       | 0.19          |
| (1,516) | 1:11:A:TRP:HH2  | 1:37:A:PRO:HD2  | 19       | 0.19          |
| (1,515) | 1:34:A:TRP:HZ3  | 2:88:B:PRO:HB3  | 15       | 0.19          |
| (1,515) | 1:34:A:TRP:HZ3  | 2:88:B:PRO:HB3  | 20       | 0.19          |
| (1,480) | 1:33:A:GLN:HE21 | 1:35:A:GLU:HG2  | 17       | 0.19          |
| (1,417) | 1:11:A:TRP:HE3  | 1:26:A:ASN:HB3  | 13       | 0.19          |
| (1,407) | 1:35:A:GLU:H    | 1:33:A:GLN:HE22 | 6        | 0.19          |
| (1,296) | 1:26:A:ASN:HD22 | 1:10:A:GLY:HA2  | 1        | 0.19          |
| (1,247) | 1:24:A:TYR:HE1  | 1:36:A:ARG:HD2  | 4        | 0.19          |
| (1,247) | 1:24:A:TYR:HE2  | 1:36:A:ARG:HD2  | 4        | 0.19          |
| (1,222) | 1:17:A:ARG:HA   | 1:17:A:ARG:HG2  | 2        | 0.19          |
| (1,220) | 1:18:A:SER:HA   | 1:17:A:ARG:HD2  | 14       | 0.19          |
| (1,220) | 1:18:A:SER:HA   | 1:17:A:ARG:HD2  | 25       | 0.19          |
| (1,167) | 2:84:B:TYR:HD1  | 2:85:B:SEP:HB2  | 9        | 0.19          |
| (1,167) | 2:84:B:TYR:HD2  | 2:85:B:SEP:HB2  | 9        | 0.19          |
| (1,129) | 1:7:A:LEU:HB2   | 1:8:A:PRO:HD3   | 6        | 0.19          |
| (1,102) | 1:23:A:TYR:HE1  | 1:25:A:PHE:HB3  | 20       | 0.19          |
| (1,102) | 1:23:A:TYR:HE2  | 1:25:A:PHE:HB3  | 20       | 0.19          |
| (1,884) | 2:87:B:PHE:HD1  | 1:34:A:TRP:HB3  | 3        | 0.18          |
| (1,884) | 2:87:B:PHE:HD2  | 1:34:A:TRP:HB3  | 3        | 0.18          |
| (1,884) | 2:87:B:PHE:HD1  | 1:34:A:TRP:HB3  | 11       | 0.18          |
| (1,884) | 2:87:B:PHE:HD2  | 1:34:A:TRP:HB3  | 11       | 0.18          |
| (1,884) | 2:87:B:PHE:HD1  | 1:34:A:TRP:HB3  | 22       | 0.18          |
| (1,884) | 2:87:B:PHE:HD2  | 1:34:A:TRP:HB3  | 22       | 0.18          |
| (1,884) | 2:87:B:PHE:HD1  | 1:34:A:TRP:HB3  | 25       | 0.18          |
| (1,884) | 2:87:B:PHE:HD2  | 1:34:A:TRP:HB3  | 25       | 0.18          |
| (1,881) | 2:89:B:GLU:HB2  | 2:90:B:GLY:HA2  | 18       | 0.18          |
| (1,861) | 1:37:A:PRO:HD2  | 1:7:A:LEU:HD21  | 24       | 0.18          |
| (1,861) | 1:37:A:PRO:HD2  | 1:7:A:LEU:HD22  | 24       | 0.18          |
| (1,861) | 1:37:A:PRO:HD2  | 1:7:A:LEU:HD23  | 24       | 0.18          |
| (1,842) | 1:37:A:PRO:HD2  | 1:7:A:LEU:HD21  | 24       | 0.18          |
| (1,842) | 1:37:A:PRO:HD2  | 1:7:A:LEU:HD22  | 24       | 0.18          |
| (1,842) | 1:37:A:PRO:HD2  | 1:7:A:LEU:HD23  | 24       | 0.18          |
| (1,825) | 2:87:B:PHE:HE1  | 2:81:B:GLY:HA2  | 22       | 0.18          |
| (1,825) | 2:87:B:PHE:HE2  | 2:81:B:GLY:HA2  | 22       | 0.18          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,760) | 2:85:B:SEP:H    | 1:34:A:TRP:HZ2 | 2        | 0.18          |
| (1,760) | 2:85:B:SEP:H    | 1:34:A:TRP:HZ2 | 8        | 0.18          |
| (1,760) | 2:85:B:SEP:H    | 1:34:A:TRP:HZ2 | 23       | 0.18          |
| (1,754) | 1:11:A:TRP:HE3  | 1:13:A:LYS:HB3 | 8        | 0.18          |
| (1,720) | 2:84:B:TYR:HE1  | 1:23:A:TYR:HE1 | 18       | 0.18          |
| (1,720) | 2:84:B:TYR:HE1  | 1:23:A:TYR:HE2 | 18       | 0.18          |
| (1,720) | 2:84:B:TYR:HE2  | 1:23:A:TYR:HE1 | 18       | 0.18          |
| (1,720) | 2:84:B:TYR:HE2  | 1:23:A:TYR:HE2 | 18       | 0.18          |
| (1,714) | 1:13:A:LYS:H    | 1:24:A:TYR:HE1 | 24       | 0.18          |
| (1,714) | 1:13:A:LYS:H    | 1:24:A:TYR:HE2 | 24       | 0.18          |
| (1,697) | 2:85:B:SEP:HB3  | 1:17:A:ARG:HA  | 9        | 0.18          |
| (1,697) | 2:85:B:SEP:HB3  | 1:17:A:ARG:HA  | 10       | 0.18          |
| (1,683) | 2:83:B:PRO:HD2  | 2:84:B:TYR:HB3 | 3        | 0.18          |
| (1,652) | 1:8:A:PRO:HD2   | 1:9:A:PRO:HA   | 16       | 0.18          |
| (1,605) | 1:33:A:GLN:HE22 | 1:24:A:TYR:HB3 | 1        | 0.18          |
| (1,562) | 1:34:A:TRP:HZ2  | 1:16:A:SER:HB3 | 18       | 0.18          |
| (1,557) | 2:84:B:TYR:HD1  | 2:82:B:SER:HA  | 6        | 0.18          |
| (1,557) | 2:84:B:TYR:HD2  | 2:82:B:SER:HA  | 6        | 0.18          |
| (1,515) | 1:34:A:TRP:HZ3  | 2:88:B:PRO:HB3 | 3        | 0.18          |
| (1,515) | 1:34:A:TRP:HZ3  | 2:88:B:PRO:HB3 | 23       | 0.18          |
| (1,430) | 1:24:A:TYR:HE1  | 1:37:A:PRO:HG2 | 17       | 0.18          |
| (1,430) | 1:24:A:TYR:HE2  | 1:37:A:PRO:HG2 | 17       | 0.18          |
| (1,430) | 1:24:A:TYR:HE1  | 1:37:A:PRO:HG2 | 18       | 0.18          |
| (1,430) | 1:24:A:TYR:HE2  | 1:37:A:PRO:HG2 | 18       | 0.18          |
| (1,291) | 1:25:A:PHE:HE1  | 1:32:A:SER:HB2 | 22       | 0.18          |
| (1,291) | 1:25:A:PHE:HE2  | 1:32:A:SER:HB2 | 22       | 0.18          |
| (1,222) | 1:17:A:ARG:HA   | 1:17:A:ARG:HG2 | 7        | 0.18          |
| (1,129) | 1:7:A:LEU:HB2   | 1:8:A:PRO:HD3  | 16       | 0.18          |
| (1,88)  | 1:33:A:GLN:HE21 | 1:37:A:PRO:HA  | 8        | 0.18          |
| (1,75)  | 1:37:A:PRO:HD3  | 1:36:A:ARG:HD2 | 20       | 0.18          |
| (1,26)  | 1:22:A:VAL:H    | 1:21:A:ARG:HG3 | 23       | 0.18          |
| (1,884) | 2:87:B:PHE:HD1  | 1:34:A:TRP:HB3 | 2        | 0.17          |
| (1,884) | 2:87:B:PHE:HD2  | 1:34:A:TRP:HB3 | 2        | 0.17          |
| (1,884) | 2:87:B:PHE:HD1  | 1:34:A:TRP:HB3 | 6        | 0.17          |
| (1,884) | 2:87:B:PHE:HD2  | 1:34:A:TRP:HB3 | 6        | 0.17          |
| (1,884) | 2:87:B:PHE:HD1  | 1:34:A:TRP:HB3 | 15       | 0.17          |
| (1,884) | 2:87:B:PHE:HD2  | 1:34:A:TRP:HB3 | 15       | 0.17          |
| (1,863) | 1:8:A:PRO:HD2   | 1:7:A:LEU:HD11 | 13       | 0.17          |
| (1,863) | 1:8:A:PRO:HD2   | 1:7:A:LEU:HD12 | 13       | 0.17          |
| (1,863) | 1:8:A:PRO:HD2   | 1:7:A:LEU:HD13 | 13       | 0.17          |
| (1,861) | 1:37:A:PRO:HD2  | 1:7:A:LEU:HD21 | 20       | 0.17          |
| (1,861) | 1:37:A:PRO:HD2  | 1:7:A:LEU:HD22 | 20       | 0.17          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,861) | 1:37:A:PRO:HD2  | 1:7:A:LEU:HD23 | 20       | 0.17          |
| (1,857) | 1:28:A:ILE:HG13 | 1:31:A:ALA:HB1 | 5        | 0.17          |
| (1,857) | 1:28:A:ILE:HG13 | 1:31:A:ALA:HB2 | 5        | 0.17          |
| (1,857) | 1:28:A:ILE:HG13 | 1:31:A:ALA:HB3 | 5        | 0.17          |
| (1,857) | 1:28:A:ILE:HG13 | 1:31:A:ALA:HB1 | 16       | 0.17          |
| (1,857) | 1:28:A:ILE:HG13 | 1:31:A:ALA:HB2 | 16       | 0.17          |
| (1,857) | 1:28:A:ILE:HG13 | 1:31:A:ALA:HB3 | 16       | 0.17          |
| (1,857) | 1:28:A:ILE:HG13 | 1:31:A:ALA:HB1 | 24       | 0.17          |
| (1,857) | 1:28:A:ILE:HG13 | 1:31:A:ALA:HB2 | 24       | 0.17          |
| (1,857) | 1:28:A:ILE:HG13 | 1:31:A:ALA:HB3 | 24       | 0.17          |
| (1,849) | 1:14:A:ARG:HB3  | 1:15:A:MET:HG3 | 4        | 0.17          |
| (1,842) | 1:37:A:PRO:HD2  | 1:7:A:LEU:HD21 | 20       | 0.17          |
| (1,842) | 1:37:A:PRO:HD2  | 1:7:A:LEU:HD22 | 20       | 0.17          |
| (1,842) | 1:37:A:PRO:HD2  | 1:7:A:LEU:HD23 | 20       | 0.17          |
| (1,808) | 1:11:A:TRP:HE3  | 1:37:A:PRO:HD2 | 15       | 0.17          |
| (1,798) | 1:34:A:TRP:HZ2  | 1:18:A:SER:HB3 | 3        | 0.17          |
| (1,790) | 1:25:A:PHE:HZ   | 1:27:A:HIS:HB2 | 9        | 0.17          |
| (1,790) | 1:25:A:PHE:HZ   | 1:27:A:HIS:HB2 | 19       | 0.17          |
| (1,777) | 1:24:A:TYR:HE1  | 1:7:A:LEU:HA   | 18       | 0.17          |
| (1,777) | 1:24:A:TYR:HE2  | 1:7:A:LEU:HA   | 18       | 0.17          |
| (1,777) | 1:24:A:TYR:HE1  | 1:7:A:LEU:HA   | 22       | 0.17          |
| (1,777) | 1:24:A:TYR:HE2  | 1:7:A:LEU:HA   | 22       | 0.17          |
| (1,776) | 1:24:A:TYR:HD1  | 1:7:A:LEU:HA   | 14       | 0.17          |
| (1,776) | 1:24:A:TYR:HD2  | 1:7:A:LEU:HA   | 14       | 0.17          |
| (1,775) | 2:84:B:TYR:HE1  | 2:82:B:SER:HA  | 7        | 0.17          |
| (1,775) | 2:84:B:TYR:HE2  | 2:82:B:SER:HA  | 7        | 0.17          |
| (1,775) | 2:84:B:TYR:HE1  | 2:82:B:SER:HA  | 18       | 0.17          |
| (1,775) | 2:84:B:TYR:HE2  | 2:82:B:SER:HA  | 18       | 0.17          |
| (1,762) | 1:23:A:TYR:HE1  | 1:17:A:ARG:HG3 | 12       | 0.17          |
| (1,762) | 1:23:A:TYR:HE2  | 1:17:A:ARG:HG3 | 12       | 0.17          |
| (1,760) | 2:85:B:SEP:H    | 1:34:A:TRP:HZ2 | 21       | 0.17          |
| (1,760) | 2:85:B:SEP:H    | 1:34:A:TRP:HZ2 | 22       | 0.17          |
| (1,756) | 1:41:A:SER:H    | 1:6:A:LYS:HB2  | 21       | 0.17          |
| (1,754) | 1:11:A:TRP:HE3  | 1:13:A:LYS:HB3 | 19       | 0.17          |
| (1,736) | 1:33:A:GLN:H    | 1:7:A:LEU:HD21 | 2        | 0.17          |
| (1,736) | 1:33:A:GLN:H    | 1:7:A:LEU:HD22 | 2        | 0.17          |
| (1,736) | 1:33:A:GLN:H    | 1:7:A:LEU:HD23 | 2        | 0.17          |
| (1,719) | 1:23:A:TYR:HD1  | 2:85:B:SEP:HB2 | 17       | 0.17          |
| (1,719) | 1:23:A:TYR:HD2  | 2:85:B:SEP:HB2 | 17       | 0.17          |
| (1,718) | 1:24:A:TYR:HE1  | 1:37:A:PRO:HD2 | 5        | 0.17          |
| (1,718) | 1:24:A:TYR:HE2  | 1:37:A:PRO:HD2 | 5        | 0.17          |
| (1,713) | 1:12:A:GLU:H    | 1:24:A:TYR:HD1 | 9        | 0.17          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,713) | 1:12:A:GLU:H    | 1:24:A:TYR:HD2 | 9        | 0.17          |
| (1,683) | 2:83:B:PRO:HD2  | 2:84:B:TYR:HB3 | 15       | 0.17          |
| (1,682) | 1:23:A:TYR:HB3  | 1:16:A:SER:HB3 | 14       | 0.17          |
| (1,652) | 1:8:A:PRO:HD2   | 1:9:A:PRO:HA   | 10       | 0.17          |
| (1,633) | 1:18:A:SER:HB2  | 1:17:A:ARG:HB3 | 24       | 0.17          |
| (1,547) | 1:11:A:TRP:HD1  | 1:7:A:LEU:HD11 | 11       | 0.17          |
| (1,547) | 1:11:A:TRP:HD1  | 1:7:A:LEU:HD12 | 11       | 0.17          |
| (1,547) | 1:11:A:TRP:HD1  | 1:7:A:LEU:HD13 | 11       | 0.17          |
| (1,515) | 1:34:A:TRP:HZ3  | 2:88:B:PRO:HB3 | 25       | 0.17          |
| (1,513) | 1:34:A:TRP:HZ3  | 2:86:B:PRO:HG2 | 24       | 0.17          |
| (1,493) | 1:24:A:TYR:HE1  | 1:7:A:LEU:HB3  | 2        | 0.17          |
| (1,493) | 1:24:A:TYR:HE2  | 1:7:A:LEU:HB3  | 2        | 0.17          |
| (1,483) | 1:24:A:TYR:HD1  | 1:37:A:PRO:HB2 | 1        | 0.17          |
| (1,483) | 1:24:A:TYR:HD2  | 1:37:A:PRO:HB2 | 1        | 0.17          |
| (1,430) | 1:24:A:TYR:HE1  | 1:37:A:PRO:HG2 | 6        | 0.17          |
| (1,430) | 1:24:A:TYR:HE2  | 1:37:A:PRO:HG2 | 6        | 0.17          |
| (1,430) | 1:24:A:TYR:HE1  | 1:37:A:PRO:HG2 | 11       | 0.17          |
| (1,430) | 1:24:A:TYR:HE2  | 1:37:A:PRO:HG2 | 11       | 0.17          |
| (1,291) | 1:25:A:PHE:HE1  | 1:32:A:SER:HB2 | 4        | 0.17          |
| (1,291) | 1:25:A:PHE:HE2  | 1:32:A:SER:HB2 | 4        | 0.17          |
| (1,291) | 1:25:A:PHE:HE1  | 1:32:A:SER:HB2 | 9        | 0.17          |
| (1,291) | 1:25:A:PHE:HE2  | 1:32:A:SER:HB2 | 9        | 0.17          |
| (1,258) | 1:33:A:GLN:H    | 1:24:A:TYR:HD1 | 9        | 0.17          |
| (1,258) | 1:33:A:GLN:H    | 1:24:A:TYR:HD2 | 9        | 0.17          |
| (1,247) | 1:24:A:TYR:HE1  | 1:36:A:ARG:HD2 | 25       | 0.17          |
| (1,247) | 1:24:A:TYR:HE2  | 1:36:A:ARG:HD2 | 25       | 0.17          |
| (1,222) | 1:17:A:ARG:HA   | 1:17:A:ARG:HG2 | 14       | 0.17          |
| (1,222) | 1:17:A:ARG:HA   | 1:17:A:ARG:HG2 | 24       | 0.17          |
| (1,220) | 1:18:A:SER:HA   | 1:17:A:ARG:HD2 | 8        | 0.17          |
| (1,210) | 1:12:A:GLU:H    | 1:11:A:TRP:HB2 | 4        | 0.17          |
| (1,100) | 1:33:A:GLN:HE22 | 1:33:A:GLN:HG2 | 2        | 0.17          |
| (1,100) | 1:33:A:GLN:HE22 | 1:33:A:GLN:HG2 | 3        | 0.17          |
| (1,88)  | 1:33:A:GLN:HE21 | 1:37:A:PRO:HA  | 12       | 0.17          |
| (1,12)  | 1:21:A:ARG:H    | 1:16:A:SER:HB2 | 11       | 0.17          |
| (1,884) | 2:87:B:PHE:HD1  | 1:34:A:TRP:HB3 | 1        | 0.16          |
| (1,884) | 2:87:B:PHE:HD2  | 1:34:A:TRP:HB3 | 1        | 0.16          |
| (1,884) | 2:87:B:PHE:HD1  | 1:34:A:TRP:HB3 | 12       | 0.16          |
| (1,884) | 2:87:B:PHE:HD2  | 1:34:A:TRP:HB3 | 12       | 0.16          |
| (1,884) | 2:87:B:PHE:HD1  | 1:34:A:TRP:HB3 | 16       | 0.16          |
| (1,884) | 2:87:B:PHE:HD2  | 1:34:A:TRP:HB3 | 16       | 0.16          |
| (1,884) | 2:87:B:PHE:HD1  | 1:34:A:TRP:HB3 | 20       | 0.16          |
| (1,884) | 2:87:B:PHE:HD2  | 1:34:A:TRP:HB3 | 20       | 0.16          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,881) | 2:89:B:GLU:HB2  | 2:90:B:GLY:HA2 | 16       | 0.16          |
| (1,881) | 2:89:B:GLU:HB2  | 2:90:B:GLY:HA2 | 25       | 0.16          |
| (1,857) | 1:28:A:ILE:HG13 | 1:31:A:ALA:HB1 | 2        | 0.16          |
| (1,857) | 1:28:A:ILE:HG13 | 1:31:A:ALA:HB2 | 2        | 0.16          |
| (1,857) | 1:28:A:ILE:HG13 | 1:31:A:ALA:HB3 | 2        | 0.16          |
| (1,857) | 1:28:A:ILE:HG13 | 1:31:A:ALA:HB1 | 3        | 0.16          |
| (1,857) | 1:28:A:ILE:HG13 | 1:31:A:ALA:HB2 | 3        | 0.16          |
| (1,857) | 1:28:A:ILE:HG13 | 1:31:A:ALA:HB3 | 3        | 0.16          |
| (1,857) | 1:28:A:ILE:HG13 | 1:31:A:ALA:HB1 | 7        | 0.16          |
| (1,857) | 1:28:A:ILE:HG13 | 1:31:A:ALA:HB2 | 7        | 0.16          |
| (1,857) | 1:28:A:ILE:HG13 | 1:31:A:ALA:HB3 | 7        | 0.16          |
| (1,857) | 1:28:A:ILE:HG13 | 1:31:A:ALA:HB1 | 20       | 0.16          |
| (1,857) | 1:28:A:ILE:HG13 | 1:31:A:ALA:HB2 | 20       | 0.16          |
| (1,857) | 1:28:A:ILE:HG13 | 1:31:A:ALA:HB3 | 20       | 0.16          |
| (1,857) | 1:28:A:ILE:HG13 | 1:31:A:ALA:HB1 | 21       | 0.16          |
| (1,857) | 1:28:A:ILE:HG13 | 1:31:A:ALA:HB2 | 21       | 0.16          |
| (1,857) | 1:28:A:ILE:HG13 | 1:31:A:ALA:HB3 | 21       | 0.16          |
| (1,851) | 1:7:A:LEU:HD11  | 1:37:A:PRO:HD3 | 16       | 0.16          |
| (1,851) | 1:7:A:LEU:HD12  | 1:37:A:PRO:HD3 | 16       | 0.16          |
| (1,851) | 1:7:A:LEU:HD13  | 1:37:A:PRO:HD3 | 16       | 0.16          |
| (1,849) | 1:14:A:ARG:HB3  | 1:15:A:MET:HG3 | 24       | 0.16          |
| (1,836) | 2:88:B:PRO:HA   | 1:17:A:ARG:HG2 | 23       | 0.16          |
| (1,836) | 2:88:B:PRO:HA   | 1:17:A:ARG:HG2 | 25       | 0.16          |
| (1,808) | 1:11:A:TRP:HE3  | 1:37:A:PRO:HD2 | 19       | 0.16          |
| (1,760) | 2:85:B:SEP:H    | 1:34:A:TRP:HZ2 | 19       | 0.16          |
| (1,754) | 1:11:A:TRP:HE3  | 1:13:A:LYS:HB3 | 22       | 0.16          |
| (1,736) | 1:33:A:GLN:H    | 1:7:A:LEU:HD21 | 4        | 0.16          |
| (1,736) | 1:33:A:GLN:H    | 1:7:A:LEU:HD22 | 4        | 0.16          |
| (1,736) | 1:33:A:GLN:H    | 1:7:A:LEU:HD23 | 4        | 0.16          |
| (1,736) | 1:33:A:GLN:H    | 1:7:A:LEU:HD21 | 10       | 0.16          |
| (1,736) | 1:33:A:GLN:H    | 1:7:A:LEU:HD22 | 10       | 0.16          |
| (1,736) | 1:33:A:GLN:H    | 1:7:A:LEU:HD23 | 10       | 0.16          |
| (1,720) | 2:84:B:TYR:HE1  | 1:23:A:TYR:HE1 | 2        | 0.16          |
| (1,720) | 2:84:B:TYR:HE1  | 1:23:A:TYR:HE2 | 2        | 0.16          |
| (1,720) | 2:84:B:TYR:HE2  | 1:23:A:TYR:HE1 | 2        | 0.16          |
| (1,720) | 2:84:B:TYR:HE2  | 1:23:A:TYR:HE2 | 2        | 0.16          |
| (1,718) | 1:24:A:TYR:HE1  | 1:37:A:PRO:HD2 | 13       | 0.16          |
| (1,718) | 1:24:A:TYR:HE2  | 1:37:A:PRO:HD2 | 13       | 0.16          |
| (1,682) | 1:23:A:TYR:HB3  | 1:16:A:SER:HB3 | 23       | 0.16          |
| (1,652) | 1:8:A:PRO:HD2   | 1:9:A:PRO:HA   | 4        | 0.16          |
| (1,652) | 1:8:A:PRO:HD2   | 1:9:A:PRO:HA   | 22       | 0.16          |
| (1,639) | 2:84:B:TYR:HD1  | 1:14:A:ARG:HG2 | 5        | 0.16          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,639) | 2:84:B:TYR:HD2  | 1:14:A:ARG:HG2 | 5        | 0.16          |
| (1,639) | 2:84:B:TYR:HD1  | 1:14:A:ARG:HG2 | 10       | 0.16          |
| (1,639) | 2:84:B:TYR:HD2  | 1:14:A:ARG:HG2 | 10       | 0.16          |
| (1,633) | 1:18:A:SER:HB2  | 1:17:A:ARG:HB3 | 13       | 0.16          |
| (1,605) | 1:33:A:GLN:HE22 | 1:24:A:TYR:HB3 | 5        | 0.16          |
| (1,605) | 1:33:A:GLN:HE22 | 1:24:A:TYR:HB3 | 11       | 0.16          |
| (1,557) | 2:84:B:TYR:HD1  | 2:82:B:SER:HA  | 18       | 0.16          |
| (1,557) | 2:84:B:TYR:HD2  | 2:82:B:SER:HA  | 18       | 0.16          |
| (1,430) | 1:24:A:TYR:HE1  | 1:37:A:PRO:HG2 | 22       | 0.16          |
| (1,430) | 1:24:A:TYR:HE2  | 1:37:A:PRO:HG2 | 22       | 0.16          |
| (1,222) | 1:17:A:ARG:HA   | 1:17:A:ARG:HG2 | 4        | 0.16          |
| (1,100) | 1:33:A:GLN:HE22 | 1:33:A:GLN:HG2 | 4        | 0.16          |
| (1,100) | 1:33:A:GLN:HE22 | 1:33:A:GLN:HG2 | 19       | 0.16          |
| (1,94)  | 1:34:A:TRP:HZ3  | 1:21:A:ARG:HG2 | 23       | 0.16          |
| (1,12)  | 1:21:A:ARG:H    | 1:16:A:SER:HB2 | 3        | 0.16          |
| (1,884) | 2:87:B:PHE:HD1  | 1:34:A:TRP:HB3 | 17       | 0.15          |
| (1,884) | 2:87:B:PHE:HD2  | 1:34:A:TRP:HB3 | 17       | 0.15          |
| (1,881) | 2:89:B:GLU:HB2  | 2:90:B:GLY:HA2 | 24       | 0.15          |
| (1,879) | 2:88:B:PRO:HD2  | 1:17:A:ARG:HD2 | 9        | 0.15          |
| (1,864) | 1:7:A:LEU:HD11  | 1:11:A:TRP:HB3 | 16       | 0.15          |
| (1,864) | 1:7:A:LEU:HD12  | 1:11:A:TRP:HB3 | 16       | 0.15          |
| (1,864) | 1:7:A:LEU:HD13  | 1:11:A:TRP:HB3 | 16       | 0.15          |
| (1,864) | 1:7:A:LEU:HD11  | 1:11:A:TRP:HB3 | 21       | 0.15          |
| (1,864) | 1:7:A:LEU:HD12  | 1:11:A:TRP:HB3 | 21       | 0.15          |
| (1,864) | 1:7:A:LEU:HD13  | 1:11:A:TRP:HB3 | 21       | 0.15          |
| (1,857) | 1:28:A:ILE:HG13 | 1:31:A:ALA:HB1 | 25       | 0.15          |
| (1,857) | 1:28:A:ILE:HG13 | 1:31:A:ALA:HB2 | 25       | 0.15          |
| (1,857) | 1:28:A:ILE:HG13 | 1:31:A:ALA:HB3 | 25       | 0.15          |
| (1,845) | 1:11:A:TRP:HB2  | 1:7:A:LEU:HB3  | 2        | 0.15          |
| (1,832) | 1:11:A:TRP:HZ2  | 1:37:A:PRO:HD2 | 5        | 0.15          |
| (1,825) | 2:87:B:PHE:HE1  | 2:81:B:GLY:HA2 | 1        | 0.15          |
| (1,825) | 2:87:B:PHE:HE2  | 2:81:B:GLY:HA2 | 1        | 0.15          |
| (1,825) | 2:87:B:PHE:HE1  | 2:81:B:GLY:HA2 | 9        | 0.15          |
| (1,825) | 2:87:B:PHE:HE2  | 2:81:B:GLY:HA2 | 9        | 0.15          |
| (1,808) | 1:11:A:TRP:HE3  | 1:37:A:PRO:HD2 | 6        | 0.15          |
| (1,775) | 2:84:B:TYR:HE1  | 2:82:B:SER:HA  | 4        | 0.15          |
| (1,775) | 2:84:B:TYR:HE2  | 2:82:B:SER:HA  | 4        | 0.15          |
| (1,770) | 1:25:A:PHE:HE1  | 1:14:A:ARG:HD2 | 12       | 0.15          |
| (1,770) | 1:25:A:PHE:HE2  | 1:14:A:ARG:HD2 | 12       | 0.15          |
| (1,762) | 1:23:A:TYR:HE1  | 1:17:A:ARG:HG3 | 2        | 0.15          |
| (1,762) | 1:23:A:TYR:HE2  | 1:17:A:ARG:HG3 | 2        | 0.15          |
| (1,760) | 2:85:B:SEP:H    | 1:34:A:TRP:HZ2 | 6        | 0.15          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,760) | 2:85:B:SEP:H    | 1:34:A:TRP:HZ2  | 9        | 0.15          |
| (1,760) | 2:85:B:SEP:H    | 1:34:A:TRP:HZ2  | 14       | 0.15          |
| (1,760) | 2:85:B:SEP:H    | 1:34:A:TRP:HZ2  | 16       | 0.15          |
| (1,760) | 2:85:B:SEP:H    | 1:34:A:TRP:HZ2  | 18       | 0.15          |
| (1,736) | 1:33:A:GLN:H    | 1:7:A:LEU:HD21  | 22       | 0.15          |
| (1,736) | 1:33:A:GLN:H    | 1:7:A:LEU:HD22  | 22       | 0.15          |
| (1,736) | 1:33:A:GLN:H    | 1:7:A:LEU:HD23  | 22       | 0.15          |
| (1,736) | 1:33:A:GLN:H    | 1:7:A:LEU:HD21  | 25       | 0.15          |
| (1,736) | 1:33:A:GLN:H    | 1:7:A:LEU:HD22  | 25       | 0.15          |
| (1,736) | 1:33:A:GLN:H    | 1:7:A:LEU:HD23  | 25       | 0.15          |
| (1,720) | 2:84:B:TYR:HE1  | 1:23:A:TYR:HE1  | 16       | 0.15          |
| (1,720) | 2:84:B:TYR:HE1  | 1:23:A:TYR:HE2  | 16       | 0.15          |
| (1,720) | 2:84:B:TYR:HE2  | 1:23:A:TYR:HE1  | 16       | 0.15          |
| (1,720) | 2:84:B:TYR:HE2  | 1:23:A:TYR:HE2  | 16       | 0.15          |
| (1,718) | 1:24:A:TYR:HE1  | 1:37:A:PRO:HD2  | 8        | 0.15          |
| (1,718) | 1:24:A:TYR:HE2  | 1:37:A:PRO:HD2  | 8        | 0.15          |
| (1,718) | 1:24:A:TYR:HE1  | 1:37:A:PRO:HD2  | 17       | 0.15          |
| (1,718) | 1:24:A:TYR:HE2  | 1:37:A:PRO:HD2  | 17       | 0.15          |
| (1,714) | 1:13:A:LYS:H    | 1:24:A:TYR:HE1  | 4        | 0.15          |
| (1,714) | 1:13:A:LYS:H    | 1:24:A:TYR:HE2  | 4        | 0.15          |
| (1,652) | 1:8:A:PRO:HD2   | 1:9:A:PRO:HA    | 6        | 0.15          |
| (1,652) | 1:8:A:PRO:HD2   | 1:9:A:PRO:HA    | 17       | 0.15          |
| (1,639) | 2:84:B:TYR:HD1  | 1:14:A:ARG:HG2  | 22       | 0.15          |
| (1,639) | 2:84:B:TYR:HD2  | 1:14:A:ARG:HG2  | 22       | 0.15          |
| (1,633) | 1:18:A:SER:HB2  | 1:17:A:ARG:HB3  | 15       | 0.15          |
| (1,578) | 1:34:A:TRP:HH2  | 1:21:A:ARG:HD3  | 20       | 0.15          |
| (1,547) | 1:11:A:TRP:HD1  | 1:7:A:LEU:HD11  | 14       | 0.15          |
| (1,547) | 1:11:A:TRP:HD1  | 1:7:A:LEU:HD12  | 14       | 0.15          |
| (1,547) | 1:11:A:TRP:HD1  | 1:7:A:LEU:HD13  | 14       | 0.15          |
| (1,515) | 1:34:A:TRP:HZ3  | 2:88:B:PRO:HB3  | 9        | 0.15          |
| (1,515) | 1:34:A:TRP:HZ3  | 2:88:B:PRO:HB3  | 19       | 0.15          |
| (1,506) | 1:25:A:PHE:HE1  | 1:32:A:SER:HB3  | 5        | 0.15          |
| (1,506) | 1:25:A:PHE:HE2  | 1:32:A:SER:HB3  | 5        | 0.15          |
| (1,466) | 1:27:A:HIS:HE1  | 1:28:A:ILE:HD11 | 4        | 0.15          |
| (1,466) | 1:27:A:HIS:HE1  | 1:28:A:ILE:HD12 | 4        | 0.15          |
| (1,466) | 1:27:A:HIS:HE1  | 1:28:A:ILE:HD13 | 4        | 0.15          |
| (1,430) | 1:24:A:TYR:HE1  | 1:37:A:PRO:HG2  | 7        | 0.15          |
| (1,430) | 1:24:A:TYR:HE2  | 1:37:A:PRO:HG2  | 7        | 0.15          |
| (1,417) | 1:11:A:TRP:HE3  | 1:26:A:ASN:HB3  | 3        | 0.15          |
| (1,379) | 1:40:A:ASN:H    | 1:9:A:PRO:HD3   | 1        | 0.15          |
| (1,296) | 1:26:A:ASN:HD22 | 1:10:A:GLY:HA2  | 19       | 0.15          |
| (1,291) | 1:25:A:PHE:HE1  | 1:32:A:SER:HB2  | 20       | 0.15          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,291) | 1:25:A:PHE:HE2  | 1:32:A:SER:HB2 | 20       | 0.15          |
| (1,220) | 1:18:A:SER:HA   | 1:17:A:ARG:HD2 | 1        | 0.15          |
| (1,210) | 1:12:A:GLU:H    | 1:11:A:TRP:HB2 | 10       | 0.15          |
| (1,210) | 1:12:A:GLU:H    | 1:11:A:TRP:HB2 | 12       | 0.15          |
| (1,210) | 1:12:A:GLU:H    | 1:11:A:TRP:HB2 | 13       | 0.15          |
| (1,137) | 2:85:B:SEP:HB2  | 1:17:A:ARG:HD3 | 25       | 0.15          |
| (1,123) | 1:25:A:PHE:HE1  | 1:25:A:PHE:HA  | 6        | 0.15          |
| (1,123) | 1:25:A:PHE:HE2  | 1:25:A:PHE:HA  | 6        | 0.15          |
| (1,107) | 1:24:A:TYR:HE1  | 1:7:A:LEU:HD11 | 19       | 0.15          |
| (1,107) | 1:24:A:TYR:HE1  | 1:7:A:LEU:HD12 | 19       | 0.15          |
| (1,107) | 1:24:A:TYR:HE1  | 1:7:A:LEU:HD13 | 19       | 0.15          |
| (1,107) | 1:24:A:TYR:HE2  | 1:7:A:LEU:HD11 | 19       | 0.15          |
| (1,107) | 1:24:A:TYR:HE2  | 1:7:A:LEU:HD12 | 19       | 0.15          |
| (1,107) | 1:24:A:TYR:HE2  | 1:7:A:LEU:HD13 | 19       | 0.15          |
| (1,100) | 1:33:A:GLN:HE22 | 1:33:A:GLN:HG2 | 1        | 0.15          |
| (1,100) | 1:33:A:GLN:HE22 | 1:33:A:GLN:HG2 | 11       | 0.15          |
| (1,100) | 1:33:A:GLN:HE22 | 1:33:A:GLN:HG2 | 14       | 0.15          |
| (1,100) | 1:33:A:GLN:HE22 | 1:33:A:GLN:HG2 | 25       | 0.15          |
| (1,884) | 2:87:B:PHE:HD1  | 1:34:A:TRP:HB3 | 7        | 0.14          |
| (1,884) | 2:87:B:PHE:HD2  | 1:34:A:TRP:HB3 | 7        | 0.14          |
| (1,884) | 2:87:B:PHE:HD1  | 1:34:A:TRP:HB3 | 13       | 0.14          |
| (1,884) | 2:87:B:PHE:HD2  | 1:34:A:TRP:HB3 | 13       | 0.14          |
| (1,884) | 2:87:B:PHE:HD1  | 1:34:A:TRP:HB3 | 24       | 0.14          |
| (1,884) | 2:87:B:PHE:HD2  | 1:34:A:TRP:HB3 | 24       | 0.14          |
| (1,881) | 2:89:B:GLU:HB2  | 2:90:B:GLY:HA2 | 6        | 0.14          |
| (1,881) | 2:89:B:GLU:HB2  | 2:90:B:GLY:HA2 | 17       | 0.14          |
| (1,881) | 2:89:B:GLU:HB2  | 2:90:B:GLY:HA2 | 20       | 0.14          |
| (1,851) | 1:7:A:LEU:HD11  | 1:37:A:PRO:HD3 | 12       | 0.14          |
| (1,851) | 1:7:A:LEU:HD12  | 1:37:A:PRO:HD3 | 12       | 0.14          |
| (1,851) | 1:7:A:LEU:HD13  | 1:37:A:PRO:HD3 | 12       | 0.14          |
| (1,845) | 1:11:A:TRP:HB2  | 1:7:A:LEU:HB3  | 25       | 0.14          |
| (1,836) | 2:88:B:PRO:HA   | 1:17:A:ARG:HG2 | 20       | 0.14          |
| (1,825) | 2:87:B:PHE:HE1  | 2:81:B:GLY:HA2 | 25       | 0.14          |
| (1,825) | 2:87:B:PHE:HE2  | 2:81:B:GLY:HA2 | 25       | 0.14          |
| (1,798) | 1:34:A:TRP:HZ2  | 1:18:A:SER:HB3 | 17       | 0.14          |
| (1,771) | 1:25:A:PHE:HD1  | 1:14:A:ARG:HD2 | 20       | 0.14          |
| (1,771) | 1:25:A:PHE:HD2  | 1:14:A:ARG:HD2 | 20       | 0.14          |
| (1,714) | 1:13:A:LYS:H    | 1:24:A:TYR:HE1 | 1        | 0.14          |
| (1,714) | 1:13:A:LYS:H    | 1:24:A:TYR:HE2 | 1        | 0.14          |
| (1,676) | 1:8:A:PRO:HD3   | 1:7:A:LEU:HD11 | 8        | 0.14          |
| (1,676) | 1:8:A:PRO:HD3   | 1:7:A:LEU:HD12 | 8        | 0.14          |
| (1,676) | 1:8:A:PRO:HD3   | 1:7:A:LEU:HD13 | 8        | 0.14          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,652) | 1:8:A:PRO:HD2   | 1:9:A:PRO:HA    | 19       | 0.14          |
| (1,652) | 1:8:A:PRO:HD2   | 1:9:A:PRO:HA    | 24       | 0.14          |
| (1,622) | 1:33:A:GLN:HG2  | 1:24:A:TYR:HB3  | 17       | 0.14          |
| (1,594) | 1:25:A:PHE:HZ   | 2:84:B:TYR:HB2  | 19       | 0.14          |
| (1,516) | 1:11:A:TRP:HH2  | 1:37:A:PRO:HD2  | 3        | 0.14          |
| (1,515) | 1:34:A:TRP:HZ3  | 2:88:B:PRO:HB3  | 8        | 0.14          |
| (1,515) | 1:34:A:TRP:HZ3  | 2:88:B:PRO:HB3  | 11       | 0.14          |
| (1,510) | 1:25:A:PHE:HD1  | 1:30:A:ASN:HA   | 23       | 0.14          |
| (1,510) | 1:25:A:PHE:HD2  | 1:30:A:ASN:HA   | 23       | 0.14          |
| (1,506) | 1:25:A:PHE:HE1  | 1:32:A:SER:HB3  | 12       | 0.14          |
| (1,506) | 1:25:A:PHE:HE2  | 1:32:A:SER:HB3  | 12       | 0.14          |
| (1,493) | 1:24:A:TYR:HE1  | 1:7:A:LEU:HB3   | 3        | 0.14          |
| (1,493) | 1:24:A:TYR:HE2  | 1:7:A:LEU:HB3   | 3        | 0.14          |
| (1,493) | 1:24:A:TYR:HE1  | 1:7:A:LEU:HB3   | 6        | 0.14          |
| (1,493) | 1:24:A:TYR:HE2  | 1:7:A:LEU:HB3   | 6        | 0.14          |
| (1,483) | 1:24:A:TYR:HD1  | 1:37:A:PRO:HB2  | 5        | 0.14          |
| (1,483) | 1:24:A:TYR:HD2  | 1:37:A:PRO:HB2  | 5        | 0.14          |
| (1,417) | 1:11:A:TRP:HE3  | 1:26:A:ASN:HB3  | 17       | 0.14          |
| (1,407) | 1:35:A:GLU:H    | 1:33:A:GLN:HE22 | 17       | 0.14          |
| (1,281) | 1:16:A:SER:H    | 2:85:B:SEP:HB2  | 3        | 0.14          |
| (1,227) | 1:34:A:TRP:HE3  | 1:21:A:ARG:HB2  | 18       | 0.14          |
| (1,217) | 1:16:A:SER:HB2  | 1:21:A:ARG:HG2  | 2        | 0.14          |
| (1,217) | 1:16:A:SER:HB2  | 1:21:A:ARG:HG2  | 21       | 0.14          |
| (1,214) | 1:14:A:ARG:H    | 1:13:A:LYS:HE2  | 7        | 0.14          |
| (1,210) | 1:12:A:GLU:H    | 1:11:A:TRP:HB2  | 19       | 0.14          |
| (1,145) | 1:27:A:HIS:HE1  | 1:25:A:PHE:HD1  | 4        | 0.14          |
| (1,145) | 1:27:A:HIS:HE1  | 1:25:A:PHE:HD2  | 4        | 0.14          |
| (1,137) | 2:85:B:SEP:HB2  | 1:17:A:ARG:HD3  | 19       | 0.14          |
| (1,114) | 2:87:B:PHE:H    | 2:88:B:PRO:HD2  | 11       | 0.14          |
| (1,102) | 1:23:A:TYR:HE1  | 1:25:A:PHE:HB3  | 12       | 0.14          |
| (1,102) | 1:23:A:TYR:HE2  | 1:25:A:PHE:HB3  | 12       | 0.14          |
| (1,100) | 1:33:A:GLN:HE22 | 1:33:A:GLN:HG2  | 7        | 0.14          |
| (1,100) | 1:33:A:GLN:HE22 | 1:33:A:GLN:HG2  | 9        | 0.14          |
| (1,100) | 1:33:A:GLN:HE22 | 1:33:A:GLN:HG2  | 13       | 0.14          |
| (1,100) | 1:33:A:GLN:HE22 | 1:33:A:GLN:HG2  | 16       | 0.14          |
| (1,100) | 1:33:A:GLN:HE22 | 1:33:A:GLN:HG2  | 20       | 0.14          |
| (1,100) | 1:33:A:GLN:HE22 | 1:33:A:GLN:HG2  | 21       | 0.14          |
| (1,100) | 1:33:A:GLN:HE22 | 1:33:A:GLN:HG2  | 22       | 0.14          |
| (1,88)  | 1:33:A:GLN:HE21 | 1:37:A:PRO:HA   | 23       | 0.14          |
| (1,879) | 2:88:B:PRO:HD2  | 1:17:A:ARG:HD2  | 24       | 0.13          |
| (1,865) | 1:28:A:ILE:HG21 | 1:27:A:HIS:HB2  | 12       | 0.13          |
| (1,865) | 1:28:A:ILE:HG22 | 1:27:A:HIS:HB2  | 12       | 0.13          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,865) | 1:28:A:ILE:HG23 | 1:27:A:HIS:HB2  | 12       | 0.13          |
| (1,857) | 1:28:A:ILE:HG13 | 1:31:A:ALA:HB1  | 23       | 0.13          |
| (1,857) | 1:28:A:ILE:HG13 | 1:31:A:ALA:HB2  | 23       | 0.13          |
| (1,857) | 1:28:A:ILE:HG13 | 1:31:A:ALA:HB3  | 23       | 0.13          |
| (1,849) | 1:14:A:ARG:HB3  | 1:15:A:MET:HG3  | 23       | 0.13          |
| (1,845) | 1:11:A:TRP:HB2  | 1:7:A:LEU:HB3   | 17       | 0.13          |
| (1,836) | 2:88:B:PRO:HA   | 1:17:A:ARG:HG2  | 14       | 0.13          |
| (1,828) | 1:11:A:TRP:HZ2  | 1:29:A:THR:HG21 | 19       | 0.13          |
| (1,828) | 1:11:A:TRP:HZ2  | 1:29:A:THR:HG22 | 19       | 0.13          |
| (1,828) | 1:11:A:TRP:HZ2  | 1:29:A:THR:HG23 | 19       | 0.13          |
| (1,790) | 1:25:A:PHE:HZ   | 1:27:A:HIS:HB2  | 20       | 0.13          |
| (1,775) | 2:84:B:TYR:HE1  | 2:82:B:SER:HA   | 9        | 0.13          |
| (1,775) | 2:84:B:TYR:HE2  | 2:82:B:SER:HA   | 9        | 0.13          |
| (1,760) | 2:85:B:SEP:H    | 1:34:A:TRP:HZ2  | 11       | 0.13          |
| (1,736) | 1:33:A:GLN:H    | 1:7:A:LEU:HD21  | 18       | 0.13          |
| (1,736) | 1:33:A:GLN:H    | 1:7:A:LEU:HD22  | 18       | 0.13          |
| (1,736) | 1:33:A:GLN:H    | 1:7:A:LEU:HD23  | 18       | 0.13          |
| (1,722) | 2:90:B:GLY:HA2  | 1:21:A:ARG:HG3  | 18       | 0.13          |
| (1,714) | 1:13:A:LYS:H    | 1:24:A:TYR:HE1  | 14       | 0.13          |
| (1,714) | 1:13:A:LYS:H    | 1:24:A:TYR:HE2  | 14       | 0.13          |
| (1,707) | 1:17:A:ARG:HD3  | 2:88:B:PRO:HD3  | 22       | 0.13          |
| (1,697) | 2:85:B:SEP:HB3  | 1:17:A:ARG:HA   | 2        | 0.13          |
| (1,674) | 2:86:B:PRO:HD3  | 1:14:A:ARG:HD2  | 2        | 0.13          |
| (1,667) | 1:37:A:PRO:HD3  | 1:36:A:ARG:HB2  | 19       | 0.13          |
| (1,652) | 1:8:A:PRO:HD2   | 1:9:A:PRO:HA    | 15       | 0.13          |
| (1,652) | 1:8:A:PRO:HD2   | 1:9:A:PRO:HA    | 18       | 0.13          |
| (1,578) | 1:34:A:TRP:HH2  | 1:21:A:ARG:HD3  | 10       | 0.13          |
| (1,557) | 2:84:B:TYR:HD1  | 2:82:B:SER:HA   | 14       | 0.13          |
| (1,557) | 2:84:B:TYR:HD2  | 2:82:B:SER:HA   | 14       | 0.13          |
| (1,557) | 2:84:B:TYR:HD1  | 2:82:B:SER:HA   | 21       | 0.13          |
| (1,557) | 2:84:B:TYR:HD2  | 2:82:B:SER:HA   | 21       | 0.13          |
| (1,515) | 1:34:A:TRP:HZ3  | 2:88:B:PRO:HB3  | 1        | 0.13          |
| (1,515) | 1:34:A:TRP:HZ3  | 2:88:B:PRO:HB3  | 4        | 0.13          |
| (1,515) | 1:34:A:TRP:HZ3  | 2:88:B:PRO:HB3  | 10       | 0.13          |
| (1,506) | 1:25:A:PHE:HE1  | 1:32:A:SER:HB3  | 10       | 0.13          |
| (1,506) | 1:25:A:PHE:HE2  | 1:32:A:SER:HB3  | 10       | 0.13          |
| (1,493) | 1:24:A:TYR:HE1  | 1:7:A:LEU:HB3   | 16       | 0.13          |
| (1,493) | 1:24:A:TYR:HE2  | 1:7:A:LEU:HB3   | 16       | 0.13          |
| (1,483) | 1:24:A:TYR:HD1  | 1:37:A:PRO:HB2  | 4        | 0.13          |
| (1,483) | 1:24:A:TYR:HD2  | 1:37:A:PRO:HB2  | 4        | 0.13          |
| (1,483) | 1:24:A:TYR:HD1  | 1:37:A:PRO:HB2  | 20       | 0.13          |
| (1,483) | 1:24:A:TYR:HD2  | 1:37:A:PRO:HB2  | 20       | 0.13          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,483) | 1:24:A:TYR:HD1  | 1:37:A:PRO:HB2  | 25       | 0.13          |
| (1,483) | 1:24:A:TYR:HD2  | 1:37:A:PRO:HB2  | 25       | 0.13          |
| (1,437) | 1:11:A:TRP:HD1  | 1:37:A:PRO:HG3  | 21       | 0.13          |
| (1,426) | 1:31:A:ALA:HB1  | 1:26:A:ASN:HB3  | 9        | 0.13          |
| (1,426) | 1:31:A:ALA:HB2  | 1:26:A:ASN:HB3  | 9        | 0.13          |
| (1,426) | 1:31:A:ALA:HB3  | 1:26:A:ASN:HB3  | 9        | 0.13          |
| (1,417) | 1:11:A:TRP:HE3  | 1:26:A:ASN:HB3  | 4        | 0.13          |
| (1,407) | 1:35:A:GLU:H    | 1:33:A:GLN:HE22 | 22       | 0.13          |
| (1,372) | 2:81:B:GLY:H    | 2:82:B:SER:HB2  | 3        | 0.13          |
| (1,372) | 2:81:B:GLY:H    | 2:82:B:SER:HB2  | 5        | 0.13          |
| (1,316) | 1:17:A:ARG:HD3  | 1:18:A:SER:HA   | 11       | 0.13          |
| (1,291) | 1:25:A:PHE:HE1  | 1:32:A:SER:HB2  | 23       | 0.13          |
| (1,291) | 1:25:A:PHE:HE2  | 1:32:A:SER:HB2  | 23       | 0.13          |
| (1,258) | 1:33:A:GLN:H    | 1:24:A:TYR:HD1  | 20       | 0.13          |
| (1,258) | 1:33:A:GLN:H    | 1:24:A:TYR:HD2  | 20       | 0.13          |
| (1,210) | 1:12:A:GLU:H    | 1:11:A:TRP:HB2  | 22       | 0.13          |
| (1,145) | 1:27:A:HIS:HE1  | 1:25:A:PHE:HD1  | 11       | 0.13          |
| (1,145) | 1:27:A:HIS:HE1  | 1:25:A:PHE:HD2  | 11       | 0.13          |
| (1,118) | 1:24:A:TYR:HA   | 1:13:A:LYS:HG3  | 4        | 0.13          |
| (1,118) | 1:24:A:TYR:HA   | 1:13:A:LYS:HG3  | 22       | 0.13          |
| (1,100) | 1:33:A:GLN:HE22 | 1:33:A:GLN:HG2  | 6        | 0.13          |
| (1,100) | 1:33:A:GLN:HE22 | 1:33:A:GLN:HG2  | 24       | 0.13          |
| (1,75)  | 1:37:A:PRO:HD3  | 1:36:A:ARG:HD2  | 1        | 0.13          |
| (1,75)  | 1:37:A:PRO:HD3  | 1:36:A:ARG:HD2  | 9        | 0.13          |
| (1,75)  | 1:37:A:PRO:HD3  | 1:36:A:ARG:HD2  | 16       | 0.13          |
| (1,21)  | 1:16:A:SER:H    | 1:15:A:MET:HG2  | 10       | 0.13          |
| (1,12)  | 1:21:A:ARG:H    | 1:16:A:SER:HB2  | 10       | 0.13          |
| (1,2)   | 1:13:A:LYS:H    | 1:12:A:GLU:HG2  | 22       | 0.13          |
| (1,865) | 1:28:A:ILE:HG21 | 1:27:A:HIS:HB2  | 8        | 0.12          |
| (1,865) | 1:28:A:ILE:HG22 | 1:27:A:HIS:HB2  | 8        | 0.12          |
| (1,865) | 1:28:A:ILE:HG23 | 1:27:A:HIS:HB2  | 8        | 0.12          |
| (1,857) | 1:28:A:ILE:HG13 | 1:31:A:ALA:HB1  | 13       | 0.12          |
| (1,857) | 1:28:A:ILE:HG13 | 1:31:A:ALA:HB2  | 13       | 0.12          |
| (1,857) | 1:28:A:ILE:HG13 | 1:31:A:ALA:HB3  | 13       | 0.12          |
| (1,856) | 1:7:A:LEU:HD11  | 1:36:A:ARG:HG3  | 15       | 0.12          |
| (1,856) | 1:7:A:LEU:HD12  | 1:36:A:ARG:HG3  | 15       | 0.12          |
| (1,856) | 1:7:A:LEU:HD13  | 1:36:A:ARG:HG3  | 15       | 0.12          |
| (1,851) | 1:7:A:LEU:HD11  | 1:37:A:PRO:HD3  | 11       | 0.12          |
| (1,851) | 1:7:A:LEU:HD12  | 1:37:A:PRO:HD3  | 11       | 0.12          |
| (1,851) | 1:7:A:LEU:HD13  | 1:37:A:PRO:HD3  | 11       | 0.12          |
| (1,845) | 1:11:A:TRP:HB2  | 1:7:A:LEU:HB3   | 4        | 0.12          |
| (1,845) | 1:11:A:TRP:HB2  | 1:7:A:LEU:HB3   | 18       | 0.12          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,845) | 1:11:A:TRP:HB2  | 1:7:A:LEU:HB3   | 19       | 0.12          |
| (1,832) | 1:11:A:TRP:HZ2  | 1:37:A:PRO:HD2  | 2        | 0.12          |
| (1,807) | 1:25:A:PHE:HZ   | 2:83:B:PRO:HB3  | 19       | 0.12          |
| (1,790) | 1:25:A:PHE:HZ   | 1:27:A:HIS:HB2  | 11       | 0.12          |
| (1,777) | 1:24:A:TYR:HE1  | 1:7:A:LEU:HA    | 7        | 0.12          |
| (1,777) | 1:24:A:TYR:HE2  | 1:7:A:LEU:HA    | 7        | 0.12          |
| (1,777) | 1:24:A:TYR:HE1  | 1:7:A:LEU:HA    | 16       | 0.12          |
| (1,777) | 1:24:A:TYR:HE2  | 1:7:A:LEU:HA    | 16       | 0.12          |
| (1,770) | 1:25:A:PHE:HE1  | 1:14:A:ARG:HD2  | 10       | 0.12          |
| (1,770) | 1:25:A:PHE:HE2  | 1:14:A:ARG:HD2  | 10       | 0.12          |
| (1,736) | 1:33:A:GLN:H    | 1:7:A:LEU:HD21  | 15       | 0.12          |
| (1,736) | 1:33:A:GLN:H    | 1:7:A:LEU:HD22  | 15       | 0.12          |
| (1,736) | 1:33:A:GLN:H    | 1:7:A:LEU:HD23  | 15       | 0.12          |
| (1,718) | 1:24:A:TYR:HE1  | 1:37:A:PRO:HD2  | 6        | 0.12          |
| (1,718) | 1:24:A:TYR:HE2  | 1:37:A:PRO:HD2  | 6        | 0.12          |
| (1,683) | 2:83:B:PRO:HD2  | 2:84:B:TYR:HB3  | 23       | 0.12          |
| (1,652) | 1:8:A:PRO:HD2   | 1:9:A:PRO:HA    | 3        | 0.12          |
| (1,652) | 1:8:A:PRO:HD2   | 1:9:A:PRO:HA    | 23       | 0.12          |
| (1,627) | 2:85:B:SEP:HB2  | 1:16:A:SER:HA   | 20       | 0.12          |
| (1,606) | 1:34:A:TRP:HD1  | 2:89:B:GLU:HG2  | 10       | 0.12          |
| (1,605) | 1:33:A:GLN:HE22 | 1:24:A:TYR:HB3  | 14       | 0.12          |
| (1,562) | 1:34:A:TRP:HZ2  | 1:16:A:SER:HB3  | 19       | 0.12          |
| (1,557) | 2:84:B:TYR:HD1  | 2:82:B:SER:HA   | 5        | 0.12          |
| (1,557) | 2:84:B:TYR:HD2  | 2:82:B:SER:HA   | 5        | 0.12          |
| (1,557) | 2:84:B:TYR:HD1  | 2:82:B:SER:HA   | 9        | 0.12          |
| (1,557) | 2:84:B:TYR:HD2  | 2:82:B:SER:HA   | 9        | 0.12          |
| (1,557) | 2:84:B:TYR:HD1  | 2:82:B:SER:HA   | 11       | 0.12          |
| (1,557) | 2:84:B:TYR:HD2  | 2:82:B:SER:HA   | 11       | 0.12          |
| (1,515) | 1:34:A:TRP:HZ3  | 2:88:B:PRO:HB3  | 5        | 0.12          |
| (1,515) | 1:34:A:TRP:HZ3  | 2:88:B:PRO:HB3  | 7        | 0.12          |
| (1,515) | 1:34:A:TRP:HZ3  | 2:88:B:PRO:HB3  | 13       | 0.12          |
| (1,513) | 1:34:A:TRP:HZ3  | 2:86:B:PRO:HG2  | 7        | 0.12          |
| (1,513) | 1:34:A:TRP:HZ3  | 2:86:B:PRO:HG2  | 9        | 0.12          |
| (1,513) | 1:34:A:TRP:HZ3  | 2:86:B:PRO:HG2  | 22       | 0.12          |
| (1,484) | 1:24:A:TYR:HE1  | 1:36:A:ARG:HG2  | 11       | 0.12          |
| (1,484) | 1:24:A:TYR:HE2  | 1:36:A:ARG:HG2  | 11       | 0.12          |
| (1,466) | 1:27:A:HIS:HE1  | 1:28:A:ILE:HD11 | 13       | 0.12          |
| (1,466) | 1:27:A:HIS:HE1  | 1:28:A:ILE:HD12 | 13       | 0.12          |
| (1,466) | 1:27:A:HIS:HE1  | 1:28:A:ILE:HD13 | 13       | 0.12          |
| (1,430) | 1:24:A:TYR:HE1  | 1:37:A:PRO:HG2  | 3        | 0.12          |
| (1,430) | 1:24:A:TYR:HE2  | 1:37:A:PRO:HG2  | 3        | 0.12          |
| (1,426) | 1:31:A:ALA:HB1  | 1:26:A:ASN:HB3  | 24       | 0.12          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,426) | 1:31:A:ALA:HB2  | 1:26:A:ASN:HB3  | 24       | 0.12          |
| (1,426) | 1:31:A:ALA:HB3  | 1:26:A:ASN:HB3  | 24       | 0.12          |
| (1,396) | 1:27:A:HIS:H    | 1:25:A:PHE:HZ   | 1        | 0.12          |
| (1,383) | 1:34:A:TRP:HE3  | 1:22:A:VAL:HG21 | 7        | 0.12          |
| (1,383) | 1:34:A:TRP:HE3  | 1:22:A:VAL:HG22 | 7        | 0.12          |
| (1,383) | 1:34:A:TRP:HE3  | 1:22:A:VAL:HG23 | 7        | 0.12          |
| (1,296) | 1:26:A:ASN:HD22 | 1:10:A:GLY:HA2  | 20       | 0.12          |
| (1,247) | 1:24:A:TYR:HE1  | 1:36:A:ARG:HD2  | 22       | 0.12          |
| (1,247) | 1:24:A:TYR:HE2  | 1:36:A:ARG:HD2  | 22       | 0.12          |
| (1,222) | 1:17:A:ARG:HA   | 1:17:A:ARG:HG2  | 8        | 0.12          |
| (1,222) | 1:17:A:ARG:HA   | 1:17:A:ARG:HG2  | 10       | 0.12          |
| (1,222) | 1:17:A:ARG:HA   | 1:17:A:ARG:HG2  | 12       | 0.12          |
| (1,217) | 1:16:A:SER:HB2  | 1:21:A:ARG:HG2  | 14       | 0.12          |
| (1,210) | 1:12:A:GLU:H    | 1:11:A:TRP:HB2  | 2        | 0.12          |
| (1,210) | 1:12:A:GLU:H    | 1:11:A:TRP:HB2  | 7        | 0.12          |
| (1,210) | 1:12:A:GLU:H    | 1:11:A:TRP:HB2  | 15       | 0.12          |
| (1,210) | 1:12:A:GLU:H    | 1:11:A:TRP:HB2  | 18       | 0.12          |
| (1,210) | 1:12:A:GLU:H    | 1:11:A:TRP:HB2  | 21       | 0.12          |
| (1,193) | 1:9:A:PRO:HD3   | 1:8:A:PRO:HG2   | 4        | 0.12          |
| (1,94)  | 1:34:A:TRP:HZ3  | 1:21:A:ARG:HG2  | 9        | 0.12          |
| (1,28)  | 2:85:B:SEP:H    | 2:83:B:PRO:HG2  | 17       | 0.12          |
| (1,8)   | 1:12:A:GLU:H    | 1:7:A:LEU:HD21  | 21       | 0.12          |
| (1,8)   | 1:12:A:GLU:H    | 1:7:A:LEU:HD22  | 21       | 0.12          |
| (1,8)   | 1:12:A:GLU:H    | 1:7:A:LEU:HD23  | 21       | 0.12          |
| (1,865) | 1:28:A:ILE:HG21 | 1:27:A:HIS:HB2  | 6        | 0.11          |
| (1,865) | 1:28:A:ILE:HG22 | 1:27:A:HIS:HB2  | 6        | 0.11          |
| (1,865) | 1:28:A:ILE:HG23 | 1:27:A:HIS:HB2  | 6        | 0.11          |
| (1,865) | 1:28:A:ILE:HG21 | 1:27:A:HIS:HB2  | 10       | 0.11          |
| (1,865) | 1:28:A:ILE:HG22 | 1:27:A:HIS:HB2  | 10       | 0.11          |
| (1,865) | 1:28:A:ILE:HG23 | 1:27:A:HIS:HB2  | 10       | 0.11          |
| (1,865) | 1:28:A:ILE:HG21 | 1:27:A:HIS:HB2  | 14       | 0.11          |
| (1,865) | 1:28:A:ILE:HG22 | 1:27:A:HIS:HB2  | 14       | 0.11          |
| (1,865) | 1:28:A:ILE:HG23 | 1:27:A:HIS:HB2  | 14       | 0.11          |
| (1,857) | 1:28:A:ILE:HG13 | 1:31:A:ALA:HB1  | 4        | 0.11          |
| (1,857) | 1:28:A:ILE:HG13 | 1:31:A:ALA:HB2  | 4        | 0.11          |
| (1,857) | 1:28:A:ILE:HG13 | 1:31:A:ALA:HB3  | 4        | 0.11          |
| (1,857) | 1:28:A:ILE:HG13 | 1:31:A:ALA:HB1  | 17       | 0.11          |
| (1,857) | 1:28:A:ILE:HG13 | 1:31:A:ALA:HB2  | 17       | 0.11          |
| (1,857) | 1:28:A:ILE:HG13 | 1:31:A:ALA:HB3  | 17       | 0.11          |
| (1,845) | 1:11:A:TRP:HB2  | 1:7:A:LEU:HB3   | 10       | 0.11          |
| (1,845) | 1:11:A:TRP:HB2  | 1:7:A:LEU:HB3   | 15       | 0.11          |
| (1,845) | 1:11:A:TRP:HB2  | 1:7:A:LEU:HB3   | 22       | 0.11          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,836) | 2:88:B:PRO:HA   | 1:17:A:ARG:HG2 | 6        | 0.11          |
| (1,832) | 1:11:A:TRP:HZ2  | 1:37:A:PRO:HD2 | 22       | 0.11          |
| (1,825) | 2:87:B:PHE:HE1  | 2:81:B:GLY:HA2 | 8        | 0.11          |
| (1,825) | 2:87:B:PHE:HE2  | 2:81:B:GLY:HA2 | 8        | 0.11          |
| (1,825) | 2:87:B:PHE:HE1  | 2:81:B:GLY:HA2 | 24       | 0.11          |
| (1,825) | 2:87:B:PHE:HE2  | 2:81:B:GLY:HA2 | 24       | 0.11          |
| (1,820) | 1:21:A:ARG:HB3  | 1:19:A:SER:HA  | 17       | 0.11          |
| (1,799) | 1:34:A:TRP:HZ2  | 2:88:B:PRO:HD2 | 24       | 0.11          |
| (1,749) | 1:34:A:TRP:HE1  | 2:88:B:PRO:HB2 | 8        | 0.11          |
| (1,742) | 1:14:A:ARG:H    | 1:15:A:MET:HE1 | 15       | 0.11          |
| (1,742) | 1:14:A:ARG:H    | 1:15:A:MET:HE2 | 15       | 0.11          |
| (1,742) | 1:14:A:ARG:H    | 1:15:A:MET:HE3 | 15       | 0.11          |
| (1,736) | 1:33:A:GLN:H    | 1:7:A:LEU:HD21 | 11       | 0.11          |
| (1,736) | 1:33:A:GLN:H    | 1:7:A:LEU:HD22 | 11       | 0.11          |
| (1,736) | 1:33:A:GLN:H    | 1:7:A:LEU:HD23 | 11       | 0.11          |
| (1,736) | 1:33:A:GLN:H    | 1:7:A:LEU:HD21 | 14       | 0.11          |
| (1,736) | 1:33:A:GLN:H    | 1:7:A:LEU:HD22 | 14       | 0.11          |
| (1,736) | 1:33:A:GLN:H    | 1:7:A:LEU:HD23 | 14       | 0.11          |
| (1,720) | 2:84:B:TYR:HE1  | 1:23:A:TYR:HE1 | 25       | 0.11          |
| (1,720) | 2:84:B:TYR:HE1  | 1:23:A:TYR:HE2 | 25       | 0.11          |
| (1,720) | 2:84:B:TYR:HE2  | 1:23:A:TYR:HE1 | 25       | 0.11          |
| (1,720) | 2:84:B:TYR:HE2  | 1:23:A:TYR:HE2 | 25       | 0.11          |
| (1,683) | 2:83:B:PRO:HD2  | 2:84:B:TYR:HB3 | 2        | 0.11          |
| (1,683) | 2:83:B:PRO:HD2  | 2:84:B:TYR:HB3 | 25       | 0.11          |
| (1,674) | 2:86:B:PRO:HD3  | 1:14:A:ARG:HD2 | 17       | 0.11          |
| (1,659) | 1:20:A:GLY:H    | 1:16:A:SER:HB2 | 5        | 0.11          |
| (1,652) | 1:8:A:PRO:HD2   | 1:9:A:PRO:HA   | 7        | 0.11          |
| (1,643) | 2:85:B:SEP:HB2  | 1:17:A:ARG:HG2 | 10       | 0.11          |
| (1,643) | 2:85:B:SEP:HB2  | 1:17:A:ARG:HG2 | 20       | 0.11          |
| (1,605) | 1:33:A:GLN:HE22 | 1:24:A:TYR:HB3 | 7        | 0.11          |
| (1,605) | 1:33:A:GLN:HE22 | 1:24:A:TYR:HB3 | 20       | 0.11          |
| (1,594) | 1:25:A:PHE:HZ   | 2:84:B:TYR:HB2 | 2        | 0.11          |
| (1,580) | 1:27:A:HIS:HD2  | 1:12:A:GLU:HG2 | 4        | 0.11          |
| (1,515) | 1:34:A:TRP:HZ3  | 2:88:B:PRO:HB3 | 14       | 0.11          |
| (1,515) | 1:34:A:TRP:HZ3  | 2:88:B:PRO:HB3 | 16       | 0.11          |
| (1,515) | 1:34:A:TRP:HZ3  | 2:88:B:PRO:HB3 | 18       | 0.11          |
| (1,513) | 1:34:A:TRP:HZ3  | 2:86:B:PRO:HG2 | 1        | 0.11          |
| (1,513) | 1:34:A:TRP:HZ3  | 2:86:B:PRO:HG2 | 5        | 0.11          |
| (1,513) | 1:34:A:TRP:HZ3  | 2:86:B:PRO:HG2 | 8        | 0.11          |
| (1,513) | 1:34:A:TRP:HZ3  | 2:86:B:PRO:HG2 | 12       | 0.11          |
| (1,513) | 1:34:A:TRP:HZ3  | 2:86:B:PRO:HG2 | 16       | 0.11          |
| (1,510) | 1:25:A:PHE:HD1  | 1:30:A:ASN:HA  | 12       | 0.11          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,510) | 1:25:A:PHE:HD2 | 1:30:A:ASN:HA   | 12       | 0.11          |
| (1,506) | 1:25:A:PHE:HE1 | 1:32:A:SER:HB3  | 24       | 0.11          |
| (1,506) | 1:25:A:PHE:HE2 | 1:32:A:SER:HB3  | 24       | 0.11          |
| (1,493) | 1:24:A:TYR:HE1 | 1:7:A:LEU:HB3   | 7        | 0.11          |
| (1,493) | 1:24:A:TYR:HE2 | 1:7:A:LEU:HB3   | 7        | 0.11          |
| (1,483) | 1:24:A:TYR:HD1 | 1:37:A:PRO:HB2  | 15       | 0.11          |
| (1,483) | 1:24:A:TYR:HD2 | 1:37:A:PRO:HB2  | 15       | 0.11          |
| (1,482) | 1:11:A:TRP:HH2 | 1:37:A:PRO:HB2  | 15       | 0.11          |
| (1,468) | 2:85:B:SEP:H   | 1:14:A:ARG:HB3  | 12       | 0.11          |
| (1,466) | 1:27:A:HIS:HE1 | 1:28:A:ILE:HD11 | 17       | 0.11          |
| (1,466) | 1:27:A:HIS:HE1 | 1:28:A:ILE:HD12 | 17       | 0.11          |
| (1,466) | 1:27:A:HIS:HE1 | 1:28:A:ILE:HD13 | 17       | 0.11          |
| (1,432) | 1:24:A:TYR:HD1 | 1:37:A:PRO:HG2  | 22       | 0.11          |
| (1,432) | 1:24:A:TYR:HD2 | 1:37:A:PRO:HG2  | 22       | 0.11          |
| (1,417) | 1:11:A:TRP:HE3 | 1:26:A:ASN:HB3  | 19       | 0.11          |
| (1,383) | 1:34:A:TRP:HE3 | 1:22:A:VAL:HG21 | 21       | 0.11          |
| (1,383) | 1:34:A:TRP:HE3 | 1:22:A:VAL:HG22 | 21       | 0.11          |
| (1,383) | 1:34:A:TRP:HE3 | 1:22:A:VAL:HG23 | 21       | 0.11          |
| (1,338) | 1:33:A:GLN:H   | 2:86:B:PRO:HB3  | 17       | 0.11          |
| (1,304) | 1:24:A:TYR:HE1 | 1:24:A:TYR:HA   | 19       | 0.11          |
| (1,304) | 1:24:A:TYR:HE2 | 1:24:A:TYR:HA   | 19       | 0.11          |
| (1,258) | 1:33:A:GLN:H   | 1:24:A:TYR:HD1  | 17       | 0.11          |
| (1,258) | 1:33:A:GLN:H   | 1:24:A:TYR:HD2  | 17       | 0.11          |
| (1,258) | 1:33:A:GLN:H   | 1:24:A:TYR:HD1  | 24       | 0.11          |
| (1,258) | 1:33:A:GLN:H   | 1:24:A:TYR:HD2  | 24       | 0.11          |
| (1,224) | 1:22:A:VAL:H   | 1:21:A:ARG:HD3  | 7        | 0.11          |
| (1,222) | 1:17:A:ARG:HA  | 1:17:A:ARG:HG2  | 3        | 0.11          |
| (1,222) | 1:17:A:ARG:HA  | 1:17:A:ARG:HG2  | 5        | 0.11          |
| (1,222) | 1:17:A:ARG:HA  | 1:17:A:ARG:HG2  | 11       | 0.11          |
| (1,222) | 1:17:A:ARG:HA  | 1:17:A:ARG:HG2  | 13       | 0.11          |
| (1,222) | 1:17:A:ARG:HA  | 1:17:A:ARG:HG2  | 25       | 0.11          |
| (1,220) | 1:18:A:SER:HA  | 1:17:A:ARG:HD2  | 23       | 0.11          |
| (1,210) | 1:12:A:GLU:H   | 1:11:A:TRP:HB2  | 1        | 0.11          |
| (1,210) | 1:12:A:GLU:H   | 1:11:A:TRP:HB2  | 3        | 0.11          |
| (1,210) | 1:12:A:GLU:H   | 1:11:A:TRP:HB2  | 8        | 0.11          |
| (1,210) | 1:12:A:GLU:H   | 1:11:A:TRP:HB2  | 17       | 0.11          |
| (1,210) | 1:12:A:GLU:H   | 1:11:A:TRP:HB2  | 20       | 0.11          |
| (1,145) | 1:27:A:HIS:HE1 | 1:25:A:PHE:HD1  | 10       | 0.11          |
| (1,145) | 1:27:A:HIS:HE1 | 1:25:A:PHE:HD2  | 10       | 0.11          |
| (1,145) | 1:27:A:HIS:HE1 | 1:25:A:PHE:HD1  | 17       | 0.11          |
| (1,145) | 1:27:A:HIS:HE1 | 1:25:A:PHE:HD2  | 17       | 0.11          |
| (1,145) | 1:27:A:HIS:HE1 | 1:25:A:PHE:HD1  | 21       | 0.11          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,145) | 1:27:A:HIS:HE1  | 1:25:A:PHE:HD2  | 21       | 0.11          |
| (1,129) | 1:7:A:LEU:HB2   | 1:8:A:PRO:HD3   | 2        | 0.11          |
| (1,129) | 1:7:A:LEU:HB2   | 1:8:A:PRO:HD3   | 9        | 0.11          |
| (1,105) | 1:24:A:TYR:HE1  | 1:7:A:LEU:HD21  | 17       | 0.11          |
| (1,105) | 1:24:A:TYR:HE1  | 1:7:A:LEU:HD22  | 17       | 0.11          |
| (1,105) | 1:24:A:TYR:HE1  | 1:7:A:LEU:HD23  | 17       | 0.11          |
| (1,105) | 1:24:A:TYR:HE2  | 1:7:A:LEU:HD21  | 17       | 0.11          |
| (1,105) | 1:24:A:TYR:HE2  | 1:7:A:LEU:HD22  | 17       | 0.11          |
| (1,105) | 1:24:A:TYR:HE2  | 1:7:A:LEU:HD23  | 17       | 0.11          |
| (1,105) | 1:24:A:TYR:HE1  | 1:7:A:LEU:HD21  | 25       | 0.11          |
| (1,105) | 1:24:A:TYR:HE1  | 1:7:A:LEU:HD22  | 25       | 0.11          |
| (1,105) | 1:24:A:TYR:HE1  | 1:7:A:LEU:HD23  | 25       | 0.11          |
| (1,105) | 1:24:A:TYR:HE2  | 1:7:A:LEU:HD21  | 25       | 0.11          |
| (1,105) | 1:24:A:TYR:HE2  | 1:7:A:LEU:HD22  | 25       | 0.11          |
| (1,105) | 1:24:A:TYR:HE2  | 1:7:A:LEU:HD23  | 25       | 0.11          |
| (1,28)  | 2:85:B:SEP:H    | 2:83:B:PRO:HG2  | 20       | 0.11          |
| (1,28)  | 2:85:B:SEP:H    | 2:83:B:PRO:HG2  | 23       | 0.11          |
| (1,865) | 1:28:A:ILE:HG21 | 1:27:A:HIS:HB2  | 19       | 0.1           |
| (1,865) | 1:28:A:ILE:HG22 | 1:27:A:HIS:HB2  | 19       | 0.1           |
| (1,865) | 1:28:A:ILE:HG23 | 1:27:A:HIS:HB2  | 19       | 0.1           |
| (1,845) | 1:11:A:TRP:HB2  | 1:7:A:LEU:HB3   | 11       | 0.1           |
| (1,836) | 2:88:B:PRO:HA   | 1:17:A:ARG:HG2  | 9        | 0.1           |
| (1,830) | 1:34:A:TRP:HD1  | 1:33:A:GLN:HG2  | 8        | 0.1           |
| (1,807) | 1:25:A:PHE:HZ   | 2:83:B:PRO:HB3  | 14       | 0.1           |
| (1,770) | 1:25:A:PHE:HE1  | 1:14:A:ARG:HD2  | 7        | 0.1           |
| (1,770) | 1:25:A:PHE:HE2  | 1:14:A:ARG:HD2  | 7        | 0.1           |
| (1,689) | 1:14:A:ARG:HD2  | 2:84:B:TYR:HA   | 8        | 0.1           |
| (1,666) | 1:37:A:PRO:HD3  | 1:36:A:ARG:HG3  | 24       | 0.1           |
| (1,605) | 1:33:A:GLN:HE22 | 1:24:A:TYR:HB3  | 12       | 0.1           |
| (1,594) | 1:25:A:PHE:HZ   | 2:84:B:TYR:HB2  | 15       | 0.1           |
| (1,578) | 1:34:A:TRP:HH2  | 1:21:A:ARG:HD3  | 8        | 0.1           |
| (1,557) | 2:84:B:TYR:HD1  | 2:82:B:SER:HA   | 7        | 0.1           |
| (1,557) | 2:84:B:TYR:HD2  | 2:82:B:SER:HA   | 7        | 0.1           |
| (1,549) | 1:11:A:TRP:HD1  | 1:28:A:ILE:HG13 | 18       | 0.1           |
| (1,515) | 1:34:A:TRP:HZ3  | 2:88:B:PRO:HB3  | 2        | 0.1           |
| (1,513) | 1:34:A:TRP:HZ3  | 2:86:B:PRO:HG2  | 2        | 0.1           |
| (1,483) | 1:24:A:TYR:HD1  | 1:37:A:PRO:HB2  | 24       | 0.1           |
| (1,483) | 1:24:A:TYR:HD2  | 1:37:A:PRO:HB2  | 24       | 0.1           |
| (1,467) | 1:27:A:HIS:HE1  | 1:28:A:ILE:HG13 | 18       | 0.1           |
| (1,426) | 1:31:A:ALA:HB1  | 1:26:A:ASN:HB3  | 18       | 0.1           |
| (1,426) | 1:31:A:ALA:HB2  | 1:26:A:ASN:HB3  | 18       | 0.1           |
| (1,426) | 1:31:A:ALA:HB3  | 1:26:A:ASN:HB3  | 18       | 0.1           |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,426) | 1:31:A:ALA:HB1 | 1:26:A:ASN:HB3 | 19       | 0.1           |
| (1,426) | 1:31:A:ALA:HB2 | 1:26:A:ASN:HB3 | 19       | 0.1           |
| (1,426) | 1:31:A:ALA:HB3 | 1:26:A:ASN:HB3 | 19       | 0.1           |
| (1,413) | 1:32:A:SER:H   | 1:26:A:ASN:HB2 | 25       | 0.1           |
| (1,372) | 2:81:B:GLY:H   | 2:82:B:SER:HB2 | 15       | 0.1           |
| (1,222) | 1:17:A:ARG:HA  | 1:17:A:ARG:HG2 | 23       | 0.1           |
| (1,28)  | 2:85:B:SEP:H   | 2:83:B:PRO:HG2 | 15       | 0.1           |

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

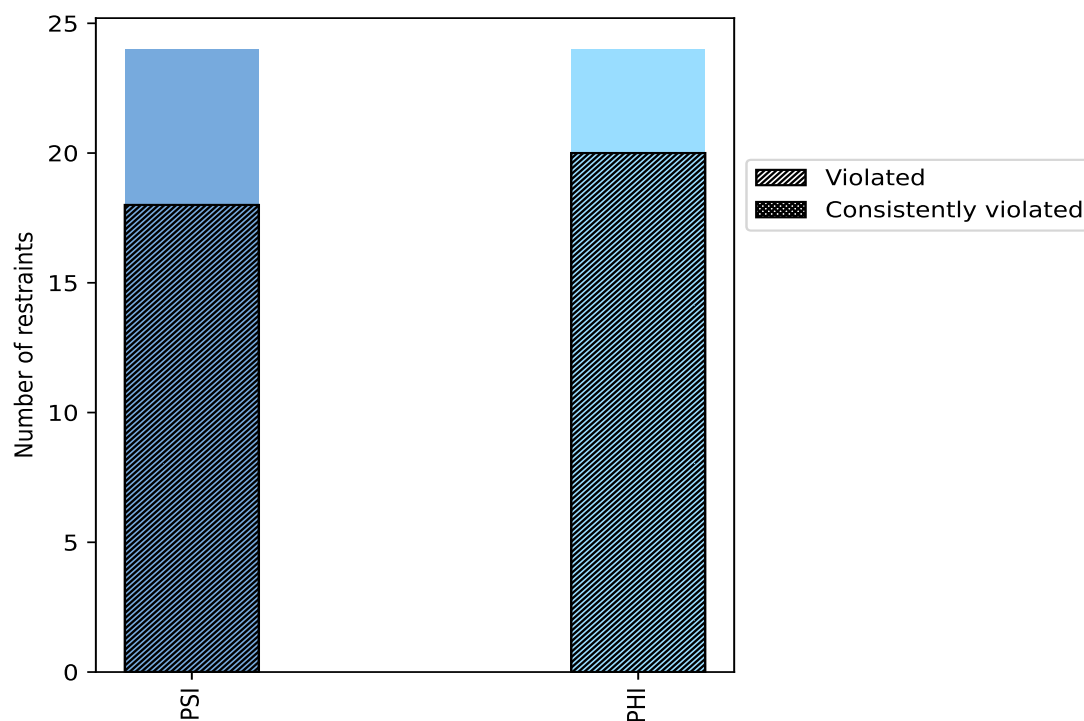
### 10.1 Summary of dihedral-angle violations [i](#)

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

| Angle type | Count | % <sup>1</sup> | Violated <sup>3</sup> |                |                | Consistently Violated <sup>4</sup> |                |                |
|------------|-------|----------------|-----------------------|----------------|----------------|------------------------------------|----------------|----------------|
|            |       |                | Count                 | % <sup>2</sup> | % <sup>1</sup> | Count                              | % <sup>2</sup> | % <sup>1</sup> |
| PSI        | 24    | 50.0           | 18                    | 75.0           | 37.5           | 0                                  | 0.0            | 0.0            |
| PHI        | 24    | 50.0           | 20                    | 83.3           | 41.7           | 0                                  | 0.0            | 0.0            |
| Total      | 48    | 100.0          | 38                    | 79.2           | 79.2           | 0                                  | 0.0            | 0.0            |

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

#### 10.1.1 Bar chart : Distribution of dihedral-angles and violations [i](#)



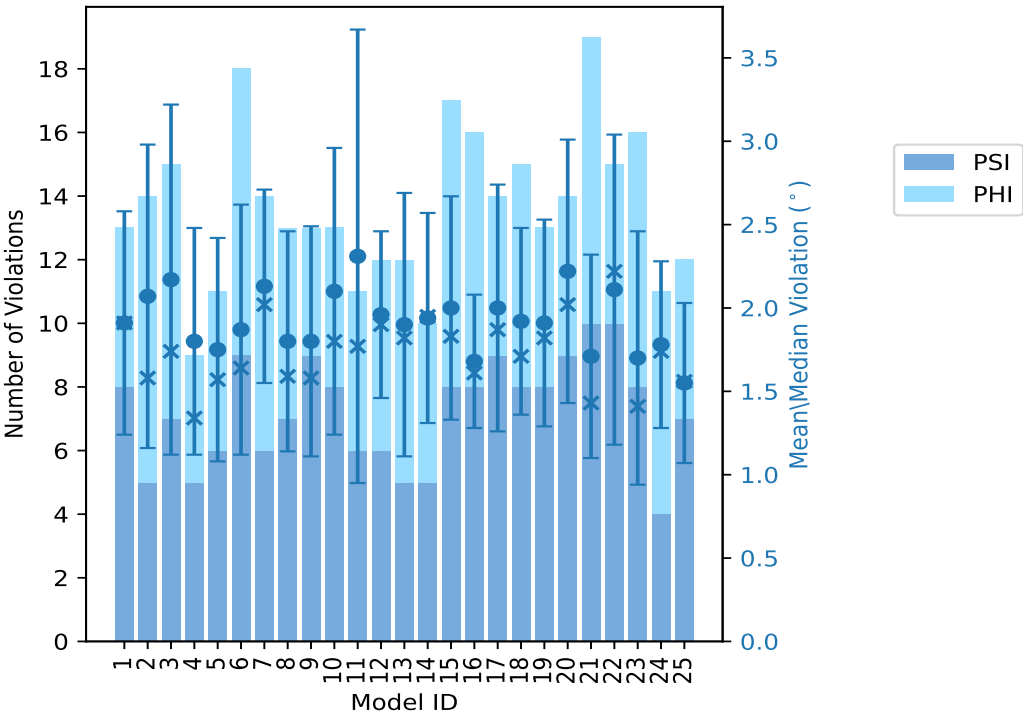
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

## 10.2 Dihedral-angle violation statistics for each model

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

| Model ID | Number of violations |     |       | Mean (°) | Max (°) | SD (°) | Median (°) |
|----------|----------------------|-----|-------|----------|---------|--------|------------|
|          | PSI                  | PHI | Total |          |         |        |            |
| 1        | 8                    | 5   | 13    | 1.91     | 3.37    | 0.67   | 1.91       |
| 2        | 5                    | 9   | 14    | 2.07     | 3.85    | 0.91   | 1.58       |
| 3        | 7                    | 8   | 15    | 2.17     | 4.85    | 1.05   | 1.74       |
| 4        | 5                    | 4   | 9     | 1.8      | 3.08    | 0.68   | 1.34       |
| 5        | 6                    | 5   | 11    | 1.75     | 3.35    | 0.67   | 1.57       |
| 6        | 9                    | 9   | 18    | 1.87     | 3.21    | 0.75   | 1.64       |
| 7        | 6                    | 8   | 14    | 2.13     | 3.4     | 0.58   | 2.02       |
| 8        | 7                    | 6   | 13    | 1.8      | 3.83    | 0.66   | 1.59       |
| 9        | 9                    | 4   | 13    | 1.8      | 3.35    | 0.69   | 1.58       |
| 10       | 8                    | 5   | 13    | 2.1      | 4.0     | 0.86   | 1.8        |
| 11       | 6                    | 5   | 11    | 2.31     | 5.41    | 1.36   | 1.77       |
| 12       | 6                    | 6   | 12    | 1.96     | 2.82    | 0.5    | 1.9        |
| 13       | 5                    | 7   | 12    | 1.9      | 4.03    | 0.79   | 1.82       |
| 14       | 5                    | 5   | 10    | 1.94     | 2.86    | 0.63   | 1.95       |
| 15       | 8                    | 9   | 17    | 2.0      | 3.79    | 0.67   | 1.83       |
| 16       | 8                    | 8   | 16    | 1.68     | 2.8     | 0.4    | 1.61       |
| 17       | 9                    | 5   | 14    | 2.0      | 4.08    | 0.74   | 1.87       |
| 18       | 8                    | 7   | 15    | 1.92     | 3.06    | 0.56   | 1.71       |
| 19       | 8                    | 5   | 13    | 1.91     | 2.97    | 0.62   | 1.82       |
| 20       | 9                    | 5   | 14    | 2.22     | 4.62    | 0.79   | 2.02       |
| 21       | 10                   | 9   | 19    | 1.71     | 2.93    | 0.61   | 1.43       |
| 22       | 10                   | 5   | 15    | 2.11     | 4.28    | 0.93   | 2.22       |
| 23       | 8                    | 8   | 16    | 1.7      | 4.18    | 0.76   | 1.41       |
| 24       | 4                    | 7   | 11    | 1.78     | 3.14    | 0.5    | 1.74       |
| 25       | 7                    | 5   | 12    | 1.55     | 2.79    | 0.48   | 1.56       |

10.2.1 Bar graph : Dihedral violation statistics for each model ⓘ



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

10.3 Dihedral-angle violation statistics for the ensemble ⓘ

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

| Number of violated restraints |     |       | Fraction of the ensemble |      |
|-------------------------------|-----|-------|--------------------------|------|
| PSI                           | PHI | Total | Count <sup>1</sup>       | %    |
| 2                             | 4   | 6     | 1                        | 4.0  |
| 2                             | 3   | 5     | 2                        | 8.0  |
| 1                             | 1   | 2     | 3                        | 12.0 |
| 1                             | 2   | 3     | 4                        | 16.0 |
| 0                             | 0   | 0     | 5                        | 20.0 |
| 1                             | 0   | 1     | 6                        | 24.0 |
| 0                             | 2   | 2     | 7                        | 28.0 |
| 0                             | 0   | 0     | 8                        | 32.0 |
| 3                             | 1   | 4     | 9                        | 36.0 |
| 0                             | 1   | 1     | 10                       | 40.0 |
| 1                             | 0   | 1     | 11                       | 44.0 |

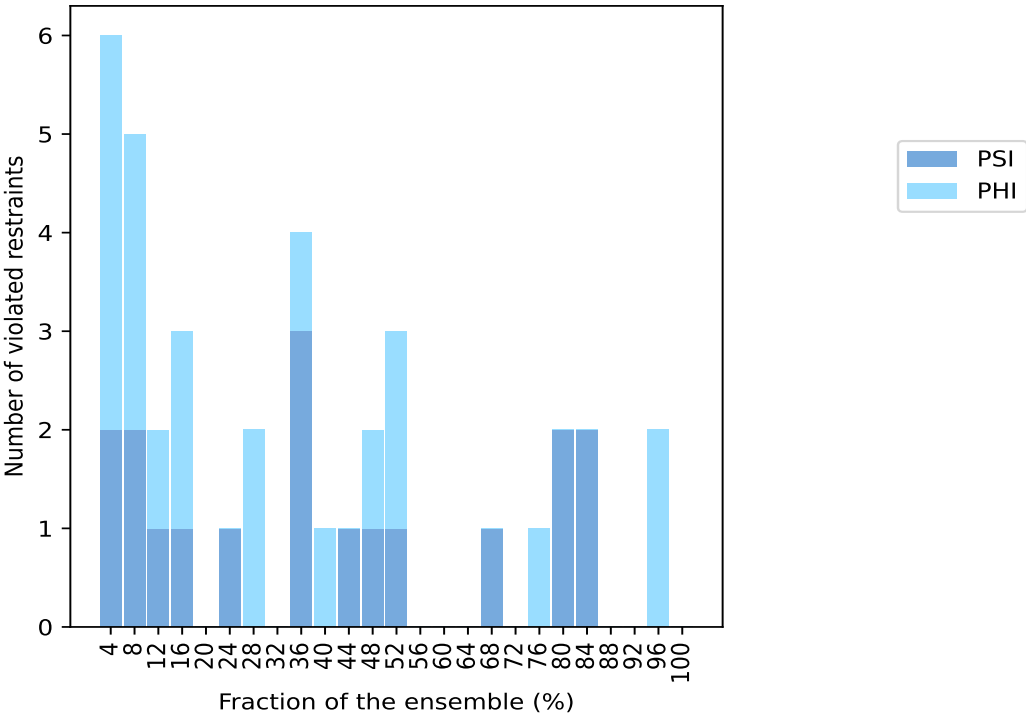
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| Number of violated restraints |     |       | Fraction of the ensemble |       |
|-------------------------------|-----|-------|--------------------------|-------|
| PSI                           | PHI | Total | Count <sup>1</sup>       | %     |
| 1                             | 1   | 2     | 12                       | 48.0  |
| 1                             | 2   | 3     | 13                       | 52.0  |
| 0                             | 0   | 0     | 14                       | 56.0  |
| 0                             | 0   | 0     | 15                       | 60.0  |
| 0                             | 0   | 0     | 16                       | 64.0  |
| 1                             | 0   | 1     | 17                       | 68.0  |
| 0                             | 0   | 0     | 18                       | 72.0  |
| 0                             | 1   | 1     | 19                       | 76.0  |
| 2                             | 0   | 2     | 20                       | 80.0  |
| 2                             | 0   | 2     | 21                       | 84.0  |
| 0                             | 0   | 0     | 22                       | 88.0  |
| 0                             | 0   | 0     | 23                       | 92.0  |
| 0                             | 2   | 2     | 24                       | 96.0  |
| 0                             | 0   | 0     | 25                       | 100.0 |

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

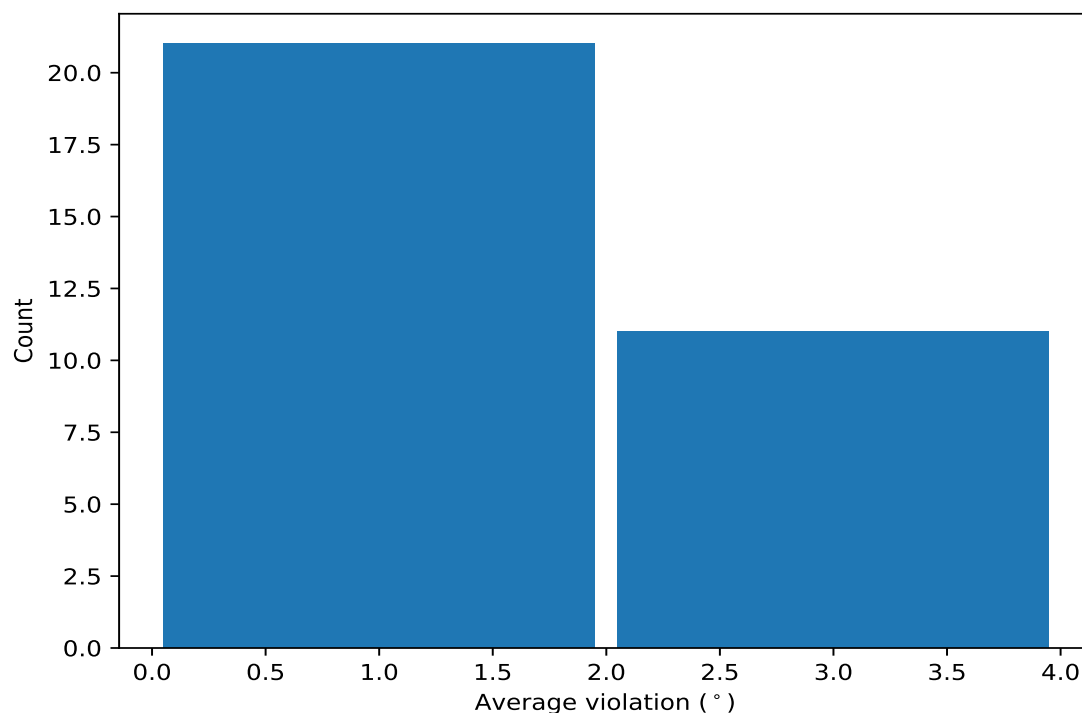
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble ⓘ



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

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

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



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

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

| Key    | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Models <sup>1</sup> | Mean | SD <sup>2</sup> | Median |
|--------|--------------|---------------|---------------|--------------|---------------------|------|-----------------|--------|
| (1,47) | 2:87:B:PHE:C | 2:88:B:PRO:N  | 2:88:B:PRO:CA | 2:88:B:PRO:C | 24                  | 2.4  | 0.9             | 2.18   |
| (1,9)  | 1:9:A:PRO:C  | 1:10:A:GLY:N  | 1:10:A:GLY:CA | 1:10:A:GLY:C | 24                  | 1.99 | 0.4             | 1.98   |
| (1,12) | 1:11:A:TRP:N | 1:11:A:TRP:CA | 1:11:A:TRP:C  | 1:12:A:GLU:N | 21                  | 2.31 | 0.8             | 2.54   |
| (1,4)  | 1:7:A:LEU:N  | 1:7:A:LEU:CA  | 1:7:A:LEU:C   | 1:8:A:PRO:N  | 21                  | 2.27 | 1.17            | 1.78   |
| (1,26) | 1:20:A:GLY:N | 1:20:A:GLY:CA | 1:20:A:GLY:C  | 1:21:A:ARG:N | 20                  | 2.35 | 0.81            | 2.32   |
| (1,38) | 1:28:A:ILE:N | 1:28:A:ILE:CA | 1:28:A:ILE:C  | 1:29:A:THR:N | 20                  | 1.48 | 0.39            | 1.4    |
| (1,43) | 1:35:A:GLU:C | 1:36:A:ARG:N  | 1:36:A:ARG:CA | 1:36:A:ARG:C | 19                  | 1.9  | 0.5             | 1.74   |
| (1,32) | 1:23:A:TYR:N | 1:23:A:TYR:CA | 1:23:A:TYR:C  | 1:24:A:TYR:N | 17                  | 1.93 | 0.62            | 1.77   |
| (1,25) | 1:19:A:SER:C | 1:20:A:GLY:N  | 1:20:A:GLY:CA | 1:20:A:GLY:C | 13                  | 2.31 | 0.88            | 2.17   |
| (1,18) | 1:14:A:ARG:N | 1:14:A:ARG:CA | 1:14:A:ARG:C  | 1:15:A:MET:N | 13                  | 2.08 | 0.55            | 2.28   |
| (1,37) | 1:27:A:HIS:C | 1:28:A:ILE:N  | 1:28:A:ILE:CA | 1:28:A:ILE:C | 13                  | 1.38 | 0.15            | 1.43   |
| (1,13) | 1:11:A:TRP:C | 1:12:A:GLU:N  | 1:12:A:GLU:CA | 1:12:A:GLU:C | 12                  | 1.73 | 0.78            | 1.23   |
| (1,24) | 1:18:A:SER:N | 1:18:A:SER:CA | 1:18:A:SER:C  | 1:19:A:SER:N | 12                  | 1.47 | 0.44            | 1.2    |

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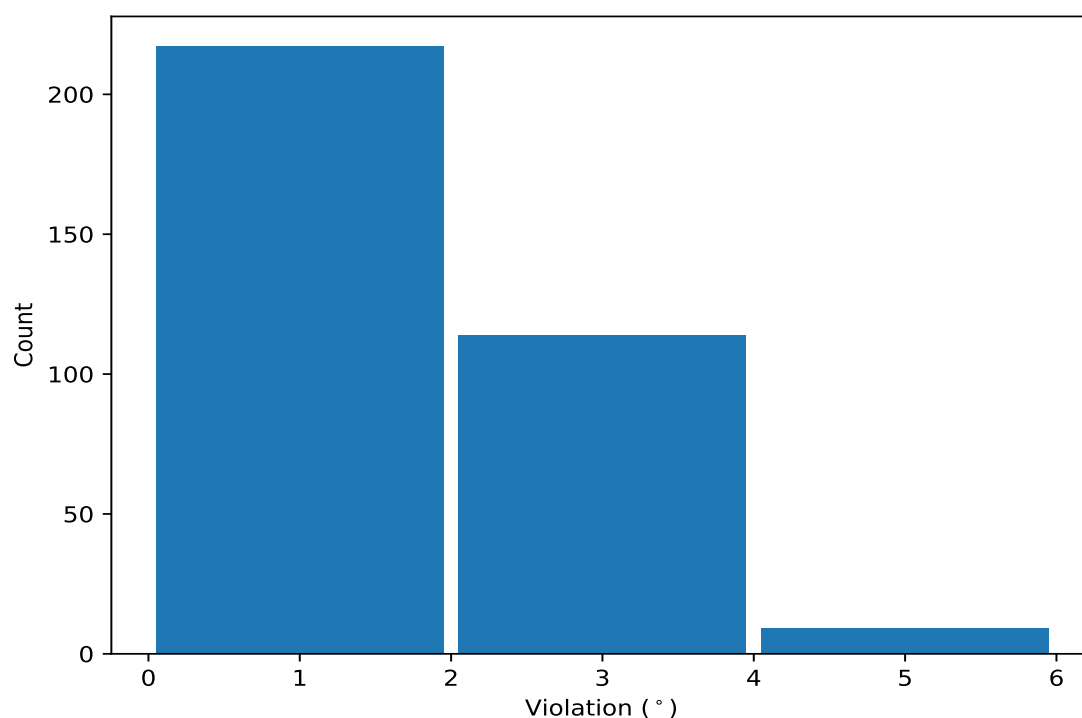
| Key    | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Models <sup>1</sup> | Mean | SD <sup>2</sup> | Median |
|--------|--------------|---------------|---------------|--------------|---------------------|------|-----------------|--------|
| (1,28) | 1:21:A:ARG:N | 1:21:A:ARG:CA | 1:21:A:ARG:C  | 1:22:A:VAL:N | 11                  | 1.84 | 0.54            | 2.01   |
| (1,27) | 1:20:A:GLY:C | 1:21:A:ARG:N  | 1:21:A:ARG:CA | 1:21:A:ARG:C | 10                  | 2.26 | 1.0             | 1.78   |
| (1,45) | 1:36:A:ARG:C | 1:37:A:PRO:N  | 1:37:A:PRO:CA | 1:37:A:PRO:C | 9                   | 2.28 | 0.97            | 2.17   |
| (1,34) | 1:24:A:TYR:N | 1:24:A:TYR:CA | 1:24:A:TYR:C  | 1:25:A:PHE:N | 9                   | 1.65 | 0.31            | 1.75   |
| (1,42) | 1:33:A:GLN:N | 1:33:A:GLN:CA | 1:33:A:GLN:C  | 1:34:A:TRP:N | 9                   | 1.61 | 0.27            | 1.55   |
| (1,40) | 1:32:A:SER:N | 1:32:A:SER:CA | 1:32:A:SER:C  | 1:33:A:GLN:N | 9                   | 1.51 | 0.45            | 1.47   |
| (1,1)  | 1:5:A:GLU:C  | 1:6:A:LYS:N   | 1:6:A:LYS:CA  | 1:6:A:LYS:C  | 7                   | 1.49 | 0.31            | 1.36   |
| (1,31) | 1:22:A:VAL:C | 1:23:A:TYR:N  | 1:23:A:TYR:CA | 1:23:A:TYR:C | 7                   | 1.41 | 0.23            | 1.35   |
| (1,36) | 1:25:A:PHE:N | 1:25:A:PHE:CA | 1:25:A:PHE:C  | 1:26:A:ASN:N | 6                   | 1.67 | 0.31            | 1.68   |
| (1,2)  | 1:6:A:LYS:N  | 1:6:A:LYS:CA  | 1:6:A:LYS:C   | 1:7:A:LEU:N  | 4                   | 1.92 | 1.13            | 1.38   |
| (1,29) | 1:21:A:ARG:C | 1:22:A:VAL:N  | 1:22:A:VAL:CA | 1:22:A:VAL:C | 4                   | 1.37 | 0.12            | 1.32   |
| (1,21) | 1:16:A:SER:C | 1:17:A:ARG:N  | 1:17:A:ARG:CA | 1:17:A:ARG:C | 4                   | 1.33 | 0.23            | 1.26   |
| (1,44) | 1:36:A:ARG:N | 1:36:A:ARG:CA | 1:36:A:ARG:C  | 1:37:A:PRO:N | 3                   | 2.19 | 0.8             | 2.54   |
| (1,39) | 1:31:A:ALA:C | 1:32:A:SER:N  | 1:32:A:SER:CA | 1:32:A:SER:C | 3                   | 1.61 | 0.25            | 1.7    |
| (1,17) | 1:13:A:LYS:C | 1:14:A:ARG:N  | 1:14:A:ARG:CA | 1:14:A:ARG:C | 2                   | 2.4  | 0.29            | 2.4    |
| (1,3)  | 1:6:A:LYS:C  | 1:7:A:LEU:N   | 1:7:A:LEU:CA  | 1:7:A:LEU:C  | 2                   | 2.06 | 0.55            | 2.06   |
| (1,15) | 1:12:A:GLU:C | 1:13:A:LYS:N  | 1:13:A:LYS:CA | 1:13:A:LYS:C | 2                   | 1.67 | 0.33            | 1.67   |
| (1,46) | 1:37:A:PRO:N | 1:37:A:PRO:CA | 1:37:A:PRO:C  | 1:38:A:SER:N | 2                   | 1.52 | 0.09            | 1.52   |
| (1,6)  | 1:8:A:PRO:N  | 1:8:A:PRO:CA  | 1:8:A:PRO:C   | 1:9:A:PRO:N  | 2                   | 1.05 | 0.01            | 1.05   |

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

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

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

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



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

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

| Key    | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Model ID | Violation (°) |
|--------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,4)  | 1:7:A:LEU:N  | 1:7:A:LEU:CA  | 1:7:A:LEU:C   | 1:8:A:PRO:N  | 11       | 5.41          |
| (1,47) | 2:87:B:PHE:C | 2:88:B:PRO:N  | 2:88:B:PRO:CA | 2:88:B:PRO:C | 3        | 4.85          |
| (1,4)  | 1:7:A:LEU:N  | 1:7:A:LEU:CA  | 1:7:A:LEU:C   | 1:8:A:PRO:N  | 20       | 4.62          |
| (1,26) | 1:20:A:GLY:N | 1:20:A:GLY:CA | 1:20:A:GLY:C  | 1:21:A:ARG:N | 22       | 4.28          |
| (1,27) | 1:20:A:GLY:C | 1:21:A:ARG:N  | 1:21:A:ARG:CA | 1:21:A:ARG:C | 11       | 4.19          |
| (1,47) | 2:87:B:PHE:C | 2:88:B:PRO:N  | 2:88:B:PRO:CA | 2:88:B:PRO:C | 23       | 4.18          |
| (1,4)  | 1:7:A:LEU:N  | 1:7:A:LEU:CA  | 1:7:A:LEU:C   | 1:8:A:PRO:N  | 17       | 4.08          |
| (1,25) | 1:19:A:SER:C | 1:20:A:GLY:N  | 1:20:A:GLY:CA | 1:20:A:GLY:C | 13       | 4.03          |
| (1,26) | 1:20:A:GLY:N | 1:20:A:GLY:CA | 1:20:A:GLY:C  | 1:21:A:ARG:N | 10       | 4.0           |
| (1,25) | 1:19:A:SER:C | 1:20:A:GLY:N  | 1:20:A:GLY:CA | 1:20:A:GLY:C | 3        | 3.9           |
| (1,2)  | 1:6:A:LYS:N  | 1:6:A:LYS:CA  | 1:6:A:LYS:C   | 1:7:A:LEU:N  | 2        | 3.85          |
| (1,45) | 1:36:A:ARG:C | 1:37:A:PRO:N  | 1:37:A:PRO:CA | 1:37:A:PRO:C | 8        | 3.83          |
| (1,12) | 1:11:A:TRP:N | 1:11:A:TRP:CA | 1:11:A:TRP:C  | 1:12:A:GLU:N | 15       | 3.79          |
| (1,45) | 1:36:A:ARG:C | 1:37:A:PRO:N  | 1:37:A:PRO:CA | 1:37:A:PRO:C | 2        | 3.62          |
| (1,47) | 2:87:B:PHE:C | 2:88:B:PRO:N  | 2:88:B:PRO:CA | 2:88:B:PRO:C | 22       | 3.48          |
| (1,27) | 1:20:A:GLY:C | 1:21:A:ARG:N  | 1:21:A:ARG:CA | 1:21:A:ARG:C | 3        | 3.46          |
| (1,12) | 1:11:A:TRP:N | 1:11:A:TRP:CA | 1:11:A:TRP:C  | 1:12:A:GLU:N | 7        | 3.4           |
| (1,12) | 1:11:A:TRP:N | 1:11:A:TRP:CA | 1:11:A:TRP:C  | 1:12:A:GLU:N | 1        | 3.37          |
| (1,4)  | 1:7:A:LEU:N  | 1:7:A:LEU:CA  | 1:7:A:LEU:C   | 1:8:A:PRO:N  | 5        | 3.35          |
| (1,4)  | 1:7:A:LEU:N  | 1:7:A:LEU:CA  | 1:7:A:LEU:C   | 1:8:A:PRO:N  | 9        | 3.35          |
| (1,26) | 1:20:A:GLY:N | 1:20:A:GLY:CA | 1:20:A:GLY:C  | 1:21:A:ARG:N | 11       | 3.25          |

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| Key    | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Model ID | Violation (°) |
|--------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,47) | 2:87:B:PHE:C | 2:88:B:PRO:N  | 2:88:B:PRO:CA | 2:88:B:PRO:C | 2        | 3.24          |
| (1,45) | 1:36:A:ARG:C | 1:37:A:PRO:N  | 1:37:A:PRO:CA | 1:37:A:PRO:C | 6        | 3.21          |
| (1,32) | 1:23:A:TYR:N | 1:23:A:TYR:CA | 1:23:A:TYR:C  | 1:24:A:TYR:N | 6        | 3.18          |
| (1,47) | 2:87:B:PHE:C | 2:88:B:PRO:N  | 2:88:B:PRO:CA | 2:88:B:PRO:C | 10       | 3.17          |
| (1,25) | 1:19:A:SER:C | 1:20:A:GLY:N  | 1:20:A:GLY:CA | 1:20:A:GLY:C | 24       | 3.14          |
| (1,27) | 1:20:A:GLY:C | 1:21:A:ARG:N  | 1:21:A:ARG:CA | 1:21:A:ARG:C | 10       | 3.08          |
| (1,12) | 1:11:A:TRP:N | 1:11:A:TRP:CA | 1:11:A:TRP:C  | 1:12:A:GLU:N | 4        | 3.08          |
| (1,47) | 2:87:B:PHE:C | 2:88:B:PRO:N  | 2:88:B:PRO:CA | 2:88:B:PRO:C | 18       | 3.06          |
| (1,28) | 1:21:A:ARG:N | 1:21:A:ARG:CA | 1:21:A:ARG:C  | 1:22:A:VAL:N | 7        | 3.05          |
| (1,13) | 1:11:A:TRP:C | 1:12:A:GLU:N  | 1:12:A:GLU:CA | 1:12:A:GLU:C | 19       | 2.97          |
| (1,44) | 1:36:A:ARG:N | 1:36:A:ARG:CA | 1:36:A:ARG:C  | 1:37:A:PRO:N | 6        | 2.94          |
| (1,13) | 1:11:A:TRP:C | 1:12:A:GLU:N  | 1:12:A:GLU:CA | 1:12:A:GLU:C | 21       | 2.93          |
| (1,18) | 1:14:A:ARG:N | 1:14:A:ARG:CA | 1:14:A:ARG:C  | 1:15:A:MET:N | 22       | 2.87          |
| (1,12) | 1:11:A:TRP:N | 1:11:A:TRP:CA | 1:11:A:TRP:C  | 1:12:A:GLU:N | 21       | 2.87          |
| (1,26) | 1:20:A:GLY:N | 1:20:A:GLY:CA | 1:20:A:GLY:C  | 1:21:A:ARG:N | 14       | 2.86          |
| (1,32) | 1:23:A:TYR:N | 1:23:A:TYR:CA | 1:23:A:TYR:C  | 1:24:A:TYR:N | 15       | 2.85          |
| (1,47) | 2:87:B:PHE:C | 2:88:B:PRO:N  | 2:88:B:PRO:CA | 2:88:B:PRO:C | 12       | 2.82          |
| (1,43) | 1:35:A:GLU:C | 1:36:A:ARG:N  | 1:36:A:ARG:CA | 1:36:A:ARG:C | 6        | 2.81          |
| (1,13) | 1:11:A:TRP:C | 1:12:A:GLU:N  | 1:12:A:GLU:CA | 1:12:A:GLU:C | 15       | 2.8           |
| (1,12) | 1:11:A:TRP:N | 1:11:A:TRP:CA | 1:11:A:TRP:C  | 1:12:A:GLU:N | 16       | 2.8           |
| (1,12) | 1:11:A:TRP:N | 1:11:A:TRP:CA | 1:11:A:TRP:C  | 1:12:A:GLU:N | 25       | 2.79          |
| (1,27) | 1:20:A:GLY:C | 1:21:A:ARG:N  | 1:21:A:ARG:CA | 1:21:A:ARG:C | 22       | 2.77          |
| (1,18) | 1:14:A:ARG:N | 1:14:A:ARG:CA | 1:14:A:ARG:C  | 1:15:A:MET:N | 1        | 2.74          |
| (1,9)  | 1:9:A:PRO:C  | 1:10:A:GLY:N  | 1:10:A:GLY:CA | 1:10:A:GLY:C | 11       | 2.71          |
| (1,43) | 1:35:A:GLU:C | 1:36:A:ARG:N  | 1:36:A:ARG:CA | 1:36:A:ARG:C | 7        | 2.7           |
| (1,12) | 1:11:A:TRP:N | 1:11:A:TRP:CA | 1:11:A:TRP:C  | 1:12:A:GLU:N | 12       | 2.7           |
| (1,26) | 1:20:A:GLY:N | 1:20:A:GLY:CA | 1:20:A:GLY:C  | 1:21:A:ARG:N | 5        | 2.69          |
| (1,17) | 1:13:A:LYS:C | 1:14:A:ARG:N  | 1:14:A:ARG:CA | 1:14:A:ARG:C | 20       | 2.69          |
| (1,25) | 1:19:A:SER:C | 1:20:A:GLY:N  | 1:20:A:GLY:CA | 1:20:A:GLY:C | 19       | 2.68          |
| (1,43) | 1:35:A:GLU:C | 1:36:A:ARG:N  | 1:36:A:ARG:CA | 1:36:A:ARG:C | 19       | 2.66          |
| (1,26) | 1:20:A:GLY:N | 1:20:A:GLY:CA | 1:20:A:GLY:C  | 1:21:A:ARG:N | 3        | 2.66          |
| (1,32) | 1:23:A:TYR:N | 1:23:A:TYR:CA | 1:23:A:TYR:C  | 1:24:A:TYR:N | 20       | 2.65          |
| (1,32) | 1:23:A:TYR:N | 1:23:A:TYR:CA | 1:23:A:TYR:C  | 1:24:A:TYR:N | 21       | 2.65          |
| (1,12) | 1:11:A:TRP:N | 1:11:A:TRP:CA | 1:11:A:TRP:C  | 1:12:A:GLU:N | 14       | 2.65          |
| (1,26) | 1:20:A:GLY:N | 1:20:A:GLY:CA | 1:20:A:GLY:C  | 1:21:A:ARG:N | 2        | 2.64          |
| (1,25) | 1:19:A:SER:C | 1:20:A:GLY:N  | 1:20:A:GLY:CA | 1:20:A:GLY:C | 18       | 2.64          |
| (1,18) | 1:14:A:ARG:N | 1:14:A:ARG:CA | 1:14:A:ARG:C  | 1:15:A:MET:N | 9        | 2.63          |
| (1,9)  | 1:9:A:PRO:C  | 1:10:A:GLY:N  | 1:10:A:GLY:CA | 1:10:A:GLY:C | 15       | 2.63          |
| (1,26) | 1:20:A:GLY:N | 1:20:A:GLY:CA | 1:20:A:GLY:C  | 1:21:A:ARG:N | 23       | 2.62          |
| (1,47) | 2:87:B:PHE:C | 2:88:B:PRO:N  | 2:88:B:PRO:CA | 2:88:B:PRO:C | 6        | 2.61          |
| (1,47) | 2:87:B:PHE:C | 2:88:B:PRO:N  | 2:88:B:PRO:CA | 2:88:B:PRO:C | 7        | 2.61          |
| (1,3)  | 1:6:A:LYS:C  | 1:7:A:LEU:N   | 1:7:A:LEU:CA  | 1:7:A:LEU:C  | 9        | 2.61          |
| (1,9)  | 1:9:A:PRO:C  | 1:10:A:GLY:N  | 1:10:A:GLY:CA | 1:10:A:GLY:C | 2        | 2.6           |
| (1,47) | 2:87:B:PHE:C | 2:88:B:PRO:N  | 2:88:B:PRO:CA | 2:88:B:PRO:C | 21       | 2.59          |
| (1,47) | 2:87:B:PHE:C | 2:88:B:PRO:N  | 2:88:B:PRO:CA | 2:88:B:PRO:C | 4        | 2.58          |
| (1,13) | 1:11:A:TRP:C | 1:12:A:GLU:N  | 1:12:A:GLU:CA | 1:12:A:GLU:C | 1        | 2.57          |
| (1,12) | 1:11:A:TRP:N | 1:11:A:TRP:CA | 1:11:A:TRP:C  | 1:12:A:GLU:N | 20       | 2.56          |
| (1,9)  | 1:9:A:PRO:C  | 1:10:A:GLY:N  | 1:10:A:GLY:CA | 1:10:A:GLY:C | 14       | 2.55          |
| (1,44) | 1:36:A:ARG:N | 1:36:A:ARG:CA | 1:36:A:ARG:C  | 1:37:A:PRO:N | 17       | 2.54          |
| (1,43) | 1:35:A:GLU:C | 1:36:A:ARG:N  | 1:36:A:ARG:CA | 1:36:A:ARG:C | 12       | 2.54          |
| (1,12) | 1:11:A:TRP:N | 1:11:A:TRP:CA | 1:11:A:TRP:C  | 1:12:A:GLU:N | 13       | 2.54          |

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| Key    | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Model ID | Violation (°) |
|--------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,18) | 1:14:A:ARG:N | 1:14:A:ARG:CA | 1:14:A:ARG:C  | 1:15:A:MET:N | 17       | 2.51          |
| (1,43) | 1:35:A:GLU:C | 1:36:A:ARG:N  | 1:36:A:ARG:CA | 1:36:A:ARG:C | 20       | 2.48          |
| (1,32) | 1:23:A:TYR:N | 1:23:A:TYR:CA | 1:23:A:TYR:C  | 1:24:A:TYR:N | 10       | 2.48          |
| (1,38) | 1:28:A:ILE:N | 1:28:A:ILE:CA | 1:28:A:ILE:C  | 1:29:A:THR:N | 18       | 2.47          |
| (1,26) | 1:20:A:GLY:N | 1:20:A:GLY:CA | 1:20:A:GLY:C  | 1:21:A:ARG:N | 17       | 2.44          |
| (1,26) | 1:20:A:GLY:N | 1:20:A:GLY:CA | 1:20:A:GLY:C  | 1:21:A:ARG:N | 18       | 2.41          |
| (1,4)  | 1:7:A:LEU:N  | 1:7:A:LEU:CA  | 1:7:A:LEU:C   | 1:8:A:PRO:N  | 19       | 2.41          |
| (1,12) | 1:11:A:TRP:N | 1:11:A:TRP:CA | 1:11:A:TRP:C  | 1:12:A:GLU:N | 22       | 2.4           |
| (1,9)  | 1:9:A:PRO:C  | 1:10:A:GLY:N  | 1:10:A:GLY:CA | 1:10:A:GLY:C | 10       | 2.4           |
| (1,9)  | 1:9:A:PRO:C  | 1:10:A:GLY:N  | 1:10:A:GLY:CA | 1:10:A:GLY:C | 18       | 2.39          |
| (1,12) | 1:11:A:TRP:N | 1:11:A:TRP:CA | 1:11:A:TRP:C  | 1:12:A:GLU:N | 19       | 2.37          |
| (1,18) | 1:14:A:ARG:N | 1:14:A:ARG:CA | 1:14:A:ARG:C  | 1:15:A:MET:N | 18       | 2.36          |
| (1,18) | 1:14:A:ARG:N | 1:14:A:ARG:CA | 1:14:A:ARG:C  | 1:15:A:MET:N | 14       | 2.35          |
| (1,40) | 1:32:A:SER:N | 1:32:A:SER:CA | 1:32:A:SER:C  | 1:33:A:GLN:N | 22       | 2.3           |
| (1,18) | 1:14:A:ARG:N | 1:14:A:ARG:CA | 1:14:A:ARG:C  | 1:15:A:MET:N | 23       | 2.28          |
| (1,24) | 1:18:A:SER:N | 1:18:A:SER:CA | 1:18:A:SER:C  | 1:19:A:SER:N | 22       | 2.26          |
| (1,26) | 1:20:A:GLY:N | 1:20:A:GLY:CA | 1:20:A:GLY:C  | 1:21:A:ARG:N | 6        | 2.23          |
| (1,47) | 2:87:B:PHE:C | 2:88:B:PRO:N  | 2:88:B:PRO:CA | 2:88:B:PRO:C | 13       | 2.22          |
| (1,36) | 1:25:A:PHE:N | 1:25:A:PHE:CA | 1:25:A:PHE:C  | 1:26:A:ASN:N | 22       | 2.22          |
| (1,26) | 1:20:A:GLY:N | 1:20:A:GLY:CA | 1:20:A:GLY:C  | 1:21:A:ARG:N | 1        | 2.22          |
| (1,43) | 1:35:A:GLU:C | 1:36:A:ARG:N  | 1:36:A:ARG:CA | 1:36:A:ARG:C | 8        | 2.21          |
| (1,25) | 1:19:A:SER:C | 1:20:A:GLY:N  | 1:20:A:GLY:CA | 1:20:A:GLY:C | 4        | 2.2           |
| (1,45) | 1:36:A:ARG:C | 1:37:A:PRO:N  | 1:37:A:PRO:CA | 1:37:A:PRO:C | 10       | 2.18          |
| (1,32) | 1:23:A:TYR:N | 1:23:A:TYR:CA | 1:23:A:TYR:C  | 1:24:A:TYR:N | 7        | 2.18          |
| (1,45) | 1:36:A:ARG:C | 1:37:A:PRO:N  | 1:37:A:PRO:CA | 1:37:A:PRO:C | 17       | 2.17          |
| (1,25) | 1:19:A:SER:C | 1:20:A:GLY:N  | 1:20:A:GLY:CA | 1:20:A:GLY:C | 9        | 2.17          |
| (1,9)  | 1:9:A:PRO:C  | 1:10:A:GLY:N  | 1:10:A:GLY:CA | 1:10:A:GLY:C | 13       | 2.17          |
| (1,4)  | 1:7:A:LEU:N  | 1:7:A:LEU:CA  | 1:7:A:LEU:C   | 1:8:A:PRO:N  | 16       | 2.17          |
| (1,9)  | 1:9:A:PRO:C  | 1:10:A:GLY:N  | 1:10:A:GLY:CA | 1:10:A:GLY:C | 7        | 2.16          |
| (1,4)  | 1:7:A:LEU:N  | 1:7:A:LEU:CA  | 1:7:A:LEU:C   | 1:8:A:PRO:N  | 15       | 2.16          |
| (1,47) | 2:87:B:PHE:C | 2:88:B:PRO:N  | 2:88:B:PRO:CA | 2:88:B:PRO:C | 14       | 2.14          |
| (1,28) | 1:21:A:ARG:N | 1:21:A:ARG:CA | 1:21:A:ARG:C  | 1:22:A:VAL:N | 20       | 2.14          |
| (1,9)  | 1:9:A:PRO:C  | 1:10:A:GLY:N  | 1:10:A:GLY:CA | 1:10:A:GLY:C | 4        | 2.13          |
| (1,9)  | 1:9:A:PRO:C  | 1:10:A:GLY:N  | 1:10:A:GLY:CA | 1:10:A:GLY:C | 21       | 2.12          |
| (1,28) | 1:21:A:ARG:N | 1:21:A:ARG:CA | 1:21:A:ARG:C  | 1:22:A:VAL:N | 24       | 2.1           |
| (1,17) | 1:13:A:LYS:C | 1:14:A:ARG:N  | 1:14:A:ARG:CA | 1:14:A:ARG:C | 7        | 2.1           |
| (1,42) | 1:33:A:GLN:N | 1:33:A:GLN:CA | 1:33:A:GLN:C  | 1:34:A:TRP:N | 17       | 2.09          |
| (1,32) | 1:23:A:TYR:N | 1:23:A:TYR:CA | 1:23:A:TYR:C  | 1:24:A:TYR:N | 12       | 2.08          |
| (1,9)  | 1:9:A:PRO:C  | 1:10:A:GLY:N  | 1:10:A:GLY:CA | 1:10:A:GLY:C | 19       | 2.08          |
| (1,47) | 2:87:B:PHE:C | 2:88:B:PRO:N  | 2:88:B:PRO:CA | 2:88:B:PRO:C | 20       | 2.06          |
| (1,28) | 1:21:A:ARG:N | 1:21:A:ARG:CA | 1:21:A:ARG:C  | 1:22:A:VAL:N | 15       | 2.06          |
| (1,4)  | 1:7:A:LEU:N  | 1:7:A:LEU:CA  | 1:7:A:LEU:C   | 1:8:A:PRO:N  | 21       | 2.06          |
| (1,34) | 1:24:A:TYR:N | 1:24:A:TYR:CA | 1:24:A:TYR:C  | 1:25:A:PHE:N | 12       | 2.05          |
| (1,28) | 1:21:A:ARG:N | 1:21:A:ARG:CA | 1:21:A:ARG:C  | 1:22:A:VAL:N | 16       | 2.02          |
| (1,1)  | 1:5:A:GLU:C  | 1:6:A:LYS:N   | 1:6:A:LYS:CA  | 1:6:A:LYS:C  | 5        | 2.02          |
| (1,40) | 1:32:A:SER:N | 1:32:A:SER:CA | 1:32:A:SER:C  | 1:33:A:GLN:N | 3        | 2.01          |
| (1,28) | 1:21:A:ARG:N | 1:21:A:ARG:CA | 1:21:A:ARG:C  | 1:22:A:VAL:N | 13       | 2.01          |
| (1,26) | 1:20:A:GLY:N | 1:20:A:GLY:CA | 1:20:A:GLY:C  | 1:21:A:ARG:N | 25       | 2.01          |
| (1,9)  | 1:9:A:PRO:C  | 1:10:A:GLY:N  | 1:10:A:GLY:CA | 1:10:A:GLY:C | 8        | 2.01          |
| (1,24) | 1:18:A:SER:N | 1:18:A:SER:CA | 1:18:A:SER:C  | 1:19:A:SER:N | 3        | 2.0           |
| (1,15) | 1:12:A:GLU:C | 1:13:A:LYS:N  | 1:13:A:LYS:CA | 1:13:A:LYS:C | 12       | 2.0           |

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| Key    | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Model ID | Violation (°) |
|--------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,43) | 1:35:A:GLU:C | 1:36:A:ARG:N  | 1:36:A:ARG:CA | 1:36:A:ARG:C | 15       | 1.99          |
| (1,24) | 1:18:A:SER:N | 1:18:A:SER:CA | 1:18:A:SER:C  | 1:19:A:SER:N | 20       | 1.99          |
| (1,38) | 1:28:A:ILE:N | 1:28:A:ILE:CA | 1:28:A:ILE:C  | 1:29:A:THR:N | 3        | 1.98          |
| (1,24) | 1:18:A:SER:N | 1:18:A:SER:CA | 1:18:A:SER:C  | 1:19:A:SER:N | 1        | 1.97          |
| (1,38) | 1:28:A:ILE:N | 1:28:A:ILE:CA | 1:28:A:ILE:C  | 1:29:A:THR:N | 6        | 1.95          |
| (1,12) | 1:11:A:TRP:N | 1:11:A:TRP:CA | 1:11:A:TRP:C  | 1:12:A:GLU:N | 17       | 1.95          |
| (1,43) | 1:35:A:GLU:C | 1:36:A:ARG:N  | 1:36:A:ARG:CA | 1:36:A:ARG:C | 1        | 1.94          |
| (1,42) | 1:33:A:GLN:N | 1:33:A:GLN:CA | 1:33:A:GLN:C  | 1:34:A:TRP:N | 23       | 1.94          |
| (1,34) | 1:24:A:TYR:N | 1:24:A:TYR:CA | 1:24:A:TYR:C  | 1:25:A:PHE:N | 8        | 1.94          |
| (1,18) | 1:14:A:ARG:N | 1:14:A:ARG:CA | 1:14:A:ARG:C  | 1:15:A:MET:N | 24       | 1.94          |
| (1,9)  | 1:9:A:PRO:C  | 1:10:A:GLY:N  | 1:10:A:GLY:CA | 1:10:A:GLY:C | 16       | 1.94          |
| (1,38) | 1:28:A:ILE:N | 1:28:A:ILE:CA | 1:28:A:ILE:C  | 1:29:A:THR:N | 7        | 1.93          |
| (1,26) | 1:20:A:GLY:N | 1:20:A:GLY:CA | 1:20:A:GLY:C  | 1:21:A:ARG:N | 9        | 1.93          |
| (1,9)  | 1:9:A:PRO:C  | 1:10:A:GLY:N  | 1:10:A:GLY:CA | 1:10:A:GLY:C | 20       | 1.92          |
| (1,47) | 2:87:B:PHE:C | 2:88:B:PRO:N  | 2:88:B:PRO:CA | 2:88:B:PRO:C | 1        | 1.91          |
| (1,34) | 1:24:A:TYR:N | 1:24:A:TYR:CA | 1:24:A:TYR:C  | 1:25:A:PHE:N | 15       | 1.9           |
| (1,4)  | 1:7:A:LEU:N  | 1:7:A:LEU:CA  | 1:7:A:LEU:C   | 1:8:A:PRO:N  | 8        | 1.9           |
| (1,10) | 1:10:A:GLY:N | 1:10:A:GLY:CA | 1:10:A:GLY:C  | 1:11:A:TRP:N | 13       | 1.89          |
| (1,9)  | 1:9:A:PRO:C  | 1:10:A:GLY:N  | 1:10:A:GLY:CA | 1:10:A:GLY:C | 24       | 1.89          |
| (1,47) | 2:87:B:PHE:C | 2:88:B:PRO:N  | 2:88:B:PRO:CA | 2:88:B:PRO:C | 9        | 1.88          |
| (1,31) | 1:22:A:VAL:C | 1:23:A:TYR:N  | 1:23:A:TYR:CA | 1:23:A:TYR:C | 6        | 1.87          |
| (1,39) | 1:31:A:ALA:C | 1:32:A:SER:N  | 1:32:A:SER:CA | 1:32:A:SER:C | 2        | 1.86          |
| (1,18) | 1:14:A:ARG:N | 1:14:A:ARG:CA | 1:14:A:ARG:C  | 1:15:A:MET:N | 15       | 1.83          |
| (1,32) | 1:23:A:TYR:N | 1:23:A:TYR:CA | 1:23:A:TYR:C  | 1:24:A:TYR:N | 19       | 1.82          |
| (1,40) | 1:32:A:SER:N | 1:32:A:SER:CA | 1:32:A:SER:C  | 1:33:A:GLN:N | 20       | 1.81          |
| (1,36) | 1:25:A:PHE:N | 1:25:A:PHE:CA | 1:25:A:PHE:C  | 1:26:A:ASN:N | 10       | 1.8           |
| (1,9)  | 1:9:A:PRO:C  | 1:10:A:GLY:N  | 1:10:A:GLY:CA | 1:10:A:GLY:C | 12       | 1.8           |
| (1,47) | 2:87:B:PHE:C | 2:88:B:PRO:N  | 2:88:B:PRO:CA | 2:88:B:PRO:C | 15       | 1.79          |
| (1,42) | 1:33:A:GLN:N | 1:33:A:GLN:CA | 1:33:A:GLN:C  | 1:34:A:TRP:N | 12       | 1.79          |
| (1,27) | 1:20:A:GLY:C | 1:21:A:ARG:N  | 1:21:A:ARG:CA | 1:21:A:ARG:C | 17       | 1.79          |
| (1,26) | 1:20:A:GLY:N | 1:20:A:GLY:CA | 1:20:A:GLY:C  | 1:21:A:ARG:N | 16       | 1.79          |
| (1,38) | 1:28:A:ILE:N | 1:28:A:ILE:CA | 1:28:A:ILE:C  | 1:29:A:THR:N | 16       | 1.78          |
| (1,28) | 1:21:A:ARG:N | 1:21:A:ARG:CA | 1:21:A:ARG:C  | 1:22:A:VAL:N | 12       | 1.78          |
| (1,27) | 1:20:A:GLY:C | 1:21:A:ARG:N  | 1:21:A:ARG:CA | 1:21:A:ARG:C | 18       | 1.78          |
| (1,26) | 1:20:A:GLY:N | 1:20:A:GLY:CA | 1:20:A:GLY:C  | 1:21:A:ARG:N | 20       | 1.78          |
| (1,4)  | 1:7:A:LEU:N  | 1:7:A:LEU:CA  | 1:7:A:LEU:C   | 1:8:A:PRO:N  | 23       | 1.78          |
| (1,43) | 1:35:A:GLU:C | 1:36:A:ARG:N  | 1:36:A:ARG:CA | 1:36:A:ARG:C | 17       | 1.77          |
| (1,40) | 1:32:A:SER:N | 1:32:A:SER:CA | 1:32:A:SER:C  | 1:33:A:GLN:N | 11       | 1.77          |
| (1,32) | 1:23:A:TYR:N | 1:23:A:TYR:CA | 1:23:A:TYR:C  | 1:24:A:TYR:N | 11       | 1.77          |
| (1,47) | 2:87:B:PHE:C | 2:88:B:PRO:N  | 2:88:B:PRO:CA | 2:88:B:PRO:C | 5        | 1.76          |
| (1,4)  | 1:7:A:LEU:N  | 1:7:A:LEU:CA  | 1:7:A:LEU:C   | 1:8:A:PRO:N  | 14       | 1.76          |
| (1,47) | 2:87:B:PHE:C | 2:88:B:PRO:N  | 2:88:B:PRO:CA | 2:88:B:PRO:C | 24       | 1.75          |
| (1,34) | 1:24:A:TYR:N | 1:24:A:TYR:CA | 1:24:A:TYR:C  | 1:25:A:PHE:N | 7        | 1.75          |
| (1,34) | 1:24:A:TYR:N | 1:24:A:TYR:CA | 1:24:A:TYR:C  | 1:25:A:PHE:N | 25       | 1.75          |
| (1,11) | 1:10:A:GLY:C | 1:11:A:TRP:N  | 1:11:A:TRP:CA | 1:11:A:TRP:C | 13       | 1.75          |
| (1,43) | 1:35:A:GLU:C | 1:36:A:ARG:N  | 1:36:A:ARG:CA | 1:36:A:ARG:C | 24       | 1.74          |
| (1,1)  | 1:5:A:GLU:C  | 1:6:A:LYS:N   | 1:6:A:LYS:CA  | 1:6:A:LYS:C  | 3        | 1.74          |
| (1,38) | 1:28:A:ILE:N | 1:28:A:ILE:CA | 1:28:A:ILE:C  | 1:29:A:THR:N | 1        | 1.73          |
| (1,25) | 1:19:A:SER:C | 1:20:A:GLY:N  | 1:20:A:GLY:CA | 1:20:A:GLY:C | 7        | 1.73          |
| (1,25) | 1:19:A:SER:C | 1:20:A:GLY:N  | 1:20:A:GLY:CA | 1:20:A:GLY:C | 15       | 1.73          |
| (1,9)  | 1:9:A:PRO:C  | 1:10:A:GLY:N  | 1:10:A:GLY:CA | 1:10:A:GLY:C | 3        | 1.72          |

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| Key    | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Model ID | Violation (°) |
|--------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,4)  | 1:7:A:LEU:N  | 1:7:A:LEU:CA  | 1:7:A:LEU:C   | 1:8:A:PRO:N  | 7        | 1.72          |
| (1,32) | 1:23:A:TYR:N | 1:23:A:TYR:CA | 1:23:A:TYR:C  | 1:24:A:TYR:N | 18       | 1.71          |
| (1,1)  | 1:5:A:GLU:C  | 1:6:A:LYS:N   | 1:6:A:LYS:CA  | 1:6:A:LYS:C  | 15       | 1.71          |
| (1,39) | 1:31:A:ALA:C | 1:32:A:SER:N  | 1:32:A:SER:CA | 1:32:A:SER:C | 15       | 1.7           |
| (1,25) | 1:19:A:SER:C | 1:20:A:GLY:N  | 1:20:A:GLY:CA | 1:20:A:GLY:C | 21       | 1.7           |
| (1,9)  | 1:9:A:PRO:C  | 1:10:A:GLY:N  | 1:10:A:GLY:CA | 1:10:A:GLY:C | 1        | 1.7           |
| (1,36) | 1:25:A:PHE:N | 1:25:A:PHE:CA | 1:25:A:PHE:C  | 1:26:A:ASN:N | 20       | 1.69          |
| (1,47) | 2:87:B:PHE:C | 2:88:B:PRO:N  | 2:88:B:PRO:CA | 2:88:B:PRO:C | 16       | 1.68          |
| (1,43) | 1:35:A:GLU:C | 1:36:A:ARG:N  | 1:36:A:ARG:CA | 1:36:A:ARG:C | 3        | 1.68          |
| (1,9)  | 1:9:A:PRO:C  | 1:10:A:GLY:N  | 1:10:A:GLY:CA | 1:10:A:GLY:C | 5        | 1.68          |
| (1,9)  | 1:9:A:PRO:C  | 1:10:A:GLY:N  | 1:10:A:GLY:CA | 1:10:A:GLY:C | 22       | 1.68          |
| (1,45) | 1:36:A:ARG:C | 1:37:A:PRO:N  | 1:37:A:PRO:CA | 1:37:A:PRO:C | 16       | 1.67          |
| (1,38) | 1:28:A:ILE:N | 1:28:A:ILE:CA | 1:28:A:ILE:C  | 1:29:A:THR:N | 8        | 1.67          |
| (1,36) | 1:25:A:PHE:N | 1:25:A:PHE:CA | 1:25:A:PHE:C  | 1:26:A:ASN:N | 17       | 1.67          |
| (1,21) | 1:16:A:SER:C | 1:17:A:ARG:N  | 1:17:A:ARG:CA | 1:17:A:ARG:C | 25       | 1.67          |
| (1,12) | 1:11:A:TRP:N | 1:11:A:TRP:CA | 1:11:A:TRP:C  | 1:12:A:GLU:N | 10       | 1.67          |
| (1,27) | 1:20:A:GLY:C | 1:21:A:ARG:N  | 1:21:A:ARG:CA | 1:21:A:ARG:C | 6        | 1.65          |
| (1,18) | 1:14:A:ARG:N | 1:14:A:ARG:CA | 1:14:A:ARG:C  | 1:15:A:MET:N | 6        | 1.63          |
| (1,12) | 1:11:A:TRP:N | 1:11:A:TRP:CA | 1:11:A:TRP:C  | 1:12:A:GLU:N | 6        | 1.62          |
| (1,4)  | 1:7:A:LEU:N  | 1:7:A:LEU:CA  | 1:7:A:LEU:C   | 1:8:A:PRO:N  | 25       | 1.62          |
| (1,46) | 1:37:A:PRO:N | 1:37:A:PRO:CA | 1:37:A:PRO:C  | 1:38:A:SER:N | 25       | 1.6           |
| (1,43) | 1:35:A:GLU:C | 1:36:A:ARG:N  | 1:36:A:ARG:CA | 1:36:A:ARG:C | 2        | 1.59          |
| (1,43) | 1:35:A:GLU:C | 1:36:A:ARG:N  | 1:36:A:ARG:CA | 1:36:A:ARG:C | 18       | 1.59          |
| (1,37) | 1:27:A:HIS:C | 1:28:A:ILE:N  | 1:28:A:ILE:CA | 1:28:A:ILE:C | 7        | 1.59          |
| (1,32) | 1:23:A:TYR:N | 1:23:A:TYR:CA | 1:23:A:TYR:C  | 1:24:A:TYR:N | 8        | 1.59          |
| (1,31) | 1:22:A:VAL:C | 1:23:A:TYR:N  | 1:23:A:TYR:CA | 1:23:A:TYR:C | 22       | 1.59          |
| (1,42) | 1:33:A:GLN:N | 1:33:A:GLN:CA | 1:33:A:GLN:C  | 1:34:A:TRP:N | 8        | 1.58          |
| (1,32) | 1:23:A:TYR:N | 1:23:A:TYR:CA | 1:23:A:TYR:C  | 1:24:A:TYR:N | 9        | 1.58          |
| (1,28) | 1:21:A:ARG:N | 1:21:A:ARG:CA | 1:21:A:ARG:C  | 1:22:A:VAL:N | 2        | 1.58          |
| (1,29) | 1:21:A:ARG:C | 1:22:A:VAL:N  | 1:22:A:VAL:CA | 1:22:A:VAL:C | 5        | 1.57          |
| (1,4)  | 1:7:A:LEU:N  | 1:7:A:LEU:CA  | 1:7:A:LEU:C   | 1:8:A:PRO:N  | 24       | 1.57          |
| (1,2)  | 1:6:A:LYS:N  | 1:6:A:LYS:CA  | 1:6:A:LYS:C   | 1:7:A:LEU:N  | 9        | 1.57          |
| (1,43) | 1:35:A:GLU:C | 1:36:A:ARG:N  | 1:36:A:ARG:CA | 1:36:A:ARG:C | 21       | 1.56          |
| (1,42) | 1:33:A:GLN:N | 1:33:A:GLN:CA | 1:33:A:GLN:C  | 1:34:A:TRP:N | 21       | 1.55          |
| (1,38) | 1:28:A:ILE:N | 1:28:A:ILE:CA | 1:28:A:ILE:C  | 1:29:A:THR:N | 2        | 1.55          |
| (1,34) | 1:24:A:TYR:N | 1:24:A:TYR:CA | 1:24:A:TYR:C  | 1:25:A:PHE:N | 19       | 1.55          |
| (1,18) | 1:14:A:ARG:N | 1:14:A:ARG:CA | 1:14:A:ARG:C  | 1:15:A:MET:N | 16       | 1.55          |
| (1,43) | 1:35:A:GLU:C | 1:36:A:ARG:N  | 1:36:A:ARG:CA | 1:36:A:ARG:C | 13       | 1.54          |
| (1,37) | 1:27:A:HIS:C | 1:28:A:ILE:N  | 1:28:A:ILE:CA | 1:28:A:ILE:C | 16       | 1.54          |
| (1,42) | 1:33:A:GLN:N | 1:33:A:GLN:CA | 1:33:A:GLN:C  | 1:34:A:TRP:N | 5        | 1.53          |
| (1,37) | 1:27:A:HIS:C | 1:28:A:ILE:N  | 1:28:A:ILE:CA | 1:28:A:ILE:C | 18       | 1.53          |
| (1,26) | 1:20:A:GLY:N | 1:20:A:GLY:CA | 1:20:A:GLY:C  | 1:21:A:ARG:N | 8        | 1.53          |
| (1,24) | 1:18:A:SER:N | 1:18:A:SER:CA | 1:18:A:SER:C  | 1:19:A:SER:N | 23       | 1.53          |
| (1,42) | 1:33:A:GLN:N | 1:33:A:GLN:CA | 1:33:A:GLN:C  | 1:34:A:TRP:N | 16       | 1.52          |
| (1,9)  | 1:9:A:PRO:C  | 1:10:A:GLY:N  | 1:10:A:GLY:CA | 1:10:A:GLY:C | 25       | 1.51          |
| (1,3)  | 1:6:A:LYS:C  | 1:7:A:LEU:N   | 1:7:A:LEU:CA  | 1:7:A:LEU:C  | 24       | 1.51          |
| (1,38) | 1:28:A:ILE:N | 1:28:A:ILE:CA | 1:28:A:ILE:C  | 1:29:A:THR:N | 10       | 1.5           |
| (1,4)  | 1:7:A:LEU:N  | 1:7:A:LEU:CA  | 1:7:A:LEU:C   | 1:8:A:PRO:N  | 3        | 1.5           |
| (1,47) | 2:87:B:PHE:C | 2:88:B:PRO:N  | 2:88:B:PRO:CA | 2:88:B:PRO:C | 17       | 1.49          |
| (1,37) | 1:27:A:HIS:C | 1:28:A:ILE:N  | 1:28:A:ILE:CA | 1:28:A:ILE:C | 3        | 1.49          |
| (1,45) | 1:36:A:ARG:C | 1:37:A:PRO:N  | 1:37:A:PRO:CA | 1:37:A:PRO:C | 14       | 1.48          |

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| Key    | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Model ID | Violation (°) |
|--------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,38) | 1:28:A:ILE:N | 1:28:A:ILE:CA | 1:28:A:ILE:C  | 1:29:A:THR:N | 20       | 1.48          |
| (1,25) | 1:19:A:SER:C | 1:20:A:GLY:N  | 1:20:A:GLY:CA | 1:20:A:GLY:C | 14       | 1.48          |
| (1,13) | 1:11:A:TRP:C | 1:12:A:GLU:N  | 1:12:A:GLU:CA | 1:12:A:GLU:C | 7        | 1.48          |
| (1,40) | 1:32:A:SER:N | 1:32:A:SER:CA | 1:32:A:SER:C  | 1:33:A:GLN:N | 19       | 1.47          |
| (1,12) | 1:11:A:TRP:N | 1:11:A:TRP:CA | 1:11:A:TRP:C  | 1:12:A:GLU:N | 2        | 1.46          |
| (1,47) | 2:87:B:PHE:C | 2:88:B:PRO:N  | 2:88:B:PRO:CA | 2:88:B:PRO:C | 8        | 1.45          |
| (1,43) | 1:35:A:GLU:C | 1:36:A:ARG:N  | 1:36:A:ARG:CA | 1:36:A:ARG:C | 11       | 1.45          |
| (1,37) | 1:27:A:HIS:C | 1:28:A:ILE:N  | 1:28:A:ILE:CA | 1:28:A:ILE:C | 2        | 1.45          |
| (1,23) | 1:17:A:ARG:C | 1:18:A:SER:N  | 1:18:A:SER:CA | 1:18:A:SER:C | 15       | 1.45          |
| (1,43) | 1:35:A:GLU:C | 1:36:A:ARG:N  | 1:36:A:ARG:CA | 1:36:A:ARG:C | 10       | 1.44          |
| (1,37) | 1:27:A:HIS:C | 1:28:A:ILE:N  | 1:28:A:ILE:CA | 1:28:A:ILE:C | 24       | 1.44          |
| (1,34) | 1:24:A:TYR:N | 1:24:A:TYR:CA | 1:24:A:TYR:C  | 1:25:A:PHE:N | 18       | 1.44          |
| (1,25) | 1:19:A:SER:C | 1:20:A:GLY:N  | 1:20:A:GLY:CA | 1:20:A:GLY:C | 2        | 1.44          |
| (1,46) | 1:37:A:PRO:N | 1:37:A:PRO:CA | 1:37:A:PRO:C  | 1:38:A:SER:N | 18       | 1.43          |
| (1,37) | 1:27:A:HIS:C | 1:28:A:ILE:N  | 1:28:A:ILE:CA | 1:28:A:ILE:C | 23       | 1.43          |
| (1,36) | 1:25:A:PHE:N | 1:25:A:PHE:CA | 1:25:A:PHE:C  | 1:26:A:ASN:N | 23       | 1.43          |
| (1,34) | 1:24:A:TYR:N | 1:24:A:TYR:CA | 1:24:A:TYR:C  | 1:25:A:PHE:N | 21       | 1.43          |
| (1,9)  | 1:9:A:PRO:C  | 1:10:A:GLY:N  | 1:10:A:GLY:CA | 1:10:A:GLY:C | 17       | 1.42          |
| (1,27) | 1:20:A:GLY:C | 1:21:A:ARG:N  | 1:21:A:ARG:CA | 1:21:A:ARG:C | 7        | 1.41          |
| (1,4)  | 1:7:A:LEU:N  | 1:7:A:LEU:CA  | 1:7:A:LEU:C   | 1:8:A:PRO:N  | 18       | 1.4           |
| (1,27) | 1:20:A:GLY:C | 1:21:A:ARG:N  | 1:21:A:ARG:CA | 1:21:A:ARG:C | 23       | 1.39          |
| (1,21) | 1:16:A:SER:C | 1:17:A:ARG:N  | 1:17:A:ARG:CA | 1:17:A:ARG:C | 16       | 1.39          |
| (1,1)  | 1:5:A:GLU:C  | 1:6:A:LYS:N   | 1:6:A:LYS:CA  | 1:6:A:LYS:C  | 18       | 1.36          |
| (1,31) | 1:22:A:VAL:C | 1:23:A:TYR:N  | 1:23:A:TYR:CA | 1:23:A:TYR:C | 16       | 1.35          |
| (1,31) | 1:22:A:VAL:C | 1:23:A:TYR:N  | 1:23:A:TYR:CA | 1:23:A:TYR:C | 21       | 1.35          |
| (1,45) | 1:36:A:ARG:C | 1:37:A:PRO:N  | 1:37:A:PRO:CA | 1:37:A:PRO:C | 21       | 1.34          |
| (1,43) | 1:35:A:GLU:C | 1:36:A:ARG:N  | 1:36:A:ARG:CA | 1:36:A:ARG:C | 23       | 1.34          |
| (1,37) | 1:27:A:HIS:C | 1:28:A:ILE:N  | 1:28:A:ILE:CA | 1:28:A:ILE:C | 4        | 1.34          |
| (1,31) | 1:22:A:VAL:C | 1:23:A:TYR:N  | 1:23:A:TYR:CA | 1:23:A:TYR:C | 11       | 1.34          |
| (1,29) | 1:21:A:ARG:C | 1:22:A:VAL:N  | 1:22:A:VAL:CA | 1:22:A:VAL:C | 9        | 1.34          |
| (1,15) | 1:12:A:GLU:C | 1:13:A:LYS:N  | 1:13:A:LYS:CA | 1:13:A:LYS:C | 16       | 1.34          |
| (1,38) | 1:28:A:ILE:N | 1:28:A:ILE:CA | 1:28:A:ILE:C  | 1:29:A:THR:N | 12       | 1.33          |
| (1,37) | 1:27:A:HIS:C | 1:28:A:ILE:N  | 1:28:A:ILE:CA | 1:28:A:ILE:C | 12       | 1.33          |
| (1,37) | 1:27:A:HIS:C | 1:28:A:ILE:N  | 1:28:A:ILE:CA | 1:28:A:ILE:C | 21       | 1.32          |
| (1,28) | 1:21:A:ARG:N | 1:21:A:ARG:CA | 1:21:A:ARG:C  | 1:22:A:VAL:N | 19       | 1.32          |
| (1,9)  | 1:9:A:PRO:C  | 1:10:A:GLY:N  | 1:10:A:GLY:CA | 1:10:A:GLY:C | 23       | 1.32          |
| (1,1)  | 1:5:A:GLU:C  | 1:6:A:LYS:N   | 1:6:A:LYS:CA  | 1:6:A:LYS:C  | 23       | 1.32          |
| (1,32) | 1:23:A:TYR:N | 1:23:A:TYR:CA | 1:23:A:TYR:C  | 1:24:A:TYR:N | 24       | 1.3           |
| (1,9)  | 1:9:A:PRO:C  | 1:10:A:GLY:N  | 1:10:A:GLY:CA | 1:10:A:GLY:C | 6        | 1.3           |
| (1,5)  | 1:7:A:LEU:C  | 1:8:A:PRO:N   | 1:8:A:PRO:CA  | 1:8:A:PRO:C  | 21       | 1.3           |
| (1,4)  | 1:7:A:LEU:N  | 1:7:A:LEU:CA  | 1:7:A:LEU:C   | 1:8:A:PRO:N  | 6        | 1.3           |
| (1,42) | 1:33:A:GLN:N | 1:33:A:GLN:CA | 1:33:A:GLN:C  | 1:34:A:TRP:N | 1        | 1.29          |
| (1,37) | 1:27:A:HIS:C | 1:28:A:ILE:N  | 1:28:A:ILE:CA | 1:28:A:ILE:C | 1        | 1.29          |
| (1,29) | 1:21:A:ARG:C | 1:22:A:VAL:N  | 1:22:A:VAL:CA | 1:22:A:VAL:C | 8        | 1.29          |
| (1,13) | 1:11:A:TRP:C | 1:12:A:GLU:N  | 1:12:A:GLU:CA | 1:12:A:GLU:C | 25       | 1.29          |
| (1,29) | 1:21:A:ARG:C | 1:22:A:VAL:N  | 1:22:A:VAL:CA | 1:22:A:VAL:C | 23       | 1.28          |
| (1,26) | 1:20:A:GLY:N | 1:20:A:GLY:CA | 1:20:A:GLY:C  | 1:21:A:ARG:N | 13       | 1.28          |
| (1,4)  | 1:7:A:LEU:N  | 1:7:A:LEU:CA  | 1:7:A:LEU:C   | 1:8:A:PRO:N  | 10       | 1.28          |
| (1,39) | 1:31:A:ALA:C | 1:32:A:SER:N  | 1:32:A:SER:CA | 1:32:A:SER:C | 3        | 1.27          |
| (1,32) | 1:23:A:TYR:N | 1:23:A:TYR:CA | 1:23:A:TYR:C  | 1:24:A:TYR:N | 3        | 1.27          |
| (1,26) | 1:20:A:GLY:N | 1:20:A:GLY:CA | 1:20:A:GLY:C  | 1:21:A:ARG:N | 21       | 1.26          |

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| Key    | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Model ID | Violation (°) |
|--------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,20) | 1:15:A:MET:N | 1:15:A:MET:CA | 1:15:A:MET:C  | 1:16:A:SER:N | 16       | 1.26          |
| (1,38) | 1:28:A:ILE:N | 1:28:A:ILE:CA | 1:28:A:ILE:C  | 1:29:A:THR:N | 22       | 1.25          |
| (1,1)  | 1:5:A:GLU:C  | 1:6:A:LYS:N   | 1:6:A:LYS:CA  | 1:6:A:LYS:C  | 24       | 1.25          |
| (1,38) | 1:28:A:ILE:N | 1:28:A:ILE:CA | 1:28:A:ILE:C  | 1:29:A:THR:N | 19       | 1.24          |
| (1,32) | 1:23:A:TYR:N | 1:23:A:TYR:CA | 1:23:A:TYR:C  | 1:24:A:TYR:N | 4        | 1.24          |
| (1,25) | 1:19:A:SER:C | 1:20:A:GLY:N  | 1:20:A:GLY:CA | 1:20:A:GLY:C | 12       | 1.24          |
| (1,36) | 1:25:A:PHE:N | 1:25:A:PHE:CA | 1:25:A:PHE:C  | 1:26:A:ASN:N | 11       | 1.23          |
| (1,32) | 1:23:A:TYR:N | 1:23:A:TYR:CA | 1:23:A:TYR:C  | 1:24:A:TYR:N | 23       | 1.23          |
| (1,47) | 2:87:B:PHE:C | 2:88:B:PRO:N  | 2:88:B:PRO:CA | 2:88:B:PRO:C | 19       | 1.22          |
| (1,42) | 1:33:A:GLN:N | 1:33:A:GLN:CA | 1:33:A:GLN:C  | 1:34:A:TRP:N | 15       | 1.22          |
| (1,18) | 1:14:A:ARG:N | 1:14:A:ARG:CA | 1:14:A:ARG:C  | 1:15:A:MET:N | 5        | 1.22          |
| (1,12) | 1:11:A:TRP:N | 1:11:A:TRP:CA | 1:11:A:TRP:C  | 1:12:A:GLU:N | 18       | 1.22          |
| (1,31) | 1:22:A:VAL:C | 1:23:A:TYR:N  | 1:23:A:TYR:CA | 1:23:A:TYR:C | 25       | 1.21          |
| (1,24) | 1:18:A:SER:N | 1:18:A:SER:CA | 1:18:A:SER:C  | 1:19:A:SER:N | 9        | 1.21          |
| (1,12) | 1:11:A:TRP:N | 1:11:A:TRP:CA | 1:11:A:TRP:C  | 1:12:A:GLU:N | 8        | 1.21          |
| (1,4)  | 1:7:A:LEU:N  | 1:7:A:LEU:CA  | 1:7:A:LEU:C   | 1:8:A:PRO:N  | 4        | 1.21          |
| (1,24) | 1:18:A:SER:N | 1:18:A:SER:CA | 1:18:A:SER:C  | 1:19:A:SER:N | 4        | 1.2           |
| (1,2)  | 1:6:A:LYS:N  | 1:6:A:LYS:CA  | 1:6:A:LYS:C   | 1:7:A:LEU:N  | 21       | 1.2           |
| (1,32) | 1:23:A:TYR:N | 1:23:A:TYR:CA | 1:23:A:TYR:C  | 1:24:A:TYR:N | 22       | 1.19          |
| (1,26) | 1:20:A:GLY:N | 1:20:A:GLY:CA | 1:20:A:GLY:C  | 1:21:A:ARG:N | 15       | 1.19          |
| (1,24) | 1:18:A:SER:N | 1:18:A:SER:CA | 1:18:A:SER:C  | 1:19:A:SER:N | 5        | 1.19          |
| (1,38) | 1:28:A:ILE:N | 1:28:A:ILE:CA | 1:28:A:ILE:C  | 1:29:A:THR:N | 4        | 1.18          |
| (1,37) | 1:27:A:HIS:C | 1:28:A:ILE:N  | 1:28:A:ILE:CA | 1:28:A:ILE:C | 13       | 1.18          |
| (1,38) | 1:28:A:ILE:N | 1:28:A:ILE:CA | 1:28:A:ILE:C  | 1:29:A:THR:N | 13       | 1.17          |
| (1,7)  | 1:8:A:PRO:C  | 1:9:A:PRO:N   | 1:9:A:PRO:CA  | 1:9:A:PRO:C  | 5        | 1.17          |
| (1,13) | 1:11:A:TRP:C | 1:12:A:GLU:N  | 1:12:A:GLU:CA | 1:12:A:GLU:C | 20       | 1.16          |
| (1,47) | 2:87:B:PHE:C | 2:88:B:PRO:N  | 2:88:B:PRO:CA | 2:88:B:PRO:C | 11       | 1.15          |
| (1,13) | 1:11:A:TRP:C | 1:12:A:GLU:N  | 1:12:A:GLU:CA | 1:12:A:GLU:C | 8        | 1.15          |
| (1,13) | 1:11:A:TRP:C | 1:12:A:GLU:N  | 1:12:A:GLU:CA | 1:12:A:GLU:C | 16       | 1.15          |
| (1,43) | 1:35:A:GLU:C | 1:36:A:ARG:N  | 1:36:A:ARG:CA | 1:36:A:ARG:C | 22       | 1.14          |
| (1,40) | 1:32:A:SER:N | 1:32:A:SER:CA | 1:32:A:SER:C  | 1:33:A:GLN:N | 10       | 1.13          |
| (1,31) | 1:22:A:VAL:C | 1:23:A:TYR:N  | 1:23:A:TYR:CA | 1:23:A:TYR:C | 15       | 1.13          |
| (1,21) | 1:16:A:SER:C | 1:17:A:ARG:N  | 1:17:A:ARG:CA | 1:17:A:ARG:C | 6        | 1.13          |
| (1,21) | 1:16:A:SER:C | 1:17:A:ARG:N  | 1:17:A:ARG:CA | 1:17:A:ARG:C | 2        | 1.12          |
| (1,13) | 1:11:A:TRP:C | 1:12:A:GLU:N  | 1:12:A:GLU:CA | 1:12:A:GLU:C | 6        | 1.12          |
| (1,28) | 1:21:A:ARG:N | 1:21:A:ARG:CA | 1:21:A:ARG:C  | 1:22:A:VAL:N | 21       | 1.11          |
| (1,18) | 1:14:A:ARG:N | 1:14:A:ARG:CA | 1:14:A:ARG:C  | 1:15:A:MET:N | 10       | 1.11          |
| (1,13) | 1:11:A:TRP:C | 1:12:A:GLU:N  | 1:12:A:GLU:CA | 1:12:A:GLU:C | 14       | 1.11          |
| (1,4)  | 1:7:A:LEU:N  | 1:7:A:LEU:CA  | 1:7:A:LEU:C   | 1:8:A:PRO:N  | 22       | 1.11          |
| (1,40) | 1:32:A:SER:N | 1:32:A:SER:CA | 1:32:A:SER:C  | 1:33:A:GLN:N | 21       | 1.09          |
| (1,38) | 1:28:A:ILE:N | 1:28:A:ILE:CA | 1:28:A:ILE:C  | 1:29:A:THR:N | 9        | 1.09          |
| (1,38) | 1:28:A:ILE:N | 1:28:A:ILE:CA | 1:28:A:ILE:C  | 1:29:A:THR:N | 11       | 1.09          |
| (1,44) | 1:36:A:ARG:N | 1:36:A:ARG:CA | 1:36:A:ARG:C  | 1:37:A:PRO:N | 19       | 1.08          |
| (1,38) | 1:28:A:ILE:N | 1:28:A:ILE:CA | 1:28:A:ILE:C  | 1:29:A:THR:N | 17       | 1.08          |
| (1,28) | 1:21:A:ARG:N | 1:21:A:ARG:CA | 1:21:A:ARG:C  | 1:22:A:VAL:N | 3        | 1.08          |
| (1,12) | 1:11:A:TRP:N | 1:11:A:TRP:CA | 1:11:A:TRP:C  | 1:12:A:GLU:N | 9        | 1.08          |
| (1,38) | 1:28:A:ILE:N | 1:28:A:ILE:CA | 1:28:A:ILE:C  | 1:29:A:THR:N | 25       | 1.07          |
| (1,24) | 1:18:A:SER:N | 1:18:A:SER:CA | 1:18:A:SER:C  | 1:19:A:SER:N | 6        | 1.07          |
| (1,38) | 1:28:A:ILE:N | 1:28:A:ILE:CA | 1:28:A:ILE:C  | 1:29:A:THR:N | 5        | 1.06          |
| (1,24) | 1:18:A:SER:N | 1:18:A:SER:CA | 1:18:A:SER:C  | 1:19:A:SER:N | 17       | 1.06          |
| (1,24) | 1:18:A:SER:N | 1:18:A:SER:CA | 1:18:A:SER:C  | 1:19:A:SER:N | 25       | 1.06          |

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| Key    | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Model ID | Violation (°) |
|--------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,12) | 1:11:A:TRP:N | 1:11:A:TRP:CA | 1:11:A:TRP:C  | 1:12:A:GLU:N | 23       | 1.06          |
| (1,6)  | 1:8:A:PRO:N  | 1:8:A:PRO:CA  | 1:8:A:PRO:C   | 1:9:A:PRO:N  | 6        | 1.06          |
| (1,2)  | 1:6:A:LYS:N  | 1:6:A:LYS:CA  | 1:6:A:LYS:C   | 1:7:A:LEU:N  | 22       | 1.06          |
| (1,1)  | 1:5:A:GLU:C  | 1:6:A:LYS:N   | 1:6:A:LYS:CA  | 1:6:A:LYS:C  | 6        | 1.06          |
| (1,37) | 1:27:A:HIS:C | 1:28:A:ILE:N  | 1:28:A:ILE:CA | 1:28:A:ILE:C | 25       | 1.05          |
| (1,24) | 1:18:A:SER:N | 1:18:A:SER:CA | 1:18:A:SER:C  | 1:19:A:SER:N | 21       | 1.05          |
| (1,45) | 1:36:A:ARG:C | 1:37:A:PRO:N  | 1:37:A:PRO:CA | 1:37:A:PRO:C | 23       | 1.04          |
| (1,6)  | 1:8:A:PRO:N  | 1:8:A:PRO:CA  | 1:8:A:PRO:C   | 1:9:A:PRO:N  | 1        | 1.04          |
| (1,27) | 1:20:A:GLY:C | 1:21:A:ARG:N  | 1:21:A:ARG:CA | 1:21:A:ARG:C | 2        | 1.03          |
| (1,40) | 1:32:A:SER:N | 1:32:A:SER:CA | 1:32:A:SER:C  | 1:33:A:GLN:N | 1        | 1.02          |
| (1,40) | 1:32:A:SER:N | 1:32:A:SER:CA | 1:32:A:SER:C  | 1:33:A:GLN:N | 9        | 1.02          |
| (1,13) | 1:11:A:TRP:C | 1:12:A:GLU:N  | 1:12:A:GLU:CA | 1:12:A:GLU:C | 13       | 1.02          |
| (1,34) | 1:24:A:TYR:N | 1:24:A:TYR:CA | 1:24:A:TYR:C  | 1:25:A:PHE:N | 14       | 1.01          |