



# Full wwPDB NMR Structure Validation Report ⓘ

Mar 19, 2026 – 09:57 PM UTC

PDB ID : 2JP9 / pdb\_00002jp9  
BMRB ID : 15532  
Title : Structure of the Wilms Tumor Suppressor Protein Zinc Finger Domain Bound to DNA  
Authors : Stoll, R.; Lee, B.M.; Debler, E.W.; Laity, J.H.; Wilson, I.A.; Dyson, H.J.; Wright, P.E.  
Deposited on : 2007-04-30

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

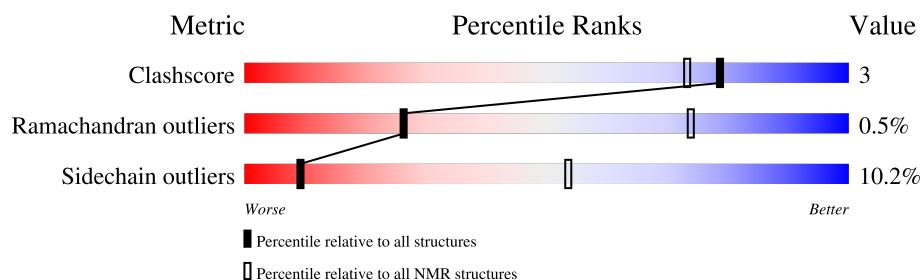
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 9%.

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   | B     | 17     | 71% 24% 6%       |
| 2   | C     | 17     | 82% 18%          |
| 3   | A     | 119    | 73% 10% • 13%    |

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 1 is the overall representative, medoid model (most similar to other models).

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:32 (26)              | 0.52              | 11           |
| 2                                    | A:37-A:39, A:46-A:119 (77) | 0.61              | 1            |

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

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

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

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

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

There are 4 unique types of molecules in this entry. The entry contains 3069 atoms, of which 1357 are hydrogens and 0 are deuteriums.

- Molecule 1 is a DNA chain called DNA (5'-D(P\*DCP\*DGP\*DCP\*DGP\*DGP\*DGP\*DGP\*DGP\*DCP\*DGP\*DTP\*DCP\*DTP\*DGP\*DCP\*DGP\*DC)-3').

| Mol | Chain | Residues | Atoms |     |     |    |     |    | Trace |
|-----|-------|----------|-------|-----|-----|----|-----|----|-------|
| 1   | B     | 17       | Total | C   | H   | N  | O   | P  | 0     |
|     |       |          | 541   | 164 | 189 | 67 | 104 | 17 |       |

- Molecule 2 is a DNA chain called DNA (5'-D(P\*DGP\*DCP\*DGP\*DCP\*DAP\*DGP\*DAP\*DCP\*DGP\*DCP\*DCP\*DCP\*DCP\*DCP\*DCP\*DGP\*DCP\*DG)-3').

| Mol | Chain | Residues | Atoms |     |     |    |     |    | Trace |
|-----|-------|----------|-------|-----|-----|----|-----|----|-------|
| 2   | C     | 17       | Total | C   | H   | N  | O   | P  | 0     |
|     |       |          | 532   | 161 | 187 | 67 | 100 | 17 |       |

- Molecule 3 is a protein called Wilms tumor 1.

| Mol | Chain | Residues | Atoms |     |     |     |     |    | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|----|-------|
| 3   | A     | 119      | Total | C   | H   | N   | O   | S  | 0     |
|     |       |          | 1992  | 622 | 981 | 210 | 168 | 11 |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | 1       | ALA      | -      | expression tag | UNP Q4VXV4 |

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

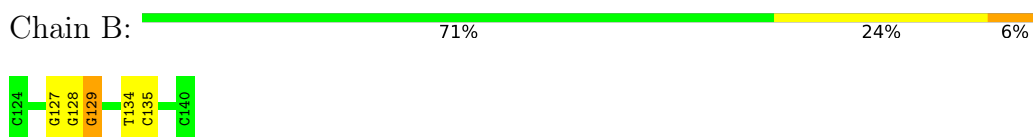
| Mol | Chain | Residues | Atoms |    |
|-----|-------|----------|-------|----|
| 4   | A     | 4        | Total | Zn |
|     |       |          | 4     | 4  |

## 4 Residue-property plots

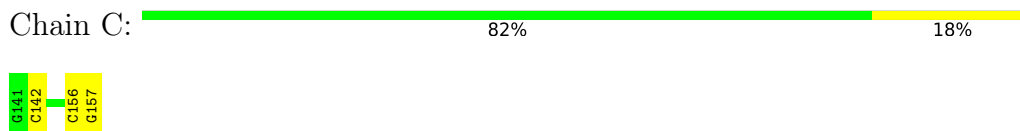
### 4.1 Average score per residue in the NMR ensemble

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

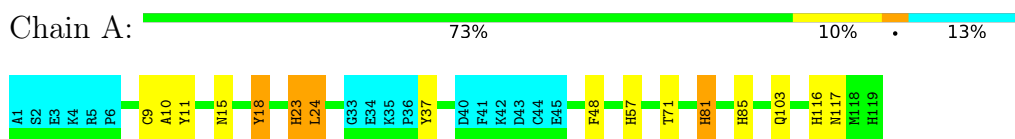
- Molecule 1: DNA (5'-D(P\*DCP\*DGP\*DCP\*DGP\*DGP\*DGP\*DGP\*DCP\*DGP\*DTP\*DCP\*DTP\*DGP\*DCP\*DGP\*DC)-3')



- Molecule 2: DNA (5'-D(P\*DGP\*DCP\*DGP\*DCP\*DAP\*DGP\*DAP\*DCP\*DGP\*DCP\*DCP\*DCP\*DCP\*DCP\*DGP\*DCP\*DG)-3')



- Molecule 3: Wilms tumor 1

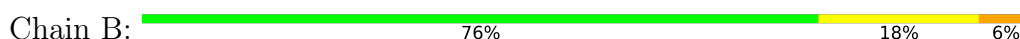


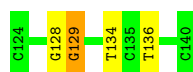
### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1 (medoid)

- Molecule 1: DNA (5'-D(P\*DCP\*DGP\*DCP\*DGP\*DGP\*DGP\*DGP\*DCP\*DGP\*DTP\*DCP\*DTP\*DGP\*DCP\*DGP\*DC)-3')

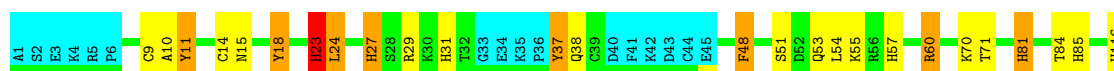




- Molecule 2: DNA (5'-D(P\*DGP\*DCP\*DGP\*DCP\*DAP\*DGP\*DAP\*DCP\*DGP\*DCP\*DCP\*DCP\*DCP\*DCP\*DCP\*DCP\*DCP\*DG)-3')

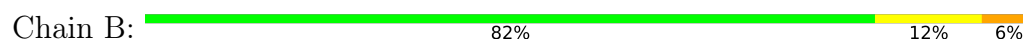


- Molecule 3: Wilms tumor 1

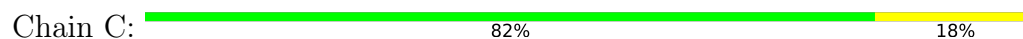


#### 4.2.2 Score per residue for model 2

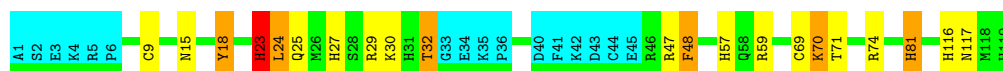
- Molecule 1: DNA (5'-D(P\*DCP\*DGP\*DCP\*DGP\*DGP\*DGP\*DGP\*DCP\*DGP\*DTP\*DCP\*DTP\*DGP\*DCP\*DGP\*DC)-3')



- Molecule 2: DNA (5'-D(P\*DGP\*DCP\*DGP\*DCP\*DAP\*DGP\*DAP\*DCP\*DGP\*DCP\*DCP\*DCP\*DCP\*DCP\*DCP\*DCP\*DCP\*DG)-3')



- Molecule 3: Wilms tumor 1



### 4.2.3 Score per residue for model 3

- Molecule 1: DNA (5'-D(P\*DCP\*DGP\*DCP\*DGP\*DGP\*DGP\*DGP\*DCP\*DGP\*DTP\*DCP\*DTP\*DGP\*DCP\*DGP\*DC)-3')

Chain B:  88% 12%



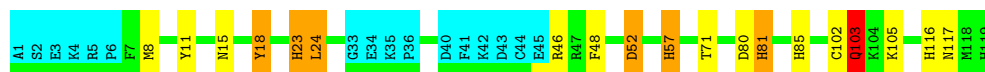
- Molecule 2: DNA (5'-D(P\*DGP\*DCP\*DGP\*DCP\*DAP\*DGP\*DAP\*DCP\*DGP\*DCP\*DCP\*DCP\*DCP\*DCP\*DGP\*DCP\*DG)-3')

Chain C:  82% 18%



- Molecule 3: Wilms tumor 1

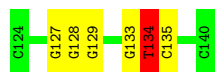
Chain A:  71% 10% 5% 13%



### 4.2.4 Score per residue for model 4

- Molecule 1: DNA (5'-D(P\*DCP\*DGP\*DCP\*DGP\*DGP\*DGP\*DGP\*DCP\*DGP\*DTP\*DCP\*DTP\*DGP\*DCP\*DGP\*DC)-3')

Chain B:  65% 29% 6%



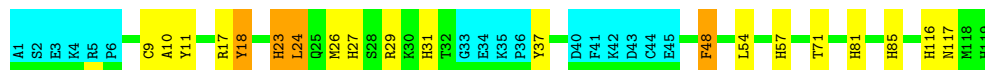
- Molecule 2: DNA (5'-D(P\*DGP\*DCP\*DGP\*DCP\*DAP\*DGP\*DAP\*DCP\*DGP\*DCP\*DCP\*DCP\*DCP\*DCP\*DGP\*DCP\*DG)-3')

Chain C:  76% 24%



- Molecule 3: Wilms tumor 1

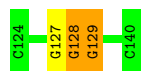
Chain A:  70% 13% 13%



### 4.2.5 Score per residue for model 5

- Molecule 1: DNA (5'-D(P\*DCP\*DGP\*DCP\*DGP\*DGP\*DGP\*DGP\*DCP\*DGP\*DTP\*DCP\*DTP\*DGP\*DCP\*DGP\*DC)-3')

Chain B:  82% 6% 12%



- Molecule 2: DNA (5'-D(P\*DGP\*DCP\*DGP\*DCP\*DAP\*DGP\*DAP\*DCP\*DGP\*DCP\*DCP\*DCP\*DCP\*DCP\*DGP\*DCP\*DG)-3')

Chain C:  76% 24%



- Molecule 3: Wilms tumor 1

Chain A:  71% 13% 13%



### 4.2.6 Score per residue for model 6

- Molecule 1: DNA (5'-D(P\*DCP\*DGP\*DCP\*DGP\*DGP\*DGP\*DGP\*DCP\*DGP\*DTP\*DCP\*DTP\*DGP\*DCP\*DGP\*DC)-3')

Chain B:  65% 24% 6% 6%



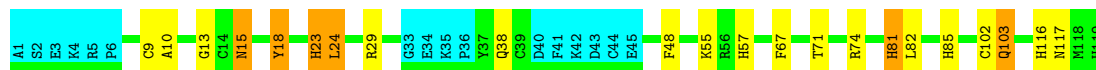
- Molecule 2: DNA (5'-D(P\*DGP\*DCP\*DGP\*DCP\*DAP\*DGP\*DAP\*DCP\*DGP\*DCP\*DCP\*DCP\*DCP\*DCP\*DGP\*DCP\*DG)-3')

Chain C:  71% 29%



- Molecule 3: Wilms tumor 1

Chain A:  68% 13% 5% 13%





### 4.2.7 Score per residue for model 7

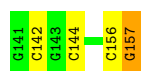
- Molecule 1: DNA (5'-D(P\*DCP\*DGP\*DCP\*DGP\*DGP\*DGP\*DGP\*DCP\*DGP\*DTP\*DCP\*DTP\*DGP\*DCP\*DGP\*DC)-3')

Chain B: 



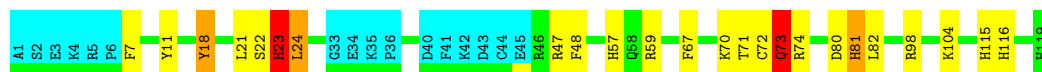
- Molecule 2: DNA (5'-D(P\*DGP\*DCP\*DGP\*DCP\*DAP\*DGP\*DAP\*DCP\*DGP\*DCP\*DCP\*DCP\*DCP\*DCP\*DGP\*DCP\*DG)-3')

Chain C: 



- Molecule 3: Wilms tumor 1

Chain A: 



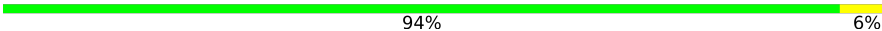
### 4.2.8 Score per residue for model 8

- Molecule 1: DNA (5'-D(P\*DCP\*DGP\*DCP\*DGP\*DGP\*DGP\*DGP\*DCP\*DGP\*DTP\*DCP\*DTP\*DGP\*DCP\*DGP\*DC)-3')

Chain B: 



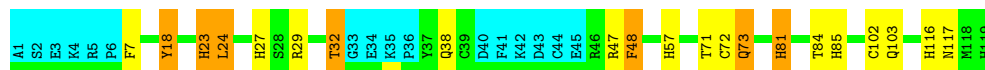
- Molecule 2: DNA (5'-D(P\*DGP\*DCP\*DGP\*DCP\*DAP\*DGP\*DAP\*DCP\*DGP\*DCP\*DCP\*DCP\*DCP\*DCP\*DGP\*DCP\*DG)-3')

Chain C: 



- Molecule 3: Wilms tumor 1

Chain A: 



### 4.2.9 Score per residue for model 9

- Molecule 1: DNA (5'-D(P\*DCP\*DGP\*DCP\*DGP\*DGP\*DGP\*DGP\*DCP\*DGP\*DTP\*DCP\*DTP\*DGP\*DCP\*DGP\*DC)-3')

Chain B:  82% 18%



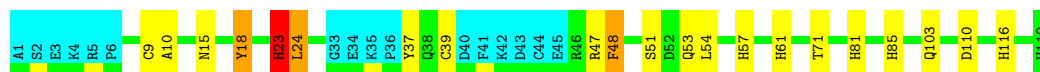
- Molecule 2: DNA (5'-D(P\*DGP\*DCP\*DGP\*DCP\*DAP\*DGP\*DAP\*DCP\*DGP\*DCP\*DCP\*DCP\*DCP\*DCP\*DGP\*DCP\*DG)-3')

Chain C:  88% 12%



- Molecule 3: Wilms tumor 1

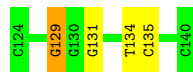
Chain A:  69% 14% 13%



### 4.2.10 Score per residue for model 10

- Molecule 1: DNA (5'-D(P\*DCP\*DGP\*DCP\*DGP\*DGP\*DGP\*DGP\*DCP\*DGP\*DTP\*DCP\*DTP\*DGP\*DCP\*DGP\*DC)-3')

Chain B:  76% 18% 6%



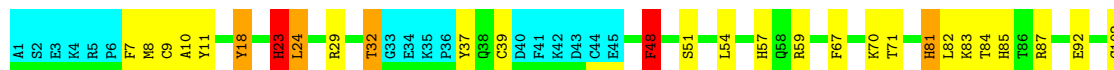
- Molecule 2: DNA (5'-D(P\*DGP\*DCP\*DGP\*DCP\*DAP\*DGP\*DAP\*DCP\*DGP\*DCP\*DCP\*DCP\*DCP\*DCP\*DGP\*DCP\*DG)-3')

Chain C:  76% 24%



- Molecule 3: Wilms tumor 1

Chain A:  60% 21% 13%





#### 4.2.11 Score per residue for model 11

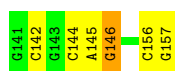
- Molecule 1: DNA (5'-D(P\*DCP\*DGP\*DCP\*DGP\*DGP\*DGP\*DGP\*DCP\*DGP\*DTP\*DCP\*DTP\*DGP\*DCP\*DGP\*DC)-3')

Chain B: 53% 18% 24% 6%



- Molecule 2: DNA (5'-D(P\*DGP\*DCP\*DGP\*DCP\*DAP\*DGP\*DAP\*DCP\*DGP\*DCP\*DCP\*DCP\*DCP\*DCP\*DGP\*DCP\*DG)-3')

Chain C: 65% 29% 6%



- Molecule 3: Wilms tumor 1

Chain A: 70% 11% 6% 13%



#### 4.2.12 Score per residue for model 12

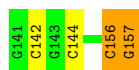
- Molecule 1: DNA (5'-D(P\*DCP\*DGP\*DCP\*DGP\*DGP\*DGP\*DGP\*DCP\*DGP\*DTP\*DCP\*DTP\*DGP\*DCP\*DGP\*DC)-3')

Chain B: 53% 41% 6%

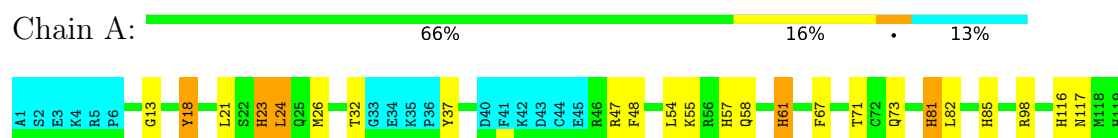


- Molecule 2: DNA (5'-D(P\*DGP\*DCP\*DGP\*DCP\*DAP\*DGP\*DAP\*DCP\*DGP\*DCP\*DCP\*DCP\*DCP\*DCP\*DGP\*DCP\*DG)-3')

Chain C: 76% 12% 12%



- Molecule 3: Wilms tumor 1

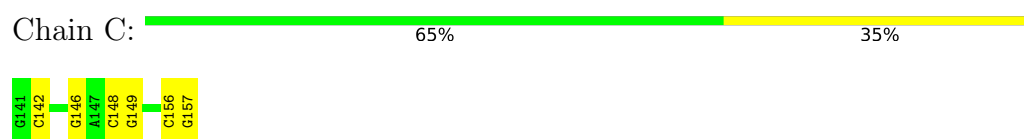


#### 4.2.13 Score per residue for model 13

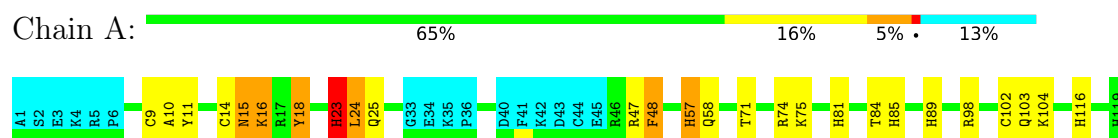
- Molecule 1: DNA (5'-D(P\*DCP\*DGP\*DCP\*DGP\*DGP\*DGP\*DGP\*DCP\*DGP\*DTP\*DCP\*DTP\*DGP\*DCP\*DGP\*DC)-3')



- Molecule 2: DNA (5'-D(P\*DGP\*DCP\*DGP\*DCP\*DAP\*DGP\*DAP\*DCP\*DGP\*DCP\*DCP\*DCP\*DCP\*DCP\*DGP\*DCP\*DG)-3')

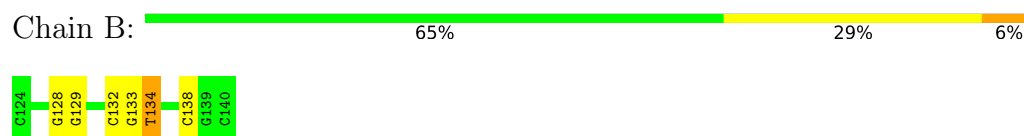


- Molecule 3: Wilms tumor 1

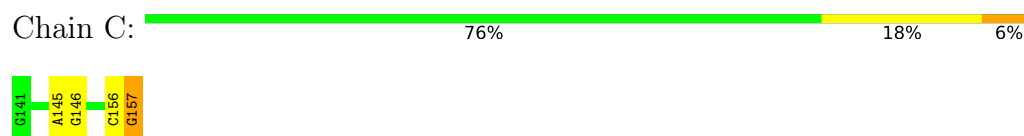


#### 4.2.14 Score per residue for model 14

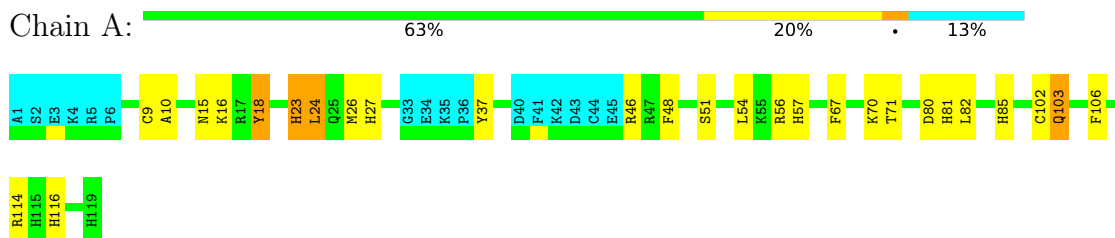
- Molecule 1: DNA (5'-D(P\*DCP\*DGP\*DCP\*DGP\*DGP\*DGP\*DGP\*DCP\*DGP\*DTP\*DCP\*DTP\*DGP\*DCP\*DGP\*DC)-3')



- Molecule 2: DNA (5'-D(P\*DGP\*DCP\*DGP\*DCP\*DAP\*DGP\*DAP\*DCP\*DGP\*DCP\*DCP\*DCP\*DCP\*DCP\*DGP\*DCP\*DG)-3')

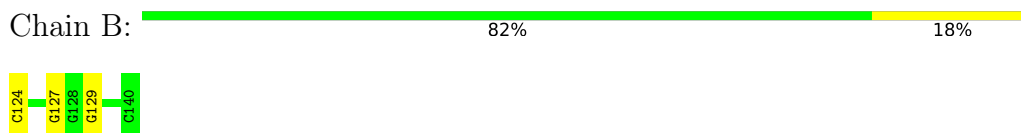


- Molecule 3: Wilms tumor 1

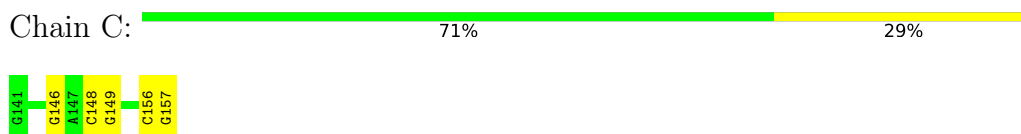


#### 4.2.15 Score per residue for model 15

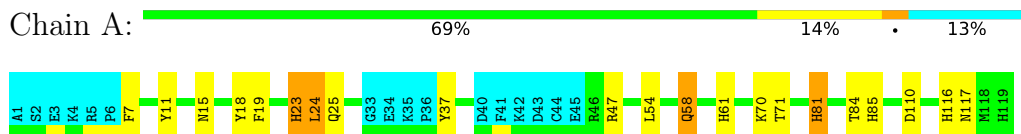
- Molecule 1: DNA (5'-D(P\*DCP\*DGP\*DCP\*DGP\*DGP\*DGP\*DGP\*DCP\*DGP\*DTP\*DCP\*DTP\*DGP\*DCP\*DGP\*DC)-3')



- Molecule 2: DNA (5'-D(P\*DGP\*DCP\*DGP\*DCP\*DAP\*DGP\*DAP\*DCP\*DGP\*DCP\*DCP\*DCP\*DCP\*DCP\*DGP\*DCP\*DG)-3')

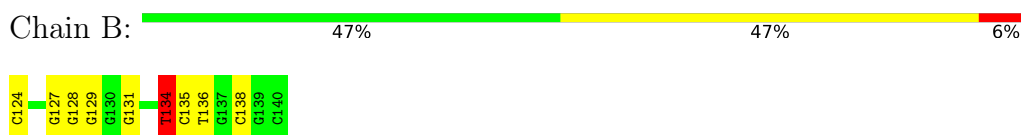


- Molecule 3: Wilms tumor 1

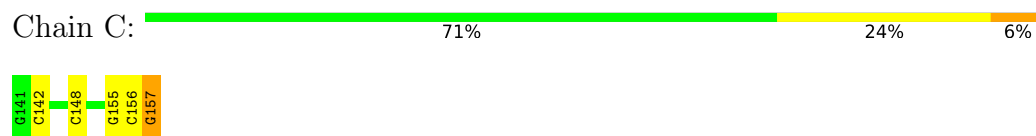


#### 4.2.16 Score per residue for model 16

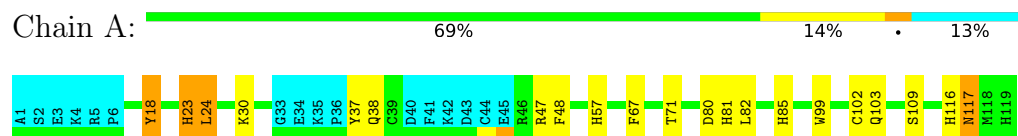
- Molecule 1: DNA (5'-D(P\*DCP\*DGP\*DCP\*DGP\*DGP\*DGP\*DGP\*DCP\*DGP\*DTP\*DCP\*DTP\*DGP\*DCP\*DGP\*DC)-3')



- Molecule 2: DNA (5'-D(P\*DGP\*DCP\*DGP\*DCP\*DAP\*DGP\*DAP\*DCP\*DGP\*DCP\*DCP\*DCP\*DCP\*DCP\*DGP\*DCP\*DG)-3')

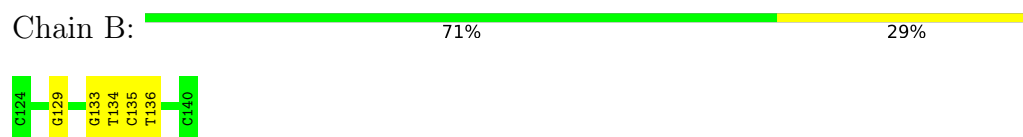


- Molecule 3: Wilms tumor 1

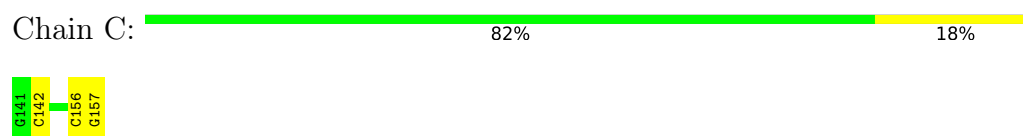


#### 4.2.17 Score per residue for model 17

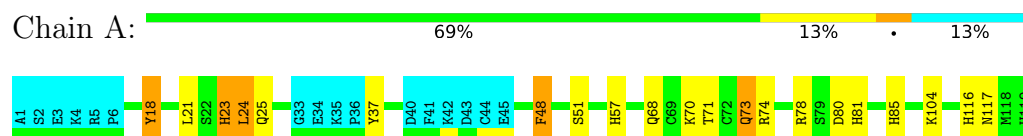
- Molecule 1: DNA (5'-D(P\*DCP\*DGP\*DCP\*DGP\*DGP\*DGP\*DGP\*DCP\*DGP\*DTP\*DCP\*DTP\*DGP\*DCP\*DGP\*DC)-3')



- Molecule 2: DNA (5'-D(P\*DGP\*DCP\*DGP\*DCP\*DAP\*DGP\*DAP\*DCP\*DGP\*DCP\*DCP\*DCP\*DCP\*DCP\*DGP\*DCP\*DG)-3')

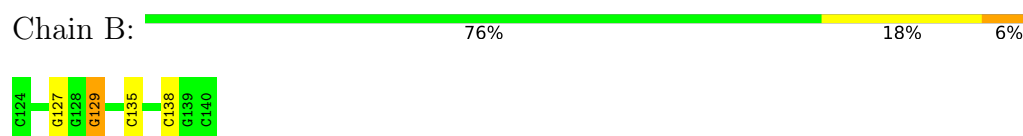


- Molecule 3: Wilms tumor 1



#### 4.2.18 Score per residue for model 18

- Molecule 1: DNA (5'-D(P\*DCP\*DGP\*DCP\*DGP\*DGP\*DGP\*DGP\*DCP\*DGP\*DTP\*DCP\*DTP\*DGP\*DCP\*DGP\*DC)-3')



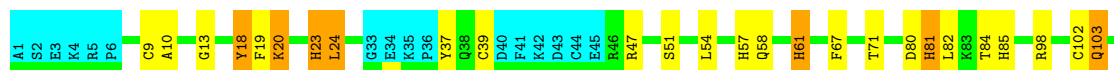
- Molecule 2: DNA (5'-D(P\*DGP\*DCP\*DGP\*DCP\*DAP\*DGP\*DAP\*DCP\*DGP\*DCP\*DCP\*DCP\*DCP\*DCP\*DGP\*DCP\*DG)-3')

Chain C:  76% 24%



- Molecule 3: Wilms tumor 1

Chain A:  63% 18% 6% 13%



#### 4.2.19 Score per residue for model 19

- Molecule 1: DNA (5'-D(P\*DCP\*DGP\*DCP\*DGP\*DGP\*DGP\*DGP\*DCP\*DGP\*DTP\*DCP\*DTP\*DGP\*DCP\*DGP\*DC)-3')

Chain B:  71% 24% 6%



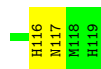
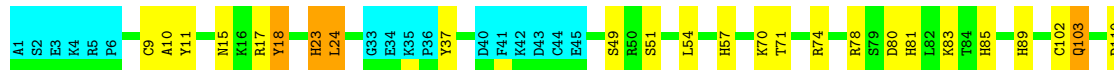
- Molecule 2: DNA (5'-D(P\*DGP\*DCP\*DGP\*DCP\*DAP\*DGP\*DAP\*DCP\*DGP\*DCP\*DCP\*DCP\*DCP\*DCP\*DGP\*DCP\*DG)-3')

Chain C:  71% 29%



- Molecule 3: Wilms tumor 1

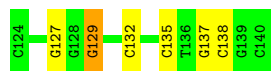
Chain A:  64% 19% 13%



#### 4.2.20 Score per residue for model 20

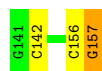
- Molecule 1: DNA (5'-D(P\*DCP\*DGP\*DCP\*DGP\*DGP\*DGP\*DGP\*DCP\*DGP\*DTP\*DCP\*DTP\*DGP\*DCP\*DGP\*DC)-3')

Chain B:  65% 29% 6%



- Molecule 2: DNA (5'-D(P\*DGP\*DCP\*DGP\*DCP\*DAP\*DGP\*DAP\*DCP\*DGP\*DCP\*DCP\*DCP\*DCP\*DCP\*DCP\*DGP\*DCP\*DG)-3')

Chain C:  82% 12% 6%



- Molecule 3: Wilms tumor 1

Chain A:  68% 15% 13%





## 5 Refinement protocol and experimental data overview

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

Of the 200 calculated structures, 20 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 |
|---------------|--------------------|---------|
| Amber         | structure solution |         |
| Amber         | refinement         |         |

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

| Chemical shift file(s)                       | working_cs.cif |
|----------------------------------------------|----------------|
| Number of chemical shift lists               | 1              |
| Total number of shifts                       | 220            |
| Number of shifts mapped to atoms             | 220            |
| Number of unparsed shifts                    | 0              |
| Number of shifts with mapping errors         | 0              |
| Number of shifts with mapping warnings       | 0              |
| Assignment completeness (well-defined parts) | 9%             |

## 6 Model quality [i](#)

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

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Chain | Bond lengths |                      | Bond angles |                       |
|-----|-------|--------------|----------------------|-------------|-----------------------|
|     |       | RMSZ         | #Z>5                 | RMSZ        | #Z>5                  |
| 1   | B     | 0.78±0.06    | 0±0/394 ( 0.0± 0.1%) | 1.22±0.06   | 3±2/607 ( 0.5± 0.3%)  |
| 2   | C     | 0.72±0.03    | 0±0/386 ( 0.0± 0.0%) | 1.18±0.03   | 2±1/592 ( 0.3± 0.1%)  |
| 3   | A     | 0.97±0.01    | 0±0/910 ( 0.0± 0.0%) | 1.24±0.03   | 6±2/1211 ( 0.5± 0.1%) |
| All | All   | 0.88         | 1/33800 ( 0.0%)      | 1.22        | 219/48200 ( 0.5%)     |

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

| Mol | Chain | Chirality | Planarity |
|-----|-------|-----------|-----------|
| 1   | B     | 0.0±0.0   | 2.1±1.5   |
| 2   | C     | 0.0±0.0   | 0.9±0.8   |
| 3   | A     | 0.0±0.0   | 2.9±1.4   |
| All | All   | 0         | 120       |

All unique bond outliers are listed below.

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) | Models |       |
|-----|-------|-----|------|-------|------|-------------|----------|--------|-------|
|     |       |     |      |       |      |             |          | Worst  | Total |
| 1   | B     | 134 | DT   | O3'-P | 5.88 | 1.70        | 1.61     | 17     | 1     |

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) | Models |       |
|-----|-------|-----|------|-----------|-------|-------------|----------|--------|-------|
|     |       |     |      |           |       |             |          | Worst  | Total |
| 3   | A     | 23  | HIS  | CA-CB-CG  | 18.67 | 132.47      | 113.80   | 15     | 20    |
| 3   | A     | 117 | ASN  | CA-CB-CG  | 8.78  | 121.38      | 112.60   | 16     | 1     |
| 1   | B     | 136 | DT   | O3'-P-O5' | -8.69 | 90.97       | 104.00   | 11     | 6     |
| 1   | B     | 128 | DG   | O3'-P-O5' | -8.12 | 91.81       | 104.00   | 6      | 3     |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) | Models |       |
|-----|-------|-----|------|-------------|-------|-------------|----------|--------|-------|
|     |       |     |      |             |       |             |          | Worst  | Total |
| 3   | A     | 113 | VAL  | CA-CB-CG2   | 7.58  | 123.29      | 110.40   | 11     | 1     |
| 3   | A     | 81  | HIS  | CA-CB-CG    | 7.57  | 121.37      | 113.80   | 7      | 8     |
| 1   | B     | 129 | DG   | O3'-P-O5'   | -7.45 | 92.83       | 104.00   | 12     | 1     |
| 3   | A     | 80  | ASP  | CA-CB-CG    | 7.09  | 119.69      | 112.60   | 19     | 9     |
| 1   | B     | 134 | DT   | C5'-C4'-C3' | -7.07 | 104.29      | 114.90   | 8      | 6     |
| 1   | B     | 133 | DG   | O3'-P-O5'   | -6.89 | 93.67       | 104.00   | 17     | 6     |
| 1   | B     | 136 | DT   | C2'-C3'-O3' | 6.65  | 121.48      | 111.50   | 1      | 2     |
| 3   | A     | 7   | PHE  | CA-CB-CG    | 6.65  | 120.45      | 113.80   | 10     | 5     |
| 1   | B     | 128 | DG   | C5'-C4'-C3' | -6.53 | 105.11      | 114.90   | 6      | 1     |
| 3   | A     | 57  | HIS  | CB-CG-CD2   | -6.49 | 122.76      | 131.20   | 5      | 7     |
| 1   | B     | 137 | DG   | O3'-P-O5'   | -6.46 | 94.31       | 104.00   | 7      | 4     |
| 3   | A     | 60  | ARG  | CD-NE-CZ    | 6.43  | 133.41      | 124.40   | 1      | 1     |
| 3   | A     | 15  | ASN  | CA-CB-CG    | 6.37  | 118.97      | 112.60   | 6      | 3     |
| 1   | B     | 131 | DG   | O3'-P-O5'   | -6.20 | 94.69       | 104.00   | 13     | 2     |
| 1   | B     | 134 | DT   | O3'-P-O5'   | -6.18 | 94.73       | 104.00   | 7      | 1     |
| 2   | C     | 148 | DC   | O3'-P-O5'   | -6.18 | 94.73       | 104.00   | 16     | 5     |
| 1   | B     | 132 | DC   | O3'-P-O5'   | -6.15 | 94.77       | 104.00   | 20     | 3     |
| 1   | B     | 135 | DC   | C5'-C4'-C3' | -6.14 | 105.69      | 114.90   | 17     | 1     |
| 3   | A     | 85  | HIS  | CB-CG-CD2   | -6.09 | 123.28      | 131.20   | 19     | 17    |
| 3   | A     | 110 | ASP  | CA-CB-CG    | 6.09  | 118.69      | 112.60   | 15     | 3     |
| 2   | C     | 146 | DG   | O5'-C5'-C4' | 6.05  | 119.87      | 110.80   | 13     | 3     |
| 1   | B     | 134 | DT   | C5'-C4'-O4' | 6.04  | 118.47      | 109.40   | 17     | 1     |
| 1   | B     | 138 | DC   | O3'-P-O5'   | -6.02 | 94.97       | 104.00   | 12     | 6     |
| 3   | A     | 116 | HIS  | CB-CG-CD2   | -5.98 | 123.43      | 131.20   | 10     | 20    |
| 3   | A     | 81  | HIS  | CB-CG-CD2   | -5.91 | 123.51      | 131.20   | 7      | 11    |
| 1   | B     | 134 | DT   | C4'-C3'-O3' | 5.89  | 118.84      | 110.00   | 17     | 1     |
| 2   | C     | 143 | DG   | O3'-P-O5'   | -5.76 | 95.37       | 104.00   | 4      | 1     |
| 3   | A     | 84  | THR  | CA-CB-CG2   | 5.75  | 120.28      | 110.50   | 18     | 7     |
| 2   | C     | 142 | DC   | C2'-C3'-O3' | 5.74  | 120.12      | 111.50   | 11     | 7     |
| 3   | A     | 61  | HIS  | CA-CB-CG    | 5.74  | 119.54      | 113.80   | 18     | 1     |
| 3   | A     | 52  | ASP  | CA-CB-CG    | 5.71  | 118.31      | 112.60   | 3      | 1     |
| 2   | C     | 153 | DC   | O3'-P-O5'   | -5.71 | 95.44       | 104.00   | 3      | 1     |
| 1   | B     | 135 | DC   | O3'-P-O5'   | -5.71 | 95.44       | 104.00   | 12     | 2     |
| 2   | C     | 142 | DC   | O3'-P-O5'   | -5.59 | 95.62       | 104.00   | 9      | 6     |
| 1   | B     | 129 | DG   | C2'-C3'-O3' | 5.52  | 119.78      | 111.50   | 5      | 1     |
| 3   | A     | 27  | HIS  | CA-CB-CG    | -5.50 | 108.30      | 113.80   | 8      | 3     |
| 3   | A     | 27  | HIS  | CB-CG-CD2   | -5.46 | 124.10      | 131.20   | 14     | 2     |
| 1   | B     | 134 | DT   | O4'-C4'-C3' | 5.46  | 113.59      | 105.40   | 11     | 2     |
| 3   | A     | 48  | PHE  | CA-CB-CG    | -5.45 | 108.35      | 113.80   | 10     | 1     |
| 1   | B     | 135 | DC   | O5'-C5'-C4' | 5.44  | 118.96      | 110.80   | 20     | 1     |
| 3   | A     | 115 | HIS  | CB-CG-CD2   | -5.43 | 124.14      | 131.20   | 7      | 1     |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) | Models |       |
|-----|-------|-----|------|-------------|-------|-------------|----------|--------|-------|
|     |       |     |      |             |       |             |          | Worst  | Total |
| 3   | A     | 32  | THR  | CA-CB-CG2   | 5.43  | 119.73      | 110.50   | 8      | 3     |
| 2   | C     | 146 | DG   | O3'-P-O5'   | -5.35 | 95.97       | 104.00   | 9      | 1     |
| 2   | C     | 144 | DC   | O3'-P-O5'   | -5.35 | 95.97       | 104.00   | 11     | 1     |
| 2   | C     | 149 | DG   | C2'-C3'-O3' | 5.33  | 119.49      | 111.50   | 6      | 3     |
| 3   | A     | 19  | PHE  | CA-CB-CG    | 5.32  | 119.11      | 113.80   | 15     | 1     |
| 2   | C     | 155 | DG   | C5'-C4'-C3' | -5.31 | 106.94      | 114.90   | 18     | 1     |
| 2   | C     | 141 | DG   | O3'-P-O5'   | -5.26 | 96.10       | 104.00   | 2      | 1     |
| 2   | C     | 144 | DC   | C4'-C3'-O3' | -5.25 | 102.12      | 110.00   | 7      | 1     |
| 1   | B     | 130 | DG   | O3'-P-O5'   | -5.25 | 96.12       | 104.00   | 12     | 1     |
| 3   | A     | 73  | GLN  | OE1-CD-NE2  | -5.25 | 117.35      | 122.60   | 17     | 1     |
| 2   | C     | 152 | DC   | O3'-P-O5'   | -5.22 | 96.16       | 104.00   | 5      | 1     |
| 3   | A     | 58  | GLN  | OE1-CD-NE2  | -5.19 | 117.41      | 122.60   | 15     | 1     |
| 2   | C     | 144 | DC   | C2'-C3'-O3' | 5.17  | 119.26      | 111.50   | 12     | 1     |
| 1   | B     | 134 | DT   | C2'-C3'-O3' | -5.17 | 103.75      | 111.50   | 16     | 1     |
| 1   | B     | 130 | DG   | C4'-C3'-O3' | 5.11  | 117.66      | 110.00   | 12     | 1     |
| 1   | B     | 135 | DC   | C5'-C4'-O4' | 5.10  | 117.06      | 109.40   | 11     | 1     |
| 2   | C     | 145 | DA   | P-O3'-C3'   | 5.10  | 127.85      | 120.20   | 14     | 1     |
| 2   | C     | 150 | DC   | C5'-C4'-C3' | -5.05 | 107.33      | 114.90   | 10     | 1     |
| 2   | C     | 150 | DC   | O3'-P-O5'   | -5.05 | 96.43       | 104.00   | 18     | 1     |
| 1   | B     | 137 | DG   | C2'-C3'-O3' | 5.03  | 119.04      | 111.50   | 13     | 1     |

There are no chirality outliers.

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

| Mol | Chain | Res | Type | Group     | Models (Total) |
|-----|-------|-----|------|-----------|----------------|
| 3   | A     | 18  | TYR  | Sidechain | 19             |
| 1   | B     | 127 | DG   | Sidechain | 12             |
| 1   | B     | 129 | DG   | Sidechain | 9              |
| 3   | A     | 11  | TYR  | Sidechain | 9              |
| 3   | A     | 48  | PHE  | Sidechain | 8              |
| 2   | C     | 157 | DG   | Sidechain | 7              |
| 3   | A     | 23  | HIS  | Sidechain | 7              |
| 1   | B     | 134 | DT   | Sidechain | 6              |
| 2   | C     | 146 | DG   | Sidechain | 5              |
| 3   | A     | 37  | TYR  | Sidechain | 4              |
| 1   | B     | 124 | DC   | Sidechain | 3              |
| 1   | B     | 128 | DG   | Sidechain | 3              |
| 2   | C     | 149 | DG   | Sidechain | 3              |
| 1   | B     | 133 | DG   | Sidechain | 3              |
| 3   | A     | 47  | ARG  | Sidechain | 3              |

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| Mol | Chain | Res | Type | Group     | Models (Total) |
|-----|-------|-----|------|-----------|----------------|
| 1   | B     | 131 | DG   | Sidechain | 3              |
| 2   | C     | 155 | DG   | Sidechain | 2              |
| 1   | B     | 130 | DG   | Sidechain | 2              |
| 3   | A     | 78  | ARG  | Sidechain | 2              |
| 3   | A     | 29  | ARG  | Sidechain | 1              |
| 3   | A     | 98  | ARG  | Sidechain | 1              |
| 1   | B     | 135 | DC   | Sidechain | 1              |
| 2   | C     | 145 | DA   | Sidechain | 1              |
| 2   | C     | 156 | DC   | Sidechain | 1              |
| 1   | B     | 132 | DC   | Sidechain | 1              |
| 3   | A     | 56  | ARG  | Sidechain | 1              |
| 3   | A     | 106 | PHE  | Sidechain | 1              |
| 3   | A     | 74  | ARG  | Sidechain | 1              |
| 3   | A     | 60  | ARG  | Sidechain | 1              |

## 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   | B     | 352   | 189      | 188      | 2±1     |
| 2   | C     | 345   | 187      | 188      | 1±0     |
| 3   | A     | 884   | 863      | 863      | 7±2     |
| All | All   | 31700 | 24780    | 24810    | 160     |

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 3.

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

| Atom-1         | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|----------------|------------------|----------|-------------|--------|-------|
|                |                  |          |             | Worst  | Total |
| 3:A:18:TYR:CD2 | 3:A:24:LEU:HD23  | 0.69     | 2.22        | 18     | 3     |
| 3:A:37:TYR:HB3 | 3:A:54:LEU:HD22  | 0.67     | 1.65        | 18     | 9     |
| 3:A:18:TYR:CD1 | 3:A:24:LEU:HD23  | 0.66     | 2.26        | 20     | 16    |
| 3:A:67:PHE:HB3 | 3:A:82:LEU:HD13  | 0.62     | 1.72        | 16     | 7     |
| 3:A:109:SER:O  | 3:A:113:VAL:HG13 | 0.56     | 2.00        | 11     | 1     |
| 1:B:128:DG:C8  | 3:A:81:HIS:CE1   | 0.52     | 2.98        | 16     | 9     |
| 1:B:129:DG:N7  | 3:A:81:HIS:CE1   | 0.50     | 2.80        | 11     | 20    |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 2:C:144:DC:N4   | 3:A:29:ARG:HH22 | 0.50     | 2.04        | 6      | 1     |
| 3:A:48:PHE:CZ   | 3:A:57:HIS:CG   | 0.50     | 3.00        | 2      | 16    |
| 1:B:129:DG:H3'  | 3:A:60:ARG:NE   | 0.49     | 2.22        | 11     | 1     |
| 3:A:9:CYS:SG    | 3:A:10:ALA:N    | 0.49     | 2.86        | 14     | 11    |
| 2:C:156:DC:H2'' | 2:C:157:DG:C8   | 0.49     | 2.43        | 18     | 15    |
| 3:A:19:PHE:O    | 3:A:20:LYS:C    | 0.47     | 2.57        | 18     | 1     |
| 3:A:24:LEU:O    | 3:A:24:LEU:HD22 | 0.46     | 2.10        | 1      | 11    |
| 1:B:134:DT:H2'' | 1:B:135:DC:C6   | 0.46     | 2.45        | 16     | 2     |
| 3:A:102:CYS:SG  | 3:A:103:GLN:N   | 0.46     | 2.89        | 6      | 8     |
| 1:B:129:DG:N7   | 3:A:81:HIS:HE1  | 0.46     | 2.09        | 4      | 4     |
| 1:B:134:DT:H2'' | 1:B:135:DC:C5   | 0.46     | 2.46        | 7      | 2     |
| 3:A:60:ARG:N    | 3:A:60:ARG:HD3  | 0.45     | 2.27        | 11     | 1     |
| 3:A:11:TYR:CD2  | 3:A:31:HIS:CE1  | 0.45     | 3.05        | 4      | 2     |
| 3:A:102:CYS:SG  | 3:A:104:LYS:CE  | 0.44     | 3.06        | 13     | 1     |
| 1:B:129:DG:H2'  | 3:A:60:ARG:CZ   | 0.44     | 2.43        | 5      | 1     |
| 1:B:135:DC:H41  | 3:A:29:ARG:NH2  | 0.43     | 2.11        | 11     | 1     |
| 3:A:14:CYS:SG   | 3:A:15:ASN:N    | 0.43     | 2.91        | 1      | 1     |
| 3:A:14:CYS:SG   | 3:A:16:LYS:HE3  | 0.43     | 2.54        | 13     | 1     |
| 1:B:134:DT:C2   | 1:B:135:DC:C4   | 0.41     | 3.08        | 4      | 1     |
| 3:A:68:GLN:NE2  | 3:A:68:GLN:H    | 0.41     | 2.13        | 17     | 1     |
| 2:C:149:DG:C4   | 2:C:150:DC:C5   | 0.41     | 3.09        | 1      | 1     |
| 3:A:25:GLN:HE21 | 3:A:29:ARG:NH1  | 0.41     | 2.14        | 2      | 1     |
| 3:A:72:CYS:SG   | 3:A:73:GLN:N    | 0.41     | 2.90        | 7      | 1     |
| 1:B:132:DC:H41  | 3:A:53:GLN:CD   | 0.41     | 2.24        | 9      | 1     |
| 3:A:19:PHE:CG   | 3:A:20:LYS:N    | 0.41     | 2.89        | 18     | 1     |
| 3:A:18:TYR:CE1  | 3:A:27:HIS:CD2  | 0.40     | 3.09        | 4      | 2     |
| 3:A:69:CYS:SG   | 3:A:70:LYS:HE2  | 0.40     | 2.56        | 2      | 1     |
| 3:A:24:LEU:HD22 | 3:A:24:LEU:O    | 0.40     | 2.17        | 16     | 4     |
| 3:A:72:CYS:O    | 3:A:73:GLN:CB   | 0.40     | 2.69        | 8      | 1     |

## 6.3 Torsion angles ⓘ

### 6.3.1 Protein backbone ⓘ

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

| Mol | Chain | Analysed      | Favoured     | Allowed    | Outliers   | Percentiles |
|-----|-------|---------------|--------------|------------|------------|-------------|
| 3   | A     | 102/119 (86%) | 95±2 (93±2%) | 6±2 (6±2%) | 1±1 (1±1%) | 26 74       |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |
|-----|-------|-----------------|------------|----------|----------|-------------|
| All | All   | 2040/2380 (86%) | 1904 (93%) | 125 (6%) | 11 (1%)  | 26 74       |

All 6 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 3   | A     | 103 | GLN  | 3              |
| 3   | A     | 13  | GLY  | 3              |
| 3   | A     | 15  | ASN  | 2              |
| 3   | A     | 73  | GLN  | 1              |
| 3   | A     | 99  | TRP  | 1              |
| 3   | A     | 20  | LYS  | 1              |

### 6.3.2 Protein sidechains ⓘ

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 |
|-----|-------|-----------------|--------------|--------------|-------------|
| 3   | A     | 98/112 (88%)    | 88±2 (90±2%) | 10±2 (10±2%) | 9 53        |
| All | All   | 1960/2240 (88%) | 1761 (90%)   | 199 (10%)    | 9 53        |

All 44 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) |
|-----|-------|-----|------|----------------|
| 3   | A     | 23  | HIS  | 20             |
| 3   | A     | 24  | LEU  | 20             |
| 3   | A     | 71  | THR  | 20             |
| 3   | A     | 117 | ASN  | 15             |
| 3   | A     | 70  | LYS  | 9              |
| 3   | A     | 51  | SER  | 8              |
| 3   | A     | 15  | ASN  | 8              |
| 3   | A     | 47  | ARG  | 7              |
| 3   | A     | 74  | ARG  | 7              |
| 3   | A     | 103 | GLN  | 6              |
| 3   | A     | 29  | ARG  | 4              |
| 3   | A     | 38  | GLN  | 4              |
| 3   | A     | 32  | THR  | 4              |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 3   | A     | 8   | MET  | 4              |
| 3   | A     | 104 | LYS  | 4              |
| 3   | A     | 73  | GLN  | 4              |
| 3   | A     | 58  | GLN  | 4              |
| 3   | A     | 55  | LYS  | 3              |
| 3   | A     | 59  | ARG  | 3              |
| 3   | A     | 26  | MET  | 3              |
| 3   | A     | 75  | LYS  | 3              |
| 3   | A     | 21  | LEU  | 3              |
| 3   | A     | 39  | CYS  | 3              |
| 3   | A     | 98  | ARG  | 3              |
| 3   | A     | 25  | GLN  | 3              |
| 3   | A     | 60  | ARG  | 2              |
| 3   | A     | 30  | LYS  | 2              |
| 3   | A     | 46  | ARG  | 2              |
| 3   | A     | 17  | ARG  | 2              |
| 3   | A     | 83  | LYS  | 2              |
| 3   | A     | 61  | HIS  | 2              |
| 3   | A     | 16  | LYS  | 2              |
| 3   | A     | 89  | HIS  | 2              |
| 3   | A     | 53  | GLN  | 1              |
| 3   | A     | 9   | CYS  | 1              |
| 3   | A     | 52  | ASP  | 1              |
| 3   | A     | 105 | LYS  | 1              |
| 3   | A     | 20  | LYS  | 1              |
| 3   | A     | 22  | SER  | 1              |
| 3   | A     | 87  | ARG  | 1              |
| 3   | A     | 92  | GLU  | 1              |
| 3   | A     | 114 | ARG  | 1              |
| 3   | A     | 109 | SER  | 1              |
| 3   | A     | 49  | SER  | 1              |

### 6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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



## 6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

## 6.7 Other polymers [i](#)

There are no such molecules in this entry.

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

There are no chain breaks in this entry.

## 7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 9% for the well-defined parts and 9% for the entire structure.

### 7.1 Chemical shift list 1

File name: working\_cs.cif

Chemical shift list name: *assigned\_chem\_shift\_list\_1*

#### 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                  | 220 |
| Number of shifts mapped to atoms        | 220 |
| Number of unparsed shifts               | 0   |
| Number of shifts with mapping errors    | 0   |
| Number of shifts with mapping warnings  | 0   |
| Number of shift outliers (ShiftChecker) | 0   |

#### 7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

| Nucleus                | # values | Correction $\pm$ precision, ppm | Suggested action           |
|------------------------|----------|---------------------------------|----------------------------|
| $^{13}\text{C}_\alpha$ | 0        | —                               | None (insufficient data)   |
| $^{13}\text{C}_\beta$  | 0        | —                               | None (insufficient data)   |
| $^{13}\text{C}'$       | 0        | —                               | None (insufficient data)   |
| $^{15}\text{N}$        | 109      | $-0.34 \pm 0.32$                | 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 9%, i.e. 196 atoms were assigned a chemical shift out of a possible 2207. 0 out of 7 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total         | $^1\text{H}$ | $^{13}\text{C}$ | $^{15}\text{N}$ |
|-----------|---------------|--------------|-----------------|-----------------|
| Backbone  | 194/510 (38%) | 97/205 (47%) | 0/206 (0%)      | 97/99 (98%)     |
| Sidechain | 0/820 (0%)    | 0/520 (0%)   | 0/238 (0%)      | 0/62 (0%)       |

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|          | Total         | <sup>1</sup> H | <sup>13</sup> C | <sup>15</sup> N |
|----------|---------------|----------------|-----------------|-----------------|
| Aromatic | 2/186 (1%)    | 1/97 (1%)      | 0/77 (0%)       | 1/12 (8%)       |
| Sugar    | 0/408 (0%)    | 0/238 (0%)     | 0/170 (0%)      | 0/0 (—%)        |
| Base     | 0/283 (0%)    | 0/181 (0%)     | 0/53 (0%)       | 0/49 (0%)       |
| Overall  | 196/2207 (9%) | 98/1241 (8%)   | 0/744 (0%)      | 98/222 (44%)    |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 9%, i.e. 220 atoms were assigned a chemical shift out of a possible 2411. 0 out of 7 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total         | <sup>1</sup> H | <sup>13</sup> C | <sup>15</sup> N |
|-----------|---------------|----------------|-----------------|-----------------|
| Backbone  | 218/587 (37%) | 109/236 (46%)  | 0/238 (0%)      | 109/113 (96%)   |
| Sidechain | 0/937 (0%)    | 0/592 (0%)     | 0/277 (0%)      | 0/68 (0%)       |
| Aromatic  | 2/196 (1%)    | 1/102 (1%)     | 0/82 (0%)       | 1/12 (8%)       |
| Sugar     | 0/408 (0%)    | 0/238 (0%)     | 0/170 (0%)      | 0/0 (—%)        |
| Base      | 0/283 (0%)    | 0/181 (0%)     | 0/53 (0%)       | 0/49 (0%)       |
| Overall   | 220/2411 (9%) | 110/1349 (8%)  | 0/820 (0%)      | 110/242 (45%)   |

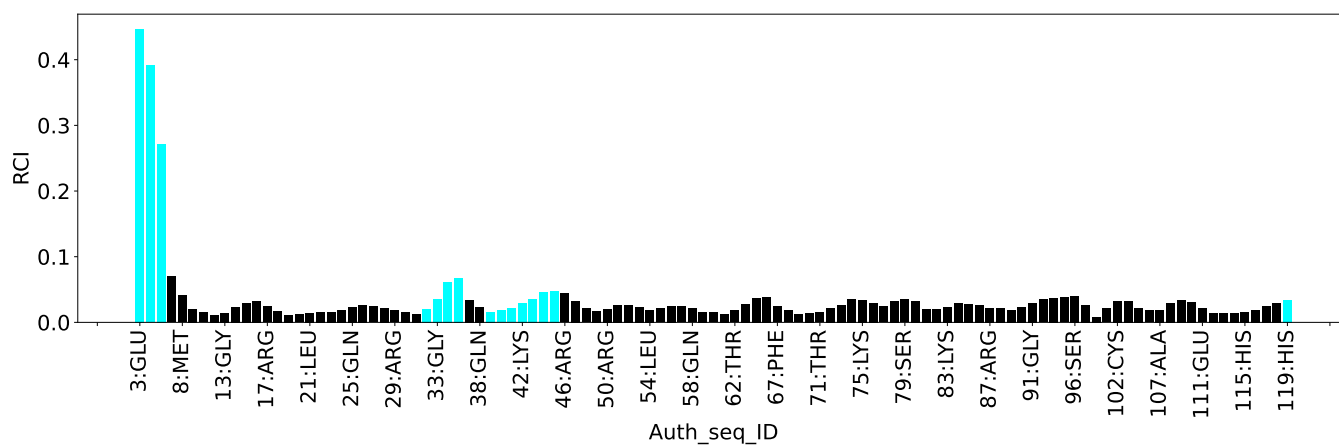
#### 7.1.4 Statistically unusual chemical shifts ⓘ

There are no statistically unusual chemical shifts.

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

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

Random coil index (RCI) for chain A:



## 8 NMR restraints analysis

### 8.1 Conformationally restricting restraints

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

| Description                                              | Value |
|----------------------------------------------------------|-------|
| Total distance restraints                                | 1012  |
| Intra-residue ( $ i-j =0$ )                              | 0     |
| Sequential ( $ i-j =1$ )                                 | 70    |
| Medium range ( $ i-j >1$ and $ i-j <5$ )                 | 309   |
| Long range ( $ i-j \geq 5$ )                             | 321   |
| Inter-chain                                              | 180   |
| Hydrogen bond restraints                                 | 132   |
| Disulfide bond restraints                                | 0     |
| Total dihedral-angle restraints                          | 108   |
| Number of unmapped restraints                            | 0     |
| Number of restraints per residue                         | 7.1   |
| Number of long range restraints per residue <sup>1</sup> | 2.3   |

<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)  | 44.3                                   | 0.2     |
| 0.2-0.5 (Medium) | 25.7                                   | 0.5     |
| >0.5 (Large)     | 27.1                                   | 2.2     |

### 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)   | 1.2                                    | 8.62    |
| 10.0-20.0 (Medium) | 0.1                                    | 18.87   |
| >20.0 (Large)      | None                                   | None    |

## 9 Distance violation analysis ⓘ

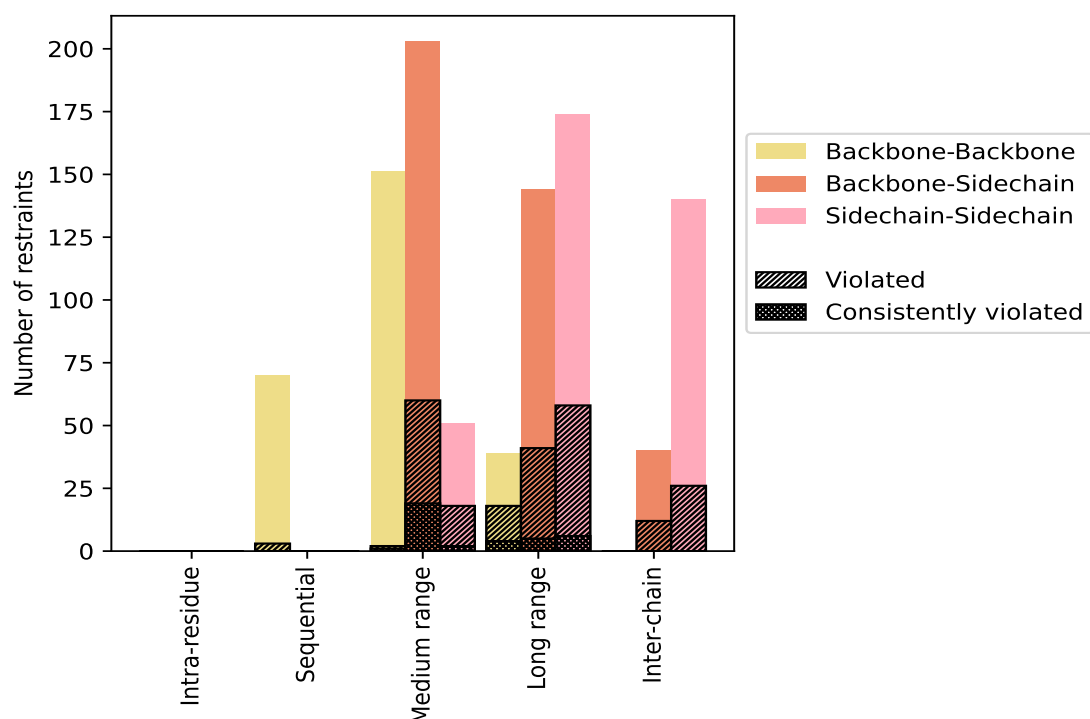
### 9.1 Summary of distance violations ⓘ

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> |
| <b>Intra-residue (<math> i-j =0</math>)</b>                                 | 0     | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Backbone                                                           | 0     | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 0     | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Sidechain-Sidechain                                                         | 0     | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| <b>Sequential (<math> i-j =1</math>)</b>                                    | 70    | 6.9            | 3                     | 4.3            | 0.3            | 0                                  | 0.0            | 0.0            |
| Backbone-Backbone                                                           | 70    | 6.9            | 3                     | 4.3            | 0.3            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 0     | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Sidechain-Sidechain                                                         | 0     | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| <b>Medium range (<math> i-j &gt;1</math> &amp; <math> i-j &lt;5</math>)</b> | 309   | 30.5           | 33                    | 10.7           | 3.3            | 3                                  | 1.0            | 0.3            |
| Backbone-Backbone                                                           | 151   | 14.9           | 2                     | 1.3            | 0.2            | 1                                  | 0.7            | 0.1            |
| Backbone-Sidechain                                                          | 107   | 10.6           | 13                    | 12.1           | 1.3            | 0                                  | 0.0            | 0.0            |
| Sidechain-Sidechain                                                         | 51    | 5.0            | 18                    | 35.3           | 1.8            | 2                                  | 3.9            | 0.2            |
| <b>Long range (<math> i-j \geq 5</math>)</b>                                | 321   | 31.7           | 110                   | 34.3           | 10.9           | 15                                 | 4.7            | 1.5            |
| Backbone-Backbone                                                           | 39    | 3.9            | 18                    | 46.2           | 1.8            | 4                                  | 10.3           | 0.4            |
| Backbone-Sidechain                                                          | 108   | 10.7           | 34                    | 31.5           | 3.4            | 5                                  | 4.6            | 0.5            |
| Sidechain-Sidechain                                                         | 174   | 17.2           | 58                    | 33.3           | 5.7            | 6                                  | 3.4            | 0.6            |
| <b>Inter-chain</b>                                                          | 180   | 17.8           | 38                    | 21.1           | 3.8            | 0                                  | 0.0            | 0.0            |
| Backbone-Backbone                                                           | 0     | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 40    | 4.0            | 12                    | 30.0           | 1.2            | 0                                  | 0.0            | 0.0            |
| Sidechain-Sidechain                                                         | 140   | 13.8           | 26                    | 18.6           | 2.6            | 0                                  | 0.0            | 0.0            |
| <b>Hydrogen bond</b>                                                        | 132   | 13.0           | 54                    | 40.9           | 5.3            | 19                                 | 14.4           | 1.9            |
| <b>Disulfide bond</b>                                                       | 0     | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| <b>Total</b>                                                                | 1012  | 100.0          | 238                   | 23.5           | 23.5           | 37                                 | 3.7            | 3.7            |
| Backbone-Backbone                                                           | 260   | 25.7           | 23                    | 8.8            | 2.3            | 5                                  | 1.9            | 0.5            |
| Backbone-Sidechain                                                          | 387   | 38.2           | 113                   | 29.2           | 11.2           | 24                                 | 6.2            | 2.4            |
| Sidechain-Sidechain                                                         | 365   | 36.1           | 102                   | 27.9           | 10.1           | 8                                  | 2.2            | 0.8            |

<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        | 0                    | 1               | 42              | 51              | 14              | 108   | 0.44     | 2.03    | 0.5                 | 0.21       |
| 2        | 0                    | 0               | 40              | 52              | 9               | 101   | 0.5      | 1.98    | 0.51                | 0.23       |
| 3        | 0                    | 0               | 41              | 46              | 5               | 92    | 0.49     | 1.96    | 0.52                | 0.22       |
| 4        | 0                    | 0               | 37              | 49              | 8               | 94    | 0.52     | 2.02    | 0.55                | 0.22       |
| 5        | 0                    | 0               | 37              | 51              | 13              | 101   | 0.46     | 2.05    | 0.52                | 0.22       |
| 6        | 0                    | 0               | 40              | 39              | 7               | 86    | 0.42     | 1.92    | 0.48                | 0.2        |
| 7        | 0                    | 2               | 40              | 59              | 8               | 109   | 0.47     | 2.2     | 0.5                 | 0.21       |
| 8        | 0                    | 0               | 43              | 49              | 11              | 103   | 0.48     | 1.88    | 0.53                | 0.2        |
| 9        | 0                    | 0               | 43              | 53              | 8               | 104   | 0.47     | 2.02    | 0.5                 | 0.22       |
| 10       | 0                    | 0               | 40              | 50              | 7               | 97    | 0.48     | 2.02    | 0.52                | 0.21       |

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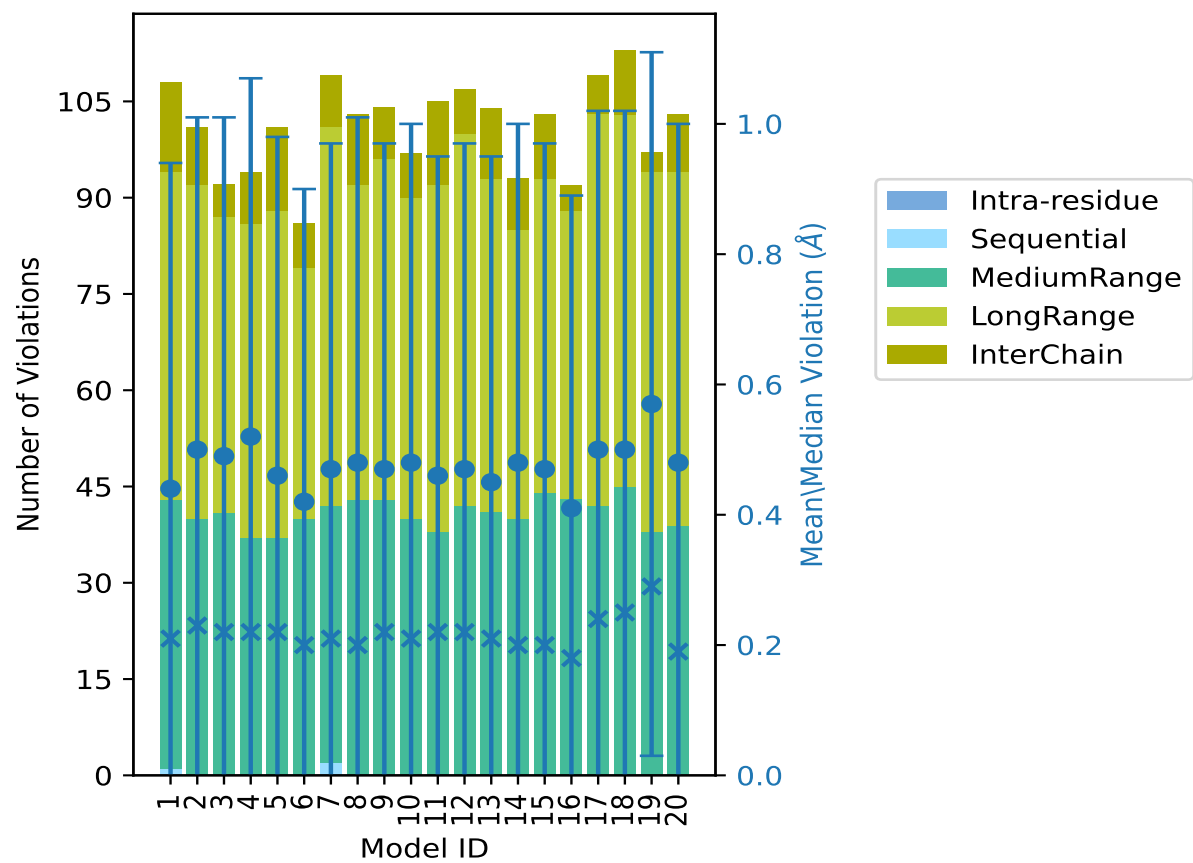


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| Model ID | Number of violations |                 |                 |                 |                 |       | Mean (Å) | Max (Å) | SD <sup>6</sup> (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
|          | IR <sup>1</sup>      | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total |          |         |                     |            |
| 11       | 0                    | 0               | 38              | 54              | 13              | 105   | 0.46     | 1.92    | 0.49                | 0.22       |
| 12       | 0                    | 0               | 42              | 58              | 7               | 107   | 0.47     | 1.89    | 0.5                 | 0.22       |
| 13       | 0                    | 0               | 41              | 52              | 11              | 104   | 0.45     | 2.05    | 0.5                 | 0.21       |
| 14       | 0                    | 0               | 40              | 45              | 8               | 93    | 0.48     | 2.02    | 0.52                | 0.2        |
| 15       | 0                    | 0               | 44              | 49              | 10              | 103   | 0.47     | 2.1     | 0.5                 | 0.2        |
| 16       | 0                    | 0               | 43              | 45              | 4               | 92    | 0.41     | 1.89    | 0.48                | 0.18       |
| 17       | 0                    | 0               | 42              | 61              | 6               | 109   | 0.5      | 2.17    | 0.52                | 0.24       |
| 18       | 0                    | 0               | 45              | 58              | 10              | 113   | 0.5      | 1.85    | 0.52                | 0.25       |
| 19       | 0                    | 0               | 38              | 56              | 3               | 97    | 0.57     | 1.95    | 0.54                | 0.29       |
| 20       | 0                    | 0               | 39              | 55              | 9               | 103   | 0.48     | 2.0     | 0.52                | 0.19       |

<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 ⓘ



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

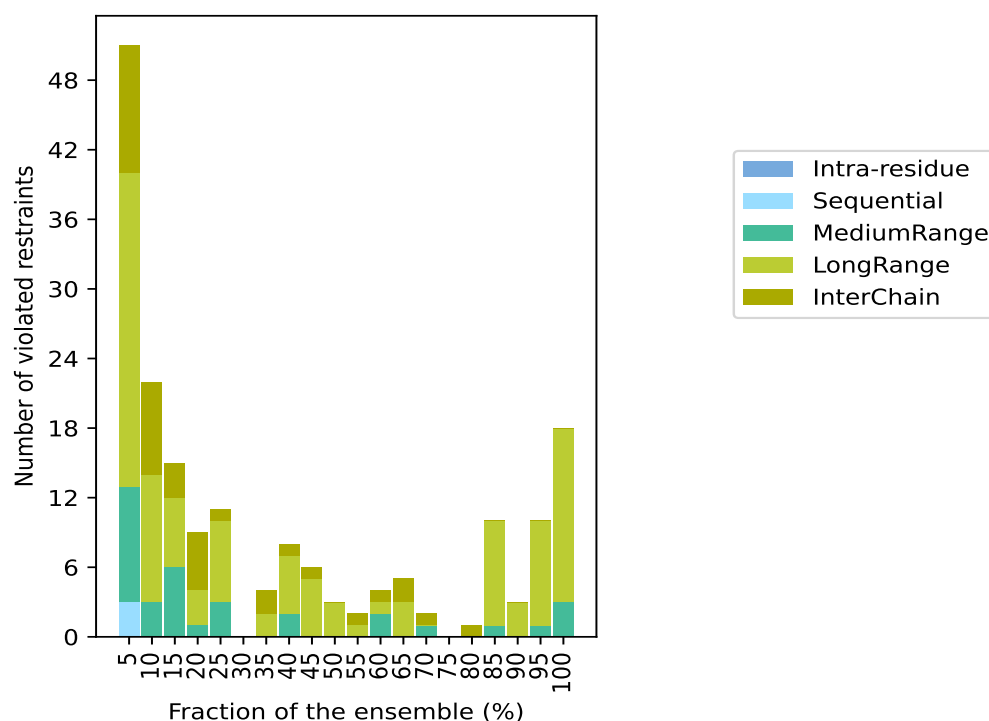
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 696(IR:0, SQ:67, MR:276, LR:211, IC:142) restraints are not violated in the ensemble.

| Number of violated restraints |                 |                 |                 |                 |       | Fraction of the ensemble |       |
|-------------------------------|-----------------|-----------------|-----------------|-----------------|-------|--------------------------|-------|
| IR <sup>1</sup>               | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total | Count <sup>6</sup>       | %     |
| 0                             | 3               | 10              | 27              | 11              | 51    | 1                        | 5.0   |
| 0                             | 0               | 3               | 11              | 8               | 22    | 2                        | 10.0  |
| 0                             | 0               | 6               | 6               | 3               | 15    | 3                        | 15.0  |
| 0                             | 0               | 1               | 3               | 5               | 9     | 4                        | 20.0  |
| 0                             | 0               | 3               | 7               | 1               | 11    | 5                        | 25.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 6                        | 30.0  |
| 0                             | 0               | 0               | 2               | 2               | 4     | 7                        | 35.0  |
| 0                             | 0               | 2               | 5               | 1               | 8     | 8                        | 40.0  |
| 0                             | 0               | 0               | 5               | 1               | 6     | 9                        | 45.0  |
| 0                             | 0               | 0               | 3               | 0               | 3     | 10                       | 50.0  |
| 0                             | 0               | 0               | 1               | 1               | 2     | 11                       | 55.0  |
| 0                             | 0               | 2               | 1               | 1               | 4     | 12                       | 60.0  |
| 0                             | 0               | 0               | 3               | 2               | 5     | 13                       | 65.0  |
| 0                             | 0               | 1               | 0               | 1               | 2     | 14                       | 70.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 15                       | 75.0  |
| 0                             | 0               | 0               | 0               | 1               | 1     | 16                       | 80.0  |
| 0                             | 0               | 1               | 9               | 0               | 10    | 17                       | 85.0  |
| 0                             | 0               | 0               | 3               | 0               | 3     | 18                       | 90.0  |
| 0                             | 0               | 1               | 9               | 0               | 10    | 19                       | 95.0  |
| 0                             | 0               | 3               | 15              | 0               | 18    | 20                       | 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

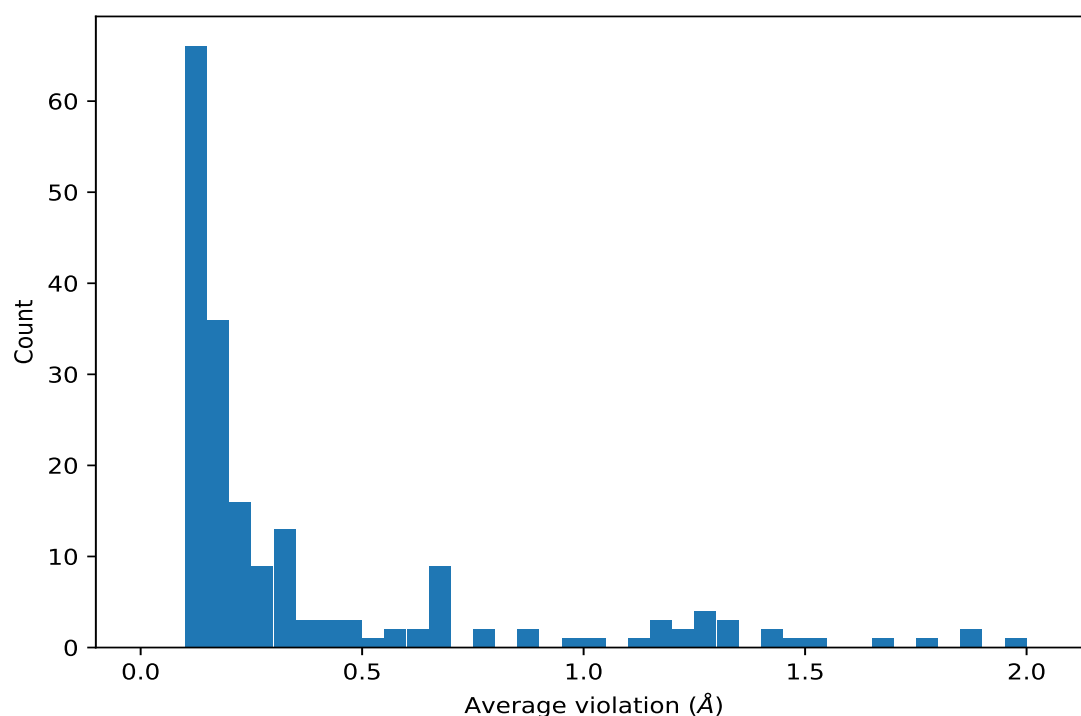
### 9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



## 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) |
|---------|----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,560) | 3:95:A:PHE:CE1 | 3:107:A:ALA:CA  | 20                  | 1.77     | 0.04                | 1.75       |
| (1,554) | 3:95:A:PHE:CD1 | 3:106:A:PHE:CA  | 20                  | 1.66     | 0.02                | 1.65       |
| (1,562) | 3:95:A:PHE:CE1 | 3:108:A:ARG:CB  | 20                  | 1.54     | 0.05                | 1.54       |
| (1,556) | 3:95:A:PHE:CD1 | 3:107:A:ALA:CA  | 20                  | 1.43     | 0.03                | 1.42       |
| (1,555) | 3:95:A:PHE:CD1 | 3:106:A:PHE:CB  | 20                  | 1.32     | 0.04                | 1.32       |
| (1,557) | 3:95:A:PHE:CD1 | 3:108:A:ARG:CA  | 20                  | 1.18     | 0.04                | 1.17       |
| (1,561) | 3:95:A:PHE:CE1 | 3:108:A:ARG:CA  | 20                  | 1.17     | 0.03                | 1.17       |
| (1,566) | 3:95:A:PHE:CE2 | 3:109:A:SER:CB  | 20                  | 1.15     | 0.02                | 1.15       |
| (1,569) | 3:95:A:PHE:CD2 | 3:112:A:LEU:CD2 | 20                  | 1.13     | 0.06                | 1.14       |
| (1,568) | 3:95:A:PHE:CD2 | 3:109:A:SER:CB  | 20                  | 0.85     | 0.03                | 0.86       |
| (2,125) | 3:112:A:LEU:N  | 3:108:A:ARG:O   | 20                  | 0.38     | 0.01                | 0.38       |
| (2,103) | 3:54:A:LEU:N   | 3:50:A:ARG:O    | 20                  | 0.34     | 0.04                | 0.35       |
| (2,119) | 3:87:A:ARG:N   | 3:84:A:THR:O    | 20                  | 0.32     | 0.03                | 0.32       |
| (2,132) | 3:119:A:HIS:N  | 3:116:A:HIS:O   | 20                  | 0.31     | 0.06                | 0.35       |
| (2,114) | 3:82:A:LEU:N   | 3:78:A:ARG:O    | 20                  | 0.3      | 0.03                | 0.31       |
| (1,351) | 3:22:A:SER:CA  | 3:24:A:LEU:CA   | 20                  | 0.3      | 0.05                | 0.29       |

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| Key     | Atom-1         | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|----------------|-----------------|---------------------|----------|---------------------|------------|
| (2,95)  | 3:27:A:HIS:N   | 3:23:A:HIS:O    | 20                  | 0.29     | 0.07                | 0.32       |
| (2,108) | 3:59:A:ARG:N   | 3:56:A:ARG:O    | 20                  | 0.29     | 0.04                | 0.3        |
| (2,97)  | 3:29:A:ARG:N   | 3:26:A:MET:O    | 20                  | 0.28     | 0.04                | 0.3        |
| (2,98)  | 3:30:A:LYS:N   | 3:27:A:HIS:O    | 20                  | 0.26     | 0.06                | 0.26       |
| (2,121) | 3:89:A:HIS:N   | 3:86:A:THR:O    | 20                  | 0.25     | 0.05                | 0.26       |
| (1,9)   | 3:17:A:ARG:HA  | 3:9:A:CYS:H     | 20                  | 0.23     | 0.05                | 0.24       |
| (1,210) | 3:107:A:ALA:HA | 3:95:A:PHE:H    | 20                  | 0.23     | 0.02                | 0.23       |
| (1,347) | 3:20:A:LYS:CB  | 3:23:A:HIS:CB   | 20                  | 0.21     | 0.03                | 0.21       |
| (2,109) | 3:60:A:ARG:N   | 3:57:A:HIS:O    | 20                  | 0.2      | 0.04                | 0.2        |
| (2,83)  | 3:117:A:ASN:H  | 3:114:A:ARG:O   | 20                  | 0.19     | 0.03                | 0.2        |
| (2,61)  | 3:87:A:ARG:H   | 3:84:A:THR:O    | 20                  | 0.18     | 0.03                | 0.18       |
| (1,77)  | 3:38:A:GLN:HA  | 3:46:A:ARG:H    | 20                  | 0.18     | 0.03                | 0.19       |
| (2,131) | 3:118:A:MET:N  | 3:115:A:HIS:O   | 20                  | 0.18     | 0.04                | 0.2        |
| (1,465) | 3:67:A:PHE:CB  | 3:82:A:LEU:CD1  | 20                  | 0.18     | 0.04                | 0.18       |
| (2,110) | 3:61:A:HIS:N   | 3:58:A:GLN:O    | 20                  | 0.17     | 0.05                | 0.16       |
| (1,142) | 3:77:A:SER:HA  | 3:67:A:PHE:H    | 20                  | 0.17     | 0.02                | 0.18       |
| (2,120) | 3:88:A:THR:N   | 3:85:A:HIS:O    | 20                  | 0.16     | 0.03                | 0.17       |
| (2,130) | 3:117:A:ASN:N  | 3:114:A:ARG:O   | 20                  | 0.16     | 0.03                | 0.15       |
| (2,17)  | 3:29:A:ARG:H   | 3:26:A:MET:O    | 20                  | 0.16     | 0.04                | 0.16       |
| (1,356) | 3:24:A:LEU:CD2 | 3:27:A:HIS:CB   | 20                  | 0.15     | 0.03                | 0.16       |
| (2,39)  | 3:59:A:ARG:H   | 3:56:A:ARG:O    | 20                  | 0.15     | 0.02                | 0.15       |
| (1,470) | 3:67:A:PHE:CE1 | 3:77:A:SER:CA   | 19                  | 1.87     | 0.11                | 1.89       |
| (1,466) | 3:67:A:PHE:CD1 | 3:77:A:SER:CA   | 19                  | 1.46     | 0.11                | 1.5        |
| (1,471) | 3:67:A:PHE:CE1 | 3:78:A:ARG:CA   | 19                  | 1.34     | 0.11                | 1.33       |
| (1,467) | 3:67:A:PHE:CD1 | 3:78:A:ARG:CA   | 19                  | 1.28     | 0.13                | 1.31       |
| (1,477) | 3:67:A:PHE:CD2 | 3:79:A:SER:CB   | 19                  | 0.97     | 0.1                 | 1.02       |
| (1,478) | 3:67:A:PHE:CD2 | 3:82:A:LEU:CD1  | 19                  | 0.79     | 0.06                | 0.8        |
| (1,475) | 3:67:A:PHE:CE2 | 3:79:A:SER:CB   | 19                  | 0.58     | 0.12                | 0.6        |
| (1,476) | 3:67:A:PHE:CD2 | 3:79:A:SER:CA   | 19                  | 0.4      | 0.13                | 0.42       |
| (1,474) | 3:67:A:PHE:CE2 | 3:79:A:SER:CA   | 19                  | 0.38     | 0.16                | 0.37       |
| (2,126) | 3:113:A:VAL:N  | 3:109:A:SER:O   | 19                  | 0.23     | 0.04                | 0.22       |
| (2,116) | 3:84:A:THR:N   | 3:80:A:ASP:O    | 19                  | 0.21     | 0.04                | 0.22       |
| (2,128) | 3:115:A:HIS:N  | 3:111:A:GLU:O   | 19                  | 0.15     | 0.03                | 0.15       |
| (1,638) | 3:110:A:ASP:CB | 3:113:A:VAL:CG2 | 19                  | 0.12     | 0.01                | 0.12       |
| (1,279) | 3:8:A:MET:CB   | 3:16:A:LYS:CA   | 18                  | 0.32     | 0.03                | 0.32       |
| (1,319) | 3:18:A:TYR:CD1 | 3:24:A:LEU:CB   | 18                  | 0.16     | 0.03                | 0.16       |
| (1,211) | 3:96:A:SER:HA  | 3:104:A:LYS:H   | 18                  | 0.14     | 0.02                | 0.14       |
| (1,278) | 3:8:A:MET:CA   | 3:18:A:TYR:CD2  | 17                  | 1.99     | 0.11                | 2.02       |
| (1,323) | 3:18:A:TYR:CE1 | 3:23:A:HIS:CE1  | 17                  | 1.87     | 0.07                | 1.88       |
| (1,316) | 3:18:A:TYR:CD1 | 3:23:A:HIS:CD2  | 17                  | 1.41     | 0.03                | 1.41       |
| (1,317) | 3:18:A:TYR:CD1 | 3:23:A:HIS:CE1  | 17                  | 1.28     | 0.07                | 1.27       |
| (1,322) | 3:18:A:TYR:CE1 | 3:23:A:HIS:CD2  | 17                  | 1.2      | 0.04                | 1.2        |

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| Key     | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,336) | 3:18:A:TYR:CD2  | 3:24:A:LEU:CD2  | 17                  | 1.03     | 0.06                | 1.0        |
| (1,330) | 3:18:A:TYR:CE2  | 3:24:A:LEU:CD2  | 17                  | 0.68     | 0.06                | 0.67       |
| (1,318) | 3:18:A:TYR:CD1  | 3:24:A:LEU:CA   | 17                  | 0.5      | 0.04                | 0.51       |
| (1,76)  | 3:49:A:SER:HA   | 3:37:A:TYR:H    | 17                  | 0.16     | 0.03                | 0.17       |
| (1,440) | 3:54:A:LEU:CA   | 3:57:A:HIS:CB   | 17                  | 0.14     | 0.02                | 0.14       |
| (2,73)  | 3:112:A:LEU:H   | 3:108:A:ARG:O   | 17                  | 0.11     | 0.01                | 0.11       |
| (2,99)  | 3:31:A:HIS:N    | 3:28:A:SER:O    | 16                  | 0.2      | 0.07                | 0.2        |
| (2,129) | 3:116:A:HIS:N   | 3:112:A:LEU:O   | 16                  | 0.18     | 0.02                | 0.18       |
| (2,92)  | 3:24:A:LEU:N    | 3:20:A:LYS:O    | 16                  | 0.17     | 0.06                | 0.15       |
| (1,791) | 3:109:A:SER:CB  | 2:150:C:DC:C3'  | 16                  | 0.13     | 0.02                | 0.13       |
| (2,112) | 3:69:A:CYS:N    | 3:74:A:ARG:O    | 15                  | 0.18     | 0.06                | 0.17       |
| (2,106) | 3:57:A:HIS:N    | 3:53:A:GLN:O    | 15                  | 0.16     | 0.04                | 0.16       |
| (1,652) | 3:115:A:HIS:CD2 | 3:119:A:HIS:CE1 | 14                  | 0.21     | 0.02                | 0.22       |
| (1,688) | 1:128:B:DG:C1'  | 3:81:A:HIS:CE1  | 14                  | 0.14     | 0.02                | 0.14       |
| (1,332) | 3:18:A:TYR:CE2  | 3:27:A:HIS:CD2  | 13                  | 0.29     | 0.15                | 0.25       |
| (1,687) | 1:128:B:DG:C2'  | 3:81:A:HIS:CE1  | 13                  | 0.2      | 0.01                | 0.2        |
| (1,694) | 1:128:B:DG:C5   | 3:81:A:HIS:CD2  | 13                  | 0.2      | 0.03                | 0.21       |
| (1,143) | 3:68:A:GLN:HA   | 3:74:A:ARG:H    | 13                  | 0.18     | 0.06                | 0.16       |
| (1,327) | 3:18:A:TYR:CE1  | 3:27:A:HIS:CB   | 13                  | 0.18     | 0.05                | 0.2        |
| (2,94)  | 3:26:A:MET:N    | 3:22:A:SER:O    | 13                  | 0.17     | 0.05                | 0.17       |
| (2,65)  | 3:89:A:HIS:H    | 3:86:A:THR:O    | 13                  | 0.13     | 0.02                | 0.13       |
| (2,19)  | 3:30:A:LYS:H    | 3:27:A:HIS:O    | 13                  | 0.12     | 0.01                | 0.13       |
| (1,11)  | 3:8:A:MET:HA    | 3:16:A:LYS:H    | 12                  | 0.2      | 0.08                | 0.18       |
| (2,107) | 3:58:A:GLN:N    | 3:54:A:LEU:O    | 12                  | 0.15     | 0.04                | 0.14       |
| (1,577) | 3:97:A:CYS:CB   | 3:99:A:TRP:CB   | 12                  | 0.14     | 0.05                | 0.12       |
| (1,739) | 1:133:B:DG:C6   | 3:50:A:ARG:CZ   | 12                  | 0.14     | 0.03                | 0.14       |
| (2,101) | 3:39:A:CYS:N    | 3:46:A:ARG:O    | 12                  | 0.14     | 0.02                | 0.14       |
| (1,197) | 3:81:A:HIS:HA   | 3:84:A:THR:HG21 | 12                  | 0.12     | 0.01                | 0.12       |
| (1,197) | 3:81:A:HIS:HA   | 3:84:A:THR:HG22 | 12                  | 0.12     | 0.01                | 0.12       |
| (1,197) | 3:81:A:HIS:HA   | 3:84:A:THR:HG23 | 12                  | 0.12     | 0.01                | 0.12       |
| (4,1)   | 3:26:A:MET:HE2  | 1:134:B:DT:H72  | 11                  | 0.68     | 0.2                 | 0.75       |
| (4,1)   | 3:26:A:MET:HE2  | 1:136:B:DT:H73  | 11                  | 0.68     | 0.2                 | 0.75       |
| (4,1)   | 3:26:A:MET:HE3  | 1:134:B:DT:H72  | 11                  | 0.68     | 0.2                 | 0.75       |
| (4,1)   | 3:26:A:MET:HE1  | 1:136:B:DT:H71  | 11                  | 0.68     | 0.2                 | 0.75       |
| (4,1)   | 3:26:A:MET:HE2  | 1:134:B:DT:H71  | 11                  | 0.68     | 0.2                 | 0.75       |
| (4,1)   | 3:26:A:MET:HE3  | 1:136:B:DT:H72  | 11                  | 0.68     | 0.2                 | 0.75       |
| (4,1)   | 3:26:A:MET:HE3  | 1:134:B:DT:H71  | 11                  | 0.68     | 0.2                 | 0.75       |
| (4,1)   | 3:26:A:MET:HE2  | 1:136:B:DT:H71  | 11                  | 0.68     | 0.2                 | 0.75       |
| (1,308) | 3:11:A:TYR:CD2  | 3:34:A:GLU:CB   | 11                  | 0.15     | 0.03                | 0.14       |
| (1,377) | 3:37:A:TYR:CD2  | 3:50:A:ARG:CA   | 10                  | 1.23     | 0.44                | 1.27       |
| (1,10)  | 3:19:A:PHE:HA   | 3:7:A:PHE:H     | 10                  | 0.13     | 0.02                | 0.12       |
| (1,208) | 3:96:A:SER:HA   | 3:106:A:PHE:H   | 10                  | 0.12     | 0.02                | 0.12       |

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| Key     | Atom-1         | Atom-2         | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|----------------|----------------|---------------------|----------|---------------------|------------|
| (1,374) | 3:37:A:TYR:CE2 | 3:50:A:ARG:CA  | 9                   | 1.28     | 0.36                | 1.26       |
| (1,378) | 3:37:A:TYR:CD2 | 3:51:A:SER:CA  | 9                   | 0.87     | 0.29                | 0.82       |
| (1,376) | 3:37:A:TYR:CE2 | 3:51:A:SER:CB  | 9                   | 0.44     | 0.28                | 0.44       |
| (1,380) | 3:37:A:TYR:CD2 | 3:54:A:LEU:CB  | 9                   | 0.35     | 0.17                | 0.29       |
| (1,333) | 3:18:A:TYR:CE2 | 3:27:A:HIS:CE1 | 9                   | 0.25     | 0.17                | 0.2        |
| (1,706) | 1:129:B:DG:C5' | 3:60:A:ARG:CD  | 9                   | 0.11     | 0.01                | 0.11       |
| (1,375) | 3:37:A:TYR:CE2 | 3:51:A:SER:CA  | 8                   | 0.62     | 0.23                | 0.61       |
| (1,299) | 3:11:A:TYR:CE1 | 3:34:A:GLU:CA  | 8                   | 0.22     | 0.2                 | 0.14       |
| (2,96)  | 3:28:A:SER:N   | 3:24:A:LEU:O   | 8                   | 0.16     | 0.06                | 0.13       |
| (1,75)  | 3:47:A:ARG:HA  | 3:39:A:CYS:H   | 8                   | 0.15     | 0.02                | 0.15       |
| (1,288) | 3:11:A:TYR:CA  | 3:31:A:HIS:CE1 | 8                   | 0.14     | 0.03                | 0.15       |
| (2,21)  | 3:31:A:HIS:H   | 3:28:A:SER:O   | 8                   | 0.14     | 0.03                | 0.12       |
| (1,452) | 3:59:A:ARG:CA  | 3:62:A:THR:CG2 | 8                   | 0.13     | 0.03                | 0.13       |
| (1,341) | 3:19:A:PHE:CB  | 3:23:A:HIS:CD2 | 8                   | 0.13     | 0.02                | 0.14       |
| (1,502) | 3:76:A:PHE:CB  | 3:82:A:LEU:CD1 | 8                   | 0.13     | 0.02                | 0.12       |
| (1,659) | 3:80:A:ASP:HA  | 2:150:C:DC:H6  | 8                   | 0.11     | 0.01                | 0.11       |
| (1,719) | 1:129:B:DG:C6  | 3:81:A:HIS:CE1 | 7                   | 0.16     | 0.02                | 0.17       |
| (1,484) | 3:69:A:CYS:CA  | 3:74:A:ARG:CA  | 7                   | 0.14     | 0.03                | 0.13       |
| (1,262) | 3:7:A:PHE:CB   | 3:18:A:TYR:CB  | 7                   | 0.14     | 0.03                | 0.14       |
| (1,696) | 1:128:B:DG:N7  | 3:81:A:HIS:CB  | 7                   | 0.12     | 0.02                | 0.13       |
| (2,123) | 3:97:A:CYS:N   | 3:104:A:LYS:O  | 7                   | 0.12     | 0.01                | 0.12       |
| (2,49)  | 3:67:A:PHE:H   | 3:76:A:PHE:O   | 6                   | 0.12     | 0.01                | 0.12       |
| (1,274) | 3:7:A:PHE:CD2  | 3:20:A:LYS:CA  | 5                   | 1.32     | 0.64                | 1.73       |
| (1,271) | 3:7:A:PHE:CE2  | 3:20:A:LYS:CA  | 5                   | 1.26     | 0.58                | 1.61       |
| (1,304) | 3:11:A:TYR:CD2 | 3:14:A:CYS:CB  | 5                   | 0.77     | 0.81                | 0.12       |
| (1,267) | 3:7:A:PHE:CD1  | 3:24:A:LEU:CD1 | 5                   | 0.62     | 0.29                | 0.63       |
| (1,379) | 3:37:A:TYR:CD2 | 3:51:A:SER:CB  | 5                   | 0.34     | 0.26                | 0.21       |
| (1,404) | 3:41:A:PHE:CE2 | 3:44:A:CYS:CB  | 5                   | 0.33     | 0.43                | 0.12       |
| (1,388) | 3:39:A:CYS:CB  | 3:41:A:PHE:CB  | 5                   | 0.18     | 0.05                | 0.16       |
| (1,209) | 3:105:A:LYS:HA | 3:97:A:CYS:H   | 5                   | 0.13     | 0.03                | 0.11       |
| (1,382) | 3:38:A:GLN:CA  | 3:47:A:ARG:CA  | 5                   | 0.13     | 0.02                | 0.12       |
| (2,5)   | 3:7:A:PHE:H    | 3:18:A:TYR:O   | 5                   | 0.13     | 0.02                | 0.12       |
| (2,105) | 3:56:A:ARG:N   | 3:52:A:ASP:O   | 5                   | 0.12     | 0.02                | 0.11       |
| (1,762) | 2:149:C:DG:N7  | 3:80:A:ASP:CB  | 5                   | 0.12     | 0.01                | 0.12       |
| (1,141) | 3:75:A:LYS:HA  | 3:69:A:CYS:H   | 5                   | 0.12     | 0.01                | 0.11       |
| (1,338) | 3:18:A:TYR:CD2 | 3:27:A:HIS:CD2 | 4                   | 0.2      | 0.14                | 0.13       |
| (1,535) | 3:87:A:ARG:CA  | 3:90:A:THR:CB  | 4                   | 0.18     | 0.02                | 0.18       |
| (1,715) | 1:129:B:DG:C2' | 3:78:A:ARG:CZ  | 4                   | 0.16     | 0.05                | 0.14       |
| (1,301) | 3:11:A:TYR:CE2 | 3:31:A:HIS:CB  | 4                   | 0.14     | 0.02                | 0.14       |
| (1,752) | 2:147:C:DA:N6  | 3:52:A:ASP:CG  | 4                   | 0.14     | 0.02                | 0.14       |
| (1,140) | 3:68:A:GLN:HA  | 3:76:A:PHE:H   | 4                   | 0.13     | 0.02                | 0.13       |
| (1,737) | 1:132:B:DC:C5  | 3:50:A:ARG:CZ  | 4                   | 0.12     | 0.01                | 0.12       |

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| Key     | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (2,43)  | 3:61:A:HIS:H    | 3:58:A:GLN:O    | 4                   | 0.12     | 0.01                | 0.12       |
| (1,738) | 1:132:B:DC:C6   | 3:50:A:ARG:CZ   | 4                   | 0.12     | 0.0                 | 0.12       |
| (1,764) | 2:149:C:DG:C8   | 3:80:A:ASP:CB   | 4                   | 0.11     | 0.02                | 0.11       |
| (2,87)  | 3:119:A:HIS:H   | 3:116:A:HIS:O   | 4                   | 0.11     | 0.01                | 0.11       |
| (1,428) | 3:48:A:PHE:CE2  | 3:57:A:HIS:CD2  | 3                   | 0.59     | 0.68                | 0.11       |
| (1,408) | 3:41:A:PHE:CD2  | 3:44:A:CYS:CA   | 3                   | 0.49     | 0.42                | 0.2        |
| (1,294) | 3:11:A:TYR:CD1  | 3:31:A:HIS:CB   | 3                   | 0.48     | 0.27                | 0.58       |
| (1,447) | 3:58:A:GLN:CA   | 3:61:A:HIS:CD2  | 3                   | 0.34     | 0.03                | 0.34       |
| (4,2)   | 3:26:A:MET:HE1  | 1:135:B:DC:H5   | 3                   | 0.33     | 0.17                | 0.32       |
| (4,2)   | 3:26:A:MET:HE3  | 1:135:B:DC:H5   | 3                   | 0.33     | 0.17                | 0.32       |
| (4,2)   | 3:26:A:MET:HE3  | 1:135:B:DC:H6   | 3                   | 0.33     | 0.17                | 0.32       |
| (1,270) | 3:7:A:PHE:CE1   | 3:21:A:LEU:CD1  | 3                   | 0.25     | 0.17                | 0.16       |
| (2,90)  | 3:9:A:CYS:N     | 3:16:A:LYS:O    | 3                   | 0.24     | 0.09                | 0.2        |
| (1,537) | 3:87:A:ARG:CB   | 3:90:A:THR:CB   | 3                   | 0.2      | 0.03                | 0.21       |
| (2,93)  | 3:25:A:GLN:N    | 3:21:A:LEU:O    | 3                   | 0.15     | 0.01                | 0.15       |
| (1,670) | 1:126:B:DC:N4   | 3:108:A:ARG:CZ  | 3                   | 0.13     | 0.02                | 0.14       |
| (1,691) | 1:128:B:DG:C6   | 3:81:A:HIS:CE1  | 3                   | 0.13     | 0.02                | 0.14       |
| (1,13)  | 3:7:A:PHE:H     | 3:18:A:TYR:H    | 3                   | 0.12     | 0.01                | 0.12       |
| (1,331) | 3:18:A:TYR:CE2  | 3:27:A:HIS:CB   | 3                   | 0.12     | 0.01                | 0.12       |
| (1,533) | 3:85:A:HIS:CE1  | 3:88:A:THR:CG2  | 3                   | 0.12     | 0.0                 | 0.12       |
| (1,583) | 3:97:A:CYS:CB   | 3:116:A:HIS:CE1 | 3                   | 0.12     | 0.02                | 0.12       |
| (1,442) | 3:55:A:LYS:CA   | 3:58:A:GLN:CA   | 3                   | 0.11     | 0.0                 | 0.11       |
| (1,200) | 3:83:A:LYS:HA   | 3:86:A:THR:HG21 | 3                   | 0.11     | 0.01                | 0.11       |
| (1,200) | 3:83:A:LYS:HA   | 3:86:A:THR:HG22 | 3                   | 0.11     | 0.01                | 0.11       |
| (1,200) | 3:83:A:LYS:HA   | 3:86:A:THR:HG23 | 3                   | 0.11     | 0.01                | 0.11       |
| (1,293) | 3:11:A:TYR:CD1  | 3:31:A:HIS:CA   | 2                   | 0.48     | 0.08                | 0.48       |
| (1,307) | 3:11:A:TYR:CD2  | 3:31:A:HIS:CE1  | 2                   | 0.44     | 0.05                | 0.44       |
| (1,710) | 1:129:B:DG:C4'  | 3:60:A:ARG:CZ   | 2                   | 0.34     | 0.01                | 0.34       |
| (1,707) | 1:129:B:DG:C5'  | 3:60:A:ARG:CZ   | 2                   | 0.26     | 0.01                | 0.26       |
| (1,709) | 1:129:B:DG:C4'  | 3:60:A:ARG:CD   | 2                   | 0.24     | 0.02                | 0.24       |
| (1,298) | 3:11:A:TYR:CE1  | 3:31:A:HIS:CB   | 2                   | 0.16     | 0.02                | 0.16       |
| (1,498) | 3:72:A:CYS:CB   | 3:89:A:HIS:CE1  | 2                   | 0.16     | 0.05                | 0.16       |
| (1,651) | 3:115:A:HIS:CD2 | 3:119:A:HIS:CD2 | 2                   | 0.16     | 0.02                | 0.16       |
| (1,300) | 3:11:A:TYR:CE1  | 3:34:A:GLU:CB   | 2                   | 0.15     | 0.04                | 0.15       |
| (1,704) | 1:129:B:DG:C5'  | 3:60:A:ARG:CB   | 2                   | 0.15     | 0.0                 | 0.15       |
| (1,282) | 3:9:A:CYS:CA    | 3:27:A:HIS:CD2  | 2                   | 0.14     | 0.03                | 0.14       |
| (1,368) | 3:31:A:HIS:CB   | 3:34:A:GLU:CB   | 2                   | 0.14     | 0.04                | 0.14       |
| (1,763) | 2:149:C:DG:N7   | 3:80:A:ASP:CG   | 2                   | 0.14     | 0.02                | 0.14       |
| (1,767) | 2:150:C:DC:N4   | 3:80:A:ASP:CB   | 2                   | 0.14     | 0.01                | 0.14       |
| (1,448) | 3:58:A:GLN:CA   | 3:62:A:THR:CG2  | 2                   | 0.13     | 0.03                | 0.13       |
| (1,680) | 1:127:B:DG:C4'  | 3:74:A:ARG:CZ   | 2                   | 0.12     | 0.02                | 0.12       |
| (1,386) | 3:38:A:GLN:CB   | 3:47:A:ARG:CB   | 2                   | 0.12     | 0.01                | 0.12       |

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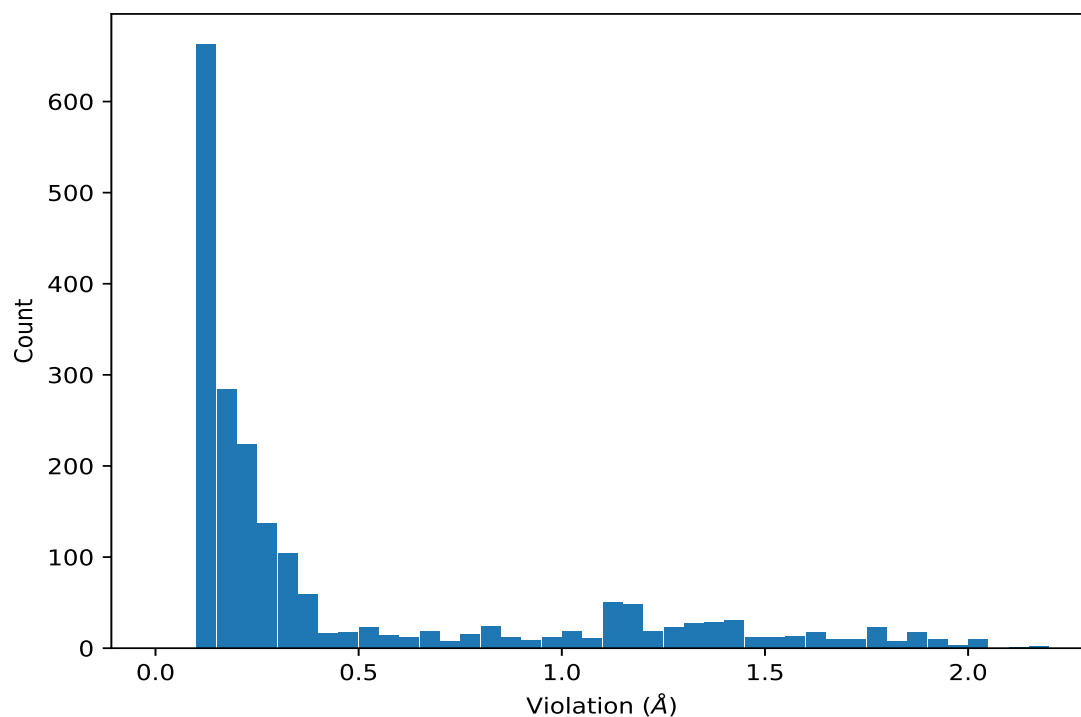
| Key     | Atom-1         | Atom-2         | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|----------------|----------------|---------------------|----------|---------------------|------------|
| (1,740) | 1:133:B:DG:C5  | 3:50:A:ARG:CZ  | 2                   | 0.12     | 0.01                | 0.12       |
| (1,268) | 3:7:A:PHE:CE1  | 3:21:A:LEU:CA  | 2                   | 0.12     | 0.02                | 0.12       |
| (1,329) | 3:18:A:TYR:CE2 | 3:24:A:LEU:CB  | 2                   | 0.12     | 0.02                | 0.12       |
| (1,458) | 3:65:A:LYS:CB  | 3:76:A:PHE:CA  | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,509) | 3:76:A:PHE:CE2 | 3:85:A:HIS:CD2 | 2                   | 0.11     | 0.0                 | 0.11       |
| (2,127) | 3:114:A:ARG:N  | 3:110:A:ASP:O  | 2                   | 0.11     | 0.0                 | 0.11       |
| (2,13)  | 3:27:A:HIS:H   | 3:23:A:HIS:O   | 2                   | 0.1      | 0.0                 | 0.1        |

<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) |
|---------|----------------|----------------|----------|---------------|
| (1,278) | 3:8:A:MET:CA   | 3:18:A:TYR:CD2 | 7        | 2.2           |
| (1,278) | 3:8:A:MET:CA   | 3:18:A:TYR:CD2 | 17       | 2.17          |
| (1,278) | 3:8:A:MET:CA   | 3:18:A:TYR:CD2 | 15       | 2.1           |
| (1,278) | 3:8:A:MET:CA   | 3:18:A:TYR:CD2 | 5        | 2.05          |
| (1,278) | 3:8:A:MET:CA   | 3:18:A:TYR:CD2 | 13       | 2.05          |
| (1,278) | 3:8:A:MET:CA   | 3:18:A:TYR:CD2 | 1        | 2.03          |
| (1,470) | 3:67:A:PHE:CE1 | 3:77:A:SER:CA  | 9        | 2.02          |
| (1,278) | 3:8:A:MET:CA   | 3:18:A:TYR:CD2 | 4        | 2.02          |
| (1,278) | 3:8:A:MET:CA   | 3:18:A:TYR:CD2 | 10       | 2.02          |
| (1,278) | 3:8:A:MET:CA   | 3:18:A:TYR:CD2 | 14       | 2.02          |
| (1,470) | 3:67:A:PHE:CE1 | 3:77:A:SER:CA  | 5        | 2.0           |
| (1,470) | 3:67:A:PHE:CE1 | 3:77:A:SER:CA  | 13       | 2.0           |
| (1,470) | 3:67:A:PHE:CE1 | 3:77:A:SER:CA  | 20       | 2.0           |
| (1,278) | 3:8:A:MET:CA   | 3:18:A:TYR:CD2 | 2        | 1.98          |
| (1,470) | 3:67:A:PHE:CE1 | 3:77:A:SER:CA  | 3        | 1.96          |
| (1,323) | 3:18:A:TYR:CE1 | 3:23:A:HIS:CE1 | 4        | 1.96          |
| (1,470) | 3:67:A:PHE:CE1 | 3:77:A:SER:CA  | 1        | 1.95          |
| (1,323) | 3:18:A:TYR:CE1 | 3:23:A:HIS:CE1 | 19       | 1.95          |
| (1,323) | 3:18:A:TYR:CE1 | 3:23:A:HIS:CE1 | 10       | 1.94          |
| (1,278) | 3:8:A:MET:CA   | 3:18:A:TYR:CD2 | 20       | 1.94          |
| (1,470) | 3:67:A:PHE:CE1 | 3:77:A:SER:CA  | 7        | 1.93          |
| (1,470) | 3:67:A:PHE:CE1 | 3:77:A:SER:CA  | 10       | 1.92          |
| (1,323) | 3:18:A:TYR:CE1 | 3:23:A:HIS:CE1 | 6        | 1.92          |
| (1,278) | 3:8:A:MET:CA   | 3:18:A:TYR:CD2 | 9        | 1.92          |
| (1,278) | 3:8:A:MET:CA   | 3:18:A:TYR:CD2 | 11       | 1.92          |
| (1,323) | 3:18:A:TYR:CE1 | 3:23:A:HIS:CE1 | 14       | 1.91          |
| (1,278) | 3:8:A:MET:CA   | 3:18:A:TYR:CD2 | 19       | 1.9           |
| (1,470) | 3:67:A:PHE:CE1 | 3:77:A:SER:CA  | 12       | 1.89          |
| (1,470) | 3:67:A:PHE:CE1 | 3:77:A:SER:CA  | 16       | 1.89          |
| (1,323) | 3:18:A:TYR:CE1 | 3:23:A:HIS:CE1 | 2        | 1.89          |
| (1,323) | 3:18:A:TYR:CE1 | 3:23:A:HIS:CE1 | 3        | 1.89          |
| (1,278) | 3:8:A:MET:CA   | 3:18:A:TYR:CD2 | 3        | 1.89          |
| (1,470) | 3:67:A:PHE:CE1 | 3:77:A:SER:CA  | 4        | 1.88          |
| (1,470) | 3:67:A:PHE:CE1 | 3:77:A:SER:CA  | 11       | 1.88          |
| (1,323) | 3:18:A:TYR:CE1 | 3:23:A:HIS:CE1 | 11       | 1.88          |
| (1,323) | 3:18:A:TYR:CE1 | 3:23:A:HIS:CE1 | 17       | 1.88          |
| (1,274) | 3:7:A:PHE:CD2  | 3:20:A:LYS:CA  | 8        | 1.88          |
| (1,323) | 3:18:A:TYR:CE1 | 3:23:A:HIS:CE1 | 5        | 1.87          |
| (1,323) | 3:18:A:TYR:CE1 | 3:23:A:HIS:CE1 | 12       | 1.87          |
| (1,323) | 3:18:A:TYR:CE1 | 3:23:A:HIS:CE1 | 20       | 1.87          |
| (1,323) | 3:18:A:TYR:CE1 | 3:23:A:HIS:CE1 | 15       | 1.86          |
| (1,560) | 3:95:A:PHE:CE1 | 3:107:A:ALA:CA | 18       | 1.85          |
| (1,323) | 3:18:A:TYR:CE1 | 3:23:A:HIS:CE1 | 1        | 1.85          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,560) | 3:95:A:PHE:CE1 | 3:107:A:ALA:CA | 10       | 1.84          |
| (1,560) | 3:95:A:PHE:CE1 | 3:107:A:ALA:CA | 17       | 1.84          |
| (1,374) | 3:37:A:TYR:CE2 | 3:50:A:ARG:CA  | 8        | 1.84          |
| (1,374) | 3:37:A:TYR:CE2 | 3:50:A:ARG:CA  | 18       | 1.84          |
| (1,470) | 3:67:A:PHE:CE1 | 3:77:A:SER:CA  | 18       | 1.83          |
| (1,560) | 3:95:A:PHE:CE1 | 3:107:A:ALA:CA | 4        | 1.81          |
| (1,377) | 3:37:A:TYR:CD2 | 3:50:A:ARG:CA  | 8        | 1.8           |
| (1,560) | 3:95:A:PHE:CE1 | 3:107:A:ALA:CA | 13       | 1.79          |
| (1,560) | 3:95:A:PHE:CE1 | 3:107:A:ALA:CA | 14       | 1.79          |
| (1,323) | 3:18:A:TYR:CE1 | 3:23:A:HIS:CE1 | 9        | 1.79          |
| (1,278) | 3:8:A:MET:CA   | 3:18:A:TYR:CD2 | 6        | 1.79          |
| (1,560) | 3:95:A:PHE:CE1 | 3:107:A:ALA:CA | 11       | 1.78          |
| (1,304) | 3:11:A:TYR:CD2 | 3:14:A:CYS:CB  | 18       | 1.78          |
| (1,274) | 3:7:A:PHE:CD2  | 3:20:A:LYS:CA  | 18       | 1.78          |
| (1,560) | 3:95:A:PHE:CE1 | 3:107:A:ALA:CA | 7        | 1.77          |
| (1,470) | 3:67:A:PHE:CE1 | 3:77:A:SER:CA  | 2        | 1.77          |
| (1,470) | 3:67:A:PHE:CE1 | 3:77:A:SER:CA  | 8        | 1.77          |
| (1,470) | 3:67:A:PHE:CE1 | 3:77:A:SER:CA  | 14       | 1.77          |
| (1,470) | 3:67:A:PHE:CE1 | 3:77:A:SER:CA  | 15       | 1.77          |
| (1,377) | 3:37:A:TYR:CD2 | 3:50:A:ARG:CA  | 18       | 1.77          |
| (1,278) | 3:8:A:MET:CA   | 3:18:A:TYR:CD2 | 12       | 1.77          |
| (1,560) | 3:95:A:PHE:CE1 | 3:107:A:ALA:CA | 2        | 1.76          |
| (1,560) | 3:95:A:PHE:CE1 | 3:107:A:ALA:CA | 3        | 1.75          |
| (1,560) | 3:95:A:PHE:CE1 | 3:107:A:ALA:CA | 8        | 1.75          |
| (1,560) | 3:95:A:PHE:CE1 | 3:107:A:ALA:CA | 9        | 1.75          |
| (1,560) | 3:95:A:PHE:CE1 | 3:107:A:ALA:CA | 15       | 1.75          |
| (1,560) | 3:95:A:PHE:CE1 | 3:107:A:ALA:CA | 16       | 1.75          |
| (1,560) | 3:95:A:PHE:CE1 | 3:107:A:ALA:CA | 19       | 1.75          |
| (1,304) | 3:11:A:TYR:CD2 | 3:14:A:CYS:CB  | 17       | 1.75          |
| (1,271) | 3:7:A:PHE:CE2  | 3:20:A:LYS:CA  | 18       | 1.75          |
| (1,560) | 3:95:A:PHE:CE1 | 3:107:A:ALA:CA | 1        | 1.74          |
| (1,560) | 3:95:A:PHE:CE1 | 3:107:A:ALA:CA | 6        | 1.74          |
| (1,560) | 3:95:A:PHE:CE1 | 3:107:A:ALA:CA | 12       | 1.74          |
| (1,432) | 3:48:A:PHE:CD2 | 3:54:A:LEU:CD1 | 19       | 1.74          |
| (1,323) | 3:18:A:TYR:CE1 | 3:23:A:HIS:CE1 | 13       | 1.73          |
| (1,274) | 3:7:A:PHE:CD2  | 3:20:A:LYS:CA  | 4        | 1.73          |
| (1,560) | 3:95:A:PHE:CE1 | 3:107:A:ALA:CA | 5        | 1.72          |
| (1,560) | 3:95:A:PHE:CE1 | 3:107:A:ALA:CA | 20       | 1.71          |
| (1,554) | 3:95:A:PHE:CD1 | 3:106:A:PHE:CA | 5        | 1.71          |
| (1,554) | 3:95:A:PHE:CD1 | 3:106:A:PHE:CA | 17       | 1.71          |
| (1,554) | 3:95:A:PHE:CD1 | 3:106:A:PHE:CA | 16       | 1.7           |
| (1,323) | 3:18:A:TYR:CE1 | 3:23:A:HIS:CE1 | 7        | 1.7           |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,554) | 3:95:A:PHE:CD1 | 3:106:A:PHE:CA | 8        | 1.68          |
| (1,470) | 3:67:A:PHE:CE1 | 3:77:A:SER:CA  | 17       | 1.68          |
| (1,554) | 3:95:A:PHE:CD1 | 3:106:A:PHE:CA | 3        | 1.67          |
| (1,554) | 3:95:A:PHE:CD1 | 3:106:A:PHE:CA | 9        | 1.67          |
| (1,554) | 3:95:A:PHE:CD1 | 3:106:A:PHE:CA | 11       | 1.67          |
| (1,554) | 3:95:A:PHE:CD1 | 3:106:A:PHE:CA | 13       | 1.67          |
| (1,554) | 3:95:A:PHE:CD1 | 3:106:A:PHE:CA | 1        | 1.66          |
| (1,554) | 3:95:A:PHE:CD1 | 3:106:A:PHE:CA | 19       | 1.66          |
| (1,554) | 3:95:A:PHE:CD1 | 3:106:A:PHE:CA | 6        | 1.65          |
| (1,554) | 3:95:A:PHE:CD1 | 3:106:A:PHE:CA | 12       | 1.65          |
| (1,554) | 3:95:A:PHE:CD1 | 3:106:A:PHE:CA | 14       | 1.65          |
| (1,554) | 3:95:A:PHE:CD1 | 3:106:A:PHE:CA | 15       | 1.65          |
| (1,554) | 3:95:A:PHE:CD1 | 3:106:A:PHE:CA | 20       | 1.65          |
| (1,271) | 3:7:A:PHE:CE2  | 3:20:A:LYS:CA  | 8        | 1.65          |
| (1,554) | 3:95:A:PHE:CD1 | 3:106:A:PHE:CA | 2        | 1.64          |
| (1,554) | 3:95:A:PHE:CD1 | 3:106:A:PHE:CA | 7        | 1.64          |
| (1,554) | 3:95:A:PHE:CD1 | 3:106:A:PHE:CA | 18       | 1.64          |
| (1,562) | 3:95:A:PHE:CE1 | 3:108:A:ARG:CB | 5        | 1.63          |
| (1,562) | 3:95:A:PHE:CE1 | 3:108:A:ARG:CB | 8        | 1.63          |
| (1,562) | 3:95:A:PHE:CE1 | 3:108:A:ARG:CB | 20       | 1.63          |
| (1,554) | 3:95:A:PHE:CD1 | 3:106:A:PHE:CA | 4        | 1.63          |
| (1,554) | 3:95:A:PHE:CD1 | 3:106:A:PHE:CA | 10       | 1.63          |
| (1,471) | 3:67:A:PHE:CE1 | 3:78:A:ARG:CA  | 16       | 1.62          |
| (1,271) | 3:7:A:PHE:CE2  | 3:20:A:LYS:CA  | 4        | 1.61          |
| (1,466) | 3:67:A:PHE:CD1 | 3:77:A:SER:CA  | 5        | 1.6           |
| (1,470) | 3:67:A:PHE:CE1 | 3:77:A:SER:CA  | 19       | 1.59          |
| (1,467) | 3:67:A:PHE:CD1 | 3:78:A:ARG:CA  | 16       | 1.59          |
| (1,562) | 3:95:A:PHE:CE1 | 3:108:A:ARG:CB | 16       | 1.58          |
| (1,562) | 3:95:A:PHE:CE1 | 3:108:A:ARG:CB | 3        | 1.57          |
| (1,562) | 3:95:A:PHE:CE1 | 3:108:A:ARG:CB | 9        | 1.57          |
| (1,562) | 3:95:A:PHE:CE1 | 3:108:A:ARG:CB | 19       | 1.57          |
| (1,466) | 3:67:A:PHE:CD1 | 3:77:A:SER:CA  | 3        | 1.57          |
| (1,562) | 3:95:A:PHE:CE1 | 3:108:A:ARG:CB | 1        | 1.56          |
| (1,562) | 3:95:A:PHE:CE1 | 3:108:A:ARG:CB | 2        | 1.56          |
| (1,466) | 3:67:A:PHE:CD1 | 3:77:A:SER:CA  | 10       | 1.56          |
| (1,466) | 3:67:A:PHE:CD1 | 3:77:A:SER:CA  | 12       | 1.56          |
| (1,466) | 3:67:A:PHE:CD1 | 3:77:A:SER:CA  | 16       | 1.55          |
| (1,428) | 3:48:A:PHE:CE2 | 3:57:A:HIS:CD2 | 19       | 1.55          |
| (1,562) | 3:95:A:PHE:CE1 | 3:108:A:ARG:CB | 6        | 1.54          |
| (1,562) | 3:95:A:PHE:CE1 | 3:108:A:ARG:CB | 12       | 1.54          |
| (1,562) | 3:95:A:PHE:CE1 | 3:108:A:ARG:CB | 15       | 1.53          |
| (1,562) | 3:95:A:PHE:CE1 | 3:108:A:ARG:CB | 17       | 1.53          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,562) | 3:95:A:PHE:CE1 | 3:108:A:ARG:CB | 7        | 1.52          |
| (1,466) | 3:67:A:PHE:CD1 | 3:77:A:SER:CA  | 7        | 1.52          |
| (1,466) | 3:67:A:PHE:CD1 | 3:77:A:SER:CA  | 9        | 1.52          |
| (1,466) | 3:67:A:PHE:CD1 | 3:77:A:SER:CA  | 13       | 1.51          |
| (1,466) | 3:67:A:PHE:CD1 | 3:77:A:SER:CA  | 20       | 1.51          |
| (1,556) | 3:95:A:PHE:CD1 | 3:107:A:ALA:CA | 17       | 1.5           |
| (1,466) | 3:67:A:PHE:CD1 | 3:77:A:SER:CA  | 1        | 1.5           |
| (1,466) | 3:67:A:PHE:CD1 | 3:77:A:SER:CA  | 11       | 1.5           |
| (1,562) | 3:95:A:PHE:CE1 | 3:108:A:ARG:CB | 4        | 1.49          |
| (1,562) | 3:95:A:PHE:CE1 | 3:108:A:ARG:CB | 10       | 1.49          |
| (1,562) | 3:95:A:PHE:CE1 | 3:108:A:ARG:CB | 13       | 1.49          |
| (1,556) | 3:95:A:PHE:CD1 | 3:107:A:ALA:CA | 18       | 1.49          |
| (1,471) | 3:67:A:PHE:CE1 | 3:78:A:ARG:CA  | 12       | 1.49          |
| (1,466) | 3:67:A:PHE:CD1 | 3:77:A:SER:CA  | 4        | 1.49          |
| (1,562) | 3:95:A:PHE:CE1 | 3:108:A:ARG:CB | 18       | 1.48          |
| (1,467) | 3:67:A:PHE:CD1 | 3:78:A:ARG:CA  | 12       | 1.48          |
| (1,562) | 3:95:A:PHE:CE1 | 3:108:A:ARG:CB | 14       | 1.47          |
| (1,556) | 3:95:A:PHE:CD1 | 3:107:A:ALA:CA | 4        | 1.46          |
| (1,556) | 3:95:A:PHE:CD1 | 3:107:A:ALA:CA | 10       | 1.46          |
| (1,378) | 3:37:A:TYR:CD2 | 3:51:A:SER:CA  | 8        | 1.46          |
| (1,562) | 3:95:A:PHE:CE1 | 3:108:A:ARG:CB | 11       | 1.45          |
| (1,556) | 3:95:A:PHE:CD1 | 3:107:A:ALA:CA | 13       | 1.45          |
| (1,556) | 3:95:A:PHE:CD1 | 3:107:A:ALA:CA | 14       | 1.45          |
| (1,316) | 3:18:A:TYR:CD1 | 3:23:A:HIS:CD2 | 7        | 1.45          |
| (1,316) | 3:18:A:TYR:CD1 | 3:23:A:HIS:CD2 | 19       | 1.45          |
| (1,556) | 3:95:A:PHE:CD1 | 3:107:A:ALA:CA | 11       | 1.44          |
| (1,471) | 3:67:A:PHE:CE1 | 3:78:A:ARG:CA  | 8        | 1.44          |
| (1,316) | 3:18:A:TYR:CD1 | 3:23:A:HIS:CD2 | 5        | 1.44          |
| (1,556) | 3:95:A:PHE:CD1 | 3:107:A:ALA:CA | 3        | 1.43          |
| (1,556) | 3:95:A:PHE:CD1 | 3:107:A:ALA:CA | 8        | 1.43          |
| (1,471) | 3:67:A:PHE:CE1 | 3:78:A:ARG:CA  | 17       | 1.43          |
| (1,471) | 3:67:A:PHE:CE1 | 3:78:A:ARG:CA  | 18       | 1.43          |
| (1,316) | 3:18:A:TYR:CD1 | 3:23:A:HIS:CD2 | 2        | 1.43          |
| (1,316) | 3:18:A:TYR:CD1 | 3:23:A:HIS:CD2 | 11       | 1.43          |
| (1,316) | 3:18:A:TYR:CD1 | 3:23:A:HIS:CD2 | 12       | 1.43          |
| (1,316) | 3:18:A:TYR:CD1 | 3:23:A:HIS:CD2 | 17       | 1.43          |
| (1,556) | 3:95:A:PHE:CD1 | 3:107:A:ALA:CA | 2        | 1.42          |
| (1,556) | 3:95:A:PHE:CD1 | 3:107:A:ALA:CA | 9        | 1.42          |
| (1,556) | 3:95:A:PHE:CD1 | 3:107:A:ALA:CA | 16       | 1.42          |
| (1,556) | 3:95:A:PHE:CD1 | 3:107:A:ALA:CA | 19       | 1.42          |
| (1,471) | 3:67:A:PHE:CE1 | 3:78:A:ARG:CA  | 10       | 1.42          |
| (1,556) | 3:95:A:PHE:CD1 | 3:107:A:ALA:CA | 1        | 1.41          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,556) | 3:95:A:PHE:CD1 | 3:107:A:ALA:CA | 5        | 1.41          |
| (1,556) | 3:95:A:PHE:CD1 | 3:107:A:ALA:CA | 7        | 1.41          |
| (1,556) | 3:95:A:PHE:CD1 | 3:107:A:ALA:CA | 12       | 1.41          |
| (1,556) | 3:95:A:PHE:CD1 | 3:107:A:ALA:CA | 15       | 1.41          |
| (1,471) | 3:67:A:PHE:CE1 | 3:78:A:ARG:CA  | 2        | 1.41          |
| (1,466) | 3:67:A:PHE:CD1 | 3:77:A:SER:CA  | 14       | 1.41          |
| (1,317) | 3:18:A:TYR:CD1 | 3:23:A:HIS:CE1 | 4        | 1.41          |
| (1,316) | 3:18:A:TYR:CD1 | 3:23:A:HIS:CD2 | 1        | 1.41          |
| (1,316) | 3:18:A:TYR:CD1 | 3:23:A:HIS:CD2 | 4        | 1.41          |
| (1,556) | 3:95:A:PHE:CD1 | 3:107:A:ALA:CA | 6        | 1.4           |
| (1,555) | 3:95:A:PHE:CD1 | 3:106:A:PHE:CB | 5        | 1.4           |
| (1,466) | 3:67:A:PHE:CD1 | 3:77:A:SER:CA  | 18       | 1.4           |
| (1,316) | 3:18:A:TYR:CD1 | 3:23:A:HIS:CD2 | 6        | 1.4           |
| (1,316) | 3:18:A:TYR:CD1 | 3:23:A:HIS:CD2 | 10       | 1.4           |
| (1,316) | 3:18:A:TYR:CD1 | 3:23:A:HIS:CD2 | 13       | 1.4           |
| (1,316) | 3:18:A:TYR:CD1 | 3:23:A:HIS:CD2 | 20       | 1.4           |
| (1,467) | 3:67:A:PHE:CD1 | 3:78:A:ARG:CA  | 10       | 1.39          |
| (1,467) | 3:67:A:PHE:CD1 | 3:78:A:ARG:CA  | 17       | 1.39          |
| (1,377) | 3:37:A:TYR:CD2 | 3:50:A:ARG:CA  | 7        | 1.39          |
| (1,377) | 3:37:A:TYR:CD2 | 3:50:A:ARG:CA  | 20       | 1.39          |
| (1,316) | 3:18:A:TYR:CD1 | 3:23:A:HIS:CD2 | 3        | 1.39          |
| (1,316) | 3:18:A:TYR:CD1 | 3:23:A:HIS:CD2 | 9        | 1.39          |
| (1,556) | 3:95:A:PHE:CD1 | 3:107:A:ALA:CA | 20       | 1.38          |
| (1,555) | 3:95:A:PHE:CD1 | 3:106:A:PHE:CB | 19       | 1.38          |
| (1,466) | 3:67:A:PHE:CD1 | 3:77:A:SER:CA  | 8        | 1.38          |
| (1,316) | 3:18:A:TYR:CD1 | 3:23:A:HIS:CD2 | 14       | 1.38          |
| (1,471) | 3:67:A:PHE:CE1 | 3:78:A:ARG:CA  | 4        | 1.37          |
| (1,471) | 3:67:A:PHE:CE1 | 3:78:A:ARG:CA  | 15       | 1.37          |
| (1,555) | 3:95:A:PHE:CD1 | 3:106:A:PHE:CB | 16       | 1.36          |
| (1,467) | 3:67:A:PHE:CD1 | 3:78:A:ARG:CA  | 8        | 1.36          |
| (1,466) | 3:67:A:PHE:CD1 | 3:77:A:SER:CA  | 2        | 1.36          |
| (1,409) | 3:41:A:PHE:CD2 | 3:44:A:CYS:CB  | 18       | 1.36          |
| (1,317) | 3:18:A:TYR:CD1 | 3:23:A:HIS:CE1 | 19       | 1.36          |
| (1,555) | 3:95:A:PHE:CD1 | 3:106:A:PHE:CB | 1        | 1.35          |
| (1,466) | 3:67:A:PHE:CD1 | 3:77:A:SER:CA  | 15       | 1.35          |
| (1,418) | 3:48:A:PHE:CD1 | 3:53:A:GLN:CB  | 19       | 1.35          |
| (1,316) | 3:18:A:TYR:CD1 | 3:23:A:HIS:CD2 | 15       | 1.35          |
| (1,555) | 3:95:A:PHE:CD1 | 3:106:A:PHE:CB | 3        | 1.34          |
| (1,467) | 3:67:A:PHE:CD1 | 3:78:A:ARG:CA  | 14       | 1.34          |
| (1,317) | 3:18:A:TYR:CD1 | 3:23:A:HIS:CE1 | 10       | 1.34          |
| (1,555) | 3:95:A:PHE:CD1 | 3:106:A:PHE:CB | 8        | 1.33          |
| (1,555) | 3:95:A:PHE:CD1 | 3:106:A:PHE:CB | 9        | 1.33          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,555) | 3:95:A:PHE:CD1 | 3:106:A:PHE:CB | 11       | 1.33          |
| (1,555) | 3:95:A:PHE:CD1 | 3:106:A:PHE:CB | 12       | 1.33          |
| (1,471) | 3:67:A:PHE:CE1 | 3:78:A:ARG:CA  | 14       | 1.33          |
| (1,317) | 3:18:A:TYR:CD1 | 3:23:A:HIS:CE1 | 2        | 1.33          |
| (1,317) | 3:18:A:TYR:CD1 | 3:23:A:HIS:CE1 | 6        | 1.33          |
| (1,555) | 3:95:A:PHE:CD1 | 3:106:A:PHE:CB | 13       | 1.32          |
| (1,555) | 3:95:A:PHE:CD1 | 3:106:A:PHE:CB | 17       | 1.32          |
| (1,555) | 3:95:A:PHE:CD1 | 3:106:A:PHE:CB | 20       | 1.32          |
| (1,467) | 3:67:A:PHE:CD1 | 3:78:A:ARG:CA  | 2        | 1.32          |
| (1,467) | 3:67:A:PHE:CD1 | 3:78:A:ARG:CA  | 5        | 1.32          |
| (1,467) | 3:67:A:PHE:CD1 | 3:78:A:ARG:CA  | 18       | 1.32          |
| (1,471) | 3:67:A:PHE:CE1 | 3:78:A:ARG:CA  | 20       | 1.31          |
| (1,467) | 3:67:A:PHE:CD1 | 3:78:A:ARG:CA  | 4        | 1.31          |
| (1,374) | 3:37:A:TYR:CE2 | 3:50:A:ARG:CA  | 20       | 1.31          |
| (1,317) | 3:18:A:TYR:CD1 | 3:23:A:HIS:CE1 | 14       | 1.31          |
| (1,555) | 3:95:A:PHE:CD1 | 3:106:A:PHE:CB | 2        | 1.3           |
| (1,555) | 3:95:A:PHE:CD1 | 3:106:A:PHE:CB | 4        | 1.3           |
| (1,555) | 3:95:A:PHE:CD1 | 3:106:A:PHE:CB | 6        | 1.3           |
| (1,555) | 3:95:A:PHE:CD1 | 3:106:A:PHE:CB | 15       | 1.3           |
| (1,471) | 3:67:A:PHE:CE1 | 3:78:A:ARG:CA  | 5        | 1.3           |
| (1,374) | 3:37:A:TYR:CE2 | 3:50:A:ARG:CA  | 7        | 1.3           |
| (1,317) | 3:18:A:TYR:CD1 | 3:23:A:HIS:CE1 | 1        | 1.3           |
| (1,555) | 3:95:A:PHE:CD1 | 3:106:A:PHE:CB | 14       | 1.29          |
| (1,555) | 3:95:A:PHE:CD1 | 3:106:A:PHE:CB | 18       | 1.29          |
| (1,471) | 3:67:A:PHE:CE1 | 3:78:A:ARG:CA  | 3        | 1.28          |
| (1,431) | 3:48:A:PHE:CD2 | 3:54:A:LEU:CB  | 19       | 1.28          |
| (1,377) | 3:37:A:TYR:CD2 | 3:50:A:ARG:CA  | 12       | 1.28          |
| (1,317) | 3:18:A:TYR:CD1 | 3:23:A:HIS:CE1 | 12       | 1.28          |
| (1,466) | 3:67:A:PHE:CD1 | 3:77:A:SER:CA  | 17       | 1.27          |
| (1,322) | 3:18:A:TYR:CE1 | 3:23:A:HIS:CD2 | 5        | 1.27          |
| (1,317) | 3:18:A:TYR:CD1 | 3:23:A:HIS:CE1 | 3        | 1.27          |
| (1,317) | 3:18:A:TYR:CD1 | 3:23:A:HIS:CE1 | 11       | 1.27          |
| (1,317) | 3:18:A:TYR:CD1 | 3:23:A:HIS:CE1 | 17       | 1.27          |
| (1,557) | 3:95:A:PHE:CD1 | 3:108:A:ARG:CA | 8        | 1.26          |
| (1,555) | 3:95:A:PHE:CD1 | 3:106:A:PHE:CB | 7        | 1.26          |
| (1,467) | 3:67:A:PHE:CD1 | 3:78:A:ARG:CA  | 3        | 1.26          |
| (1,467) | 3:67:A:PHE:CD1 | 3:78:A:ARG:CA  | 15       | 1.26          |
| (1,377) | 3:37:A:TYR:CD2 | 3:50:A:ARG:CA  | 17       | 1.26          |
| (1,374) | 3:37:A:TYR:CE2 | 3:50:A:ARG:CA  | 17       | 1.26          |
| (1,322) | 3:18:A:TYR:CE1 | 3:23:A:HIS:CD2 | 7        | 1.26          |
| (1,317) | 3:18:A:TYR:CD1 | 3:23:A:HIS:CE1 | 20       | 1.26          |
| (1,555) | 3:95:A:PHE:CD1 | 3:106:A:PHE:CB | 10       | 1.25          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,471) | 3:67:A:PHE:CE1 | 3:78:A:ARG:CA   | 1        | 1.25          |
| (1,322) | 3:18:A:TYR:CE1 | 3:23:A:HIS:CD2  | 19       | 1.25          |
| (1,317) | 3:18:A:TYR:CD1 | 3:23:A:HIS:CE1  | 5        | 1.25          |
| (1,557) | 3:95:A:PHE:CD1 | 3:108:A:ARG:CA  | 3        | 1.24          |
| (1,557) | 3:95:A:PHE:CD1 | 3:108:A:ARG:CA  | 5        | 1.24          |
| (1,322) | 3:18:A:TYR:CE1 | 3:23:A:HIS:CD2  | 11       | 1.24          |
| (1,317) | 3:18:A:TYR:CD1 | 3:23:A:HIS:CE1  | 15       | 1.24          |
| (1,557) | 3:95:A:PHE:CD1 | 3:108:A:ARG:CA  | 20       | 1.23          |
| (1,471) | 3:67:A:PHE:CE1 | 3:78:A:ARG:CA   | 9        | 1.23          |
| (1,374) | 3:37:A:TYR:CE2 | 3:50:A:ARG:CA   | 2        | 1.23          |
| (1,322) | 3:18:A:TYR:CE1 | 3:23:A:HIS:CD2  | 12       | 1.23          |
| (1,322) | 3:18:A:TYR:CE1 | 3:23:A:HIS:CD2  | 17       | 1.23          |
| (1,317) | 3:18:A:TYR:CD1 | 3:23:A:HIS:CE1  | 9        | 1.23          |
| (1,561) | 3:95:A:PHE:CE1 | 3:108:A:ARG:CA  | 5        | 1.22          |
| (1,561) | 3:95:A:PHE:CE1 | 3:108:A:ARG:CA  | 8        | 1.22          |
| (1,561) | 3:95:A:PHE:CE1 | 3:108:A:ARG:CA  | 20       | 1.22          |
| (1,471) | 3:67:A:PHE:CE1 | 3:78:A:ARG:CA   | 19       | 1.22          |
| (1,569) | 3:95:A:PHE:CD2 | 3:112:A:LEU:CD2 | 17       | 1.21          |
| (1,561) | 3:95:A:PHE:CE1 | 3:108:A:ARG:CA  | 3        | 1.21          |
| (1,420) | 3:48:A:PHE:CE1 | 3:53:A:GLN:CB   | 19       | 1.21          |
| (1,322) | 3:18:A:TYR:CE1 | 3:23:A:HIS:CD2  | 10       | 1.21          |
| (1,322) | 3:18:A:TYR:CE1 | 3:23:A:HIS:CD2  | 20       | 1.21          |
| (1,569) | 3:95:A:PHE:CD2 | 3:112:A:LEU:CD2 | 4        | 1.2           |
| (1,561) | 3:95:A:PHE:CE1 | 3:108:A:ARG:CA  | 16       | 1.2           |
| (1,561) | 3:95:A:PHE:CE1 | 3:108:A:ARG:CA  | 19       | 1.2           |
| (1,557) | 3:95:A:PHE:CD1 | 3:108:A:ARG:CA  | 12       | 1.2           |
| (1,467) | 3:67:A:PHE:CD1 | 3:78:A:ARG:CA   | 11       | 1.2           |
| (1,466) | 3:67:A:PHE:CD1 | 3:77:A:SER:CA   | 19       | 1.2           |
| (1,404) | 3:41:A:PHE:CE2 | 3:44:A:CYS:CB   | 18       | 1.2           |
| (1,322) | 3:18:A:TYR:CE1 | 3:23:A:HIS:CD2  | 3        | 1.2           |
| (1,569) | 3:95:A:PHE:CD2 | 3:112:A:LEU:CD2 | 20       | 1.19          |
| (1,566) | 3:95:A:PHE:CE2 | 3:109:A:SER:CB  | 14       | 1.19          |
| (1,557) | 3:95:A:PHE:CD1 | 3:108:A:ARG:CA  | 2        | 1.19          |
| (1,557) | 3:95:A:PHE:CD1 | 3:108:A:ARG:CA  | 9        | 1.19          |
| (1,557) | 3:95:A:PHE:CD1 | 3:108:A:ARG:CA  | 19       | 1.19          |
| (1,471) | 3:67:A:PHE:CE1 | 3:78:A:ARG:CA   | 7        | 1.19          |
| (1,471) | 3:67:A:PHE:CE1 | 3:78:A:ARG:CA   | 11       | 1.19          |
| (1,471) | 3:67:A:PHE:CE1 | 3:78:A:ARG:CA   | 13       | 1.19          |
| (1,400) | 3:41:A:PHE:CE1 | 3:61:A:HIS:CA   | 18       | 1.19          |
| (1,322) | 3:18:A:TYR:CE1 | 3:23:A:HIS:CD2  | 2        | 1.19          |
| (1,322) | 3:18:A:TYR:CE1 | 3:23:A:HIS:CD2  | 13       | 1.19          |
| (1,569) | 3:95:A:PHE:CD2 | 3:112:A:LEU:CD2 | 2        | 1.18          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,569) | 3:95:A:PHE:CD2 | 3:112:A:LEU:CD2 | 14       | 1.18          |
| (1,566) | 3:95:A:PHE:CE2 | 3:109:A:SER:CB  | 13       | 1.18          |
| (1,561) | 3:95:A:PHE:CE1 | 3:108:A:ARG:CA  | 2        | 1.18          |
| (1,561) | 3:95:A:PHE:CE1 | 3:108:A:ARG:CA  | 9        | 1.18          |
| (1,557) | 3:95:A:PHE:CD1 | 3:108:A:ARG:CA  | 1        | 1.18          |
| (1,557) | 3:95:A:PHE:CD1 | 3:108:A:ARG:CA  | 16       | 1.18          |
| (1,377) | 3:37:A:TYR:CD2 | 3:50:A:ARG:CA   | 2        | 1.18          |
| (1,322) | 3:18:A:TYR:CE1 | 3:23:A:HIS:CD2  | 1        | 1.18          |
| (1,569) | 3:95:A:PHE:CD2 | 3:112:A:LEU:CD2 | 15       | 1.17          |
| (1,566) | 3:95:A:PHE:CE2 | 3:109:A:SER:CB  | 4        | 1.17          |
| (1,566) | 3:95:A:PHE:CE2 | 3:109:A:SER:CB  | 11       | 1.17          |
| (1,566) | 3:95:A:PHE:CE2 | 3:109:A:SER:CB  | 15       | 1.17          |
| (1,566) | 3:95:A:PHE:CE2 | 3:109:A:SER:CB  | 17       | 1.17          |
| (1,561) | 3:95:A:PHE:CE1 | 3:108:A:ARG:CA  | 1        | 1.17          |
| (1,561) | 3:95:A:PHE:CE1 | 3:108:A:ARG:CA  | 6        | 1.17          |
| (1,561) | 3:95:A:PHE:CE1 | 3:108:A:ARG:CA  | 12       | 1.17          |
| (1,561) | 3:95:A:PHE:CE1 | 3:108:A:ARG:CA  | 15       | 1.17          |
| (1,561) | 3:95:A:PHE:CE1 | 3:108:A:ARG:CA  | 17       | 1.17          |
| (1,557) | 3:95:A:PHE:CD1 | 3:108:A:ARG:CA  | 6        | 1.17          |
| (1,322) | 3:18:A:TYR:CE1 | 3:23:A:HIS:CD2  | 6        | 1.17          |
| (1,569) | 3:95:A:PHE:CD2 | 3:112:A:LEU:CD2 | 8        | 1.16          |
| (1,566) | 3:95:A:PHE:CE2 | 3:109:A:SER:CB  | 2        | 1.16          |
| (1,566) | 3:95:A:PHE:CE2 | 3:109:A:SER:CB  | 6        | 1.16          |
| (1,557) | 3:95:A:PHE:CD1 | 3:108:A:ARG:CA  | 7        | 1.16          |
| (1,467) | 3:67:A:PHE:CD1 | 3:78:A:ARG:CA   | 1        | 1.16          |
| (1,467) | 3:67:A:PHE:CD1 | 3:78:A:ARG:CA   | 20       | 1.16          |
| (1,336) | 3:18:A:TYR:CD2 | 3:24:A:LEU:CD2  | 15       | 1.16          |
| (1,322) | 3:18:A:TYR:CE1 | 3:23:A:HIS:CD2  | 9        | 1.16          |
| (1,569) | 3:95:A:PHE:CD2 | 3:112:A:LEU:CD2 | 1        | 1.15          |
| (1,569) | 3:95:A:PHE:CD2 | 3:112:A:LEU:CD2 | 10       | 1.15          |
| (1,566) | 3:95:A:PHE:CE2 | 3:109:A:SER:CB  | 1        | 1.15          |
| (1,566) | 3:95:A:PHE:CE2 | 3:109:A:SER:CB  | 9        | 1.15          |
| (1,566) | 3:95:A:PHE:CE2 | 3:109:A:SER:CB  | 10       | 1.15          |
| (1,566) | 3:95:A:PHE:CE2 | 3:109:A:SER:CB  | 12       | 1.15          |
| (1,566) | 3:95:A:PHE:CE2 | 3:109:A:SER:CB  | 18       | 1.15          |
| (1,561) | 3:95:A:PHE:CE1 | 3:108:A:ARG:CA  | 7        | 1.15          |
| (1,561) | 3:95:A:PHE:CE1 | 3:108:A:ARG:CA  | 10       | 1.15          |
| (1,557) | 3:95:A:PHE:CD1 | 3:108:A:ARG:CA  | 10       | 1.15          |
| (1,557) | 3:95:A:PHE:CD1 | 3:108:A:ARG:CA  | 15       | 1.15          |
| (1,467) | 3:67:A:PHE:CD1 | 3:78:A:ARG:CA   | 7        | 1.15          |
| (1,467) | 3:67:A:PHE:CD1 | 3:78:A:ARG:CA   | 19       | 1.15          |
| (1,317) | 3:18:A:TYR:CD1 | 3:23:A:HIS:CE1  | 13       | 1.15          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,569) | 3:95:A:PHE:CD2 | 3:112:A:LEU:CD2 | 13       | 1.14          |
| (1,569) | 3:95:A:PHE:CD2 | 3:112:A:LEU:CD2 | 18       | 1.14          |
| (1,566) | 3:95:A:PHE:CE2 | 3:109:A:SER:CB  | 19       | 1.14          |
| (1,561) | 3:95:A:PHE:CE1 | 3:108:A:ARG:CA  | 4        | 1.14          |
| (1,561) | 3:95:A:PHE:CE1 | 3:108:A:ARG:CA  | 18       | 1.14          |
| (1,557) | 3:95:A:PHE:CD1 | 3:108:A:ARG:CA  | 13       | 1.14          |
| (1,557) | 3:95:A:PHE:CD1 | 3:108:A:ARG:CA  | 14       | 1.14          |
| (1,322) | 3:18:A:TYR:CE1 | 3:23:A:HIS:CD2  | 14       | 1.14          |
| (1,569) | 3:95:A:PHE:CD2 | 3:112:A:LEU:CD2 | 7        | 1.13          |
| (1,569) | 3:95:A:PHE:CD2 | 3:112:A:LEU:CD2 | 16       | 1.13          |
| (1,569) | 3:95:A:PHE:CD2 | 3:112:A:LEU:CD2 | 19       | 1.13          |
| (1,566) | 3:95:A:PHE:CE2 | 3:109:A:SER:CB  | 7        | 1.13          |
| (1,566) | 3:95:A:PHE:CE2 | 3:109:A:SER:CB  | 8        | 1.13          |
| (1,566) | 3:95:A:PHE:CE2 | 3:109:A:SER:CB  | 16       | 1.13          |
| (1,566) | 3:95:A:PHE:CE2 | 3:109:A:SER:CB  | 20       | 1.13          |
| (1,561) | 3:95:A:PHE:CE1 | 3:108:A:ARG:CA  | 13       | 1.13          |
| (1,557) | 3:95:A:PHE:CD1 | 3:108:A:ARG:CA  | 4        | 1.13          |
| (1,557) | 3:95:A:PHE:CD1 | 3:108:A:ARG:CA  | 11       | 1.13          |
| (1,377) | 3:37:A:TYR:CD2 | 3:50:A:ARG:CA   | 9        | 1.13          |
| (1,336) | 3:18:A:TYR:CD2 | 3:24:A:LEU:CD2  | 5        | 1.13          |
| (1,322) | 3:18:A:TYR:CE1 | 3:23:A:HIS:CD2  | 4        | 1.13          |
| (1,566) | 3:95:A:PHE:CE2 | 3:109:A:SER:CB  | 3        | 1.12          |
| (1,566) | 3:95:A:PHE:CE2 | 3:109:A:SER:CB  | 5        | 1.12          |
| (1,561) | 3:95:A:PHE:CE1 | 3:108:A:ARG:CA  | 14       | 1.12          |
| (1,557) | 3:95:A:PHE:CD1 | 3:108:A:ARG:CA  | 17       | 1.12          |
| (1,557) | 3:95:A:PHE:CD1 | 3:108:A:ARG:CA  | 18       | 1.12          |
| (1,374) | 3:37:A:TYR:CE2 | 3:50:A:ARG:CA   | 9        | 1.12          |
| (1,317) | 3:18:A:TYR:CD1 | 3:23:A:HIS:CE1  | 7        | 1.12          |
| (1,569) | 3:95:A:PHE:CD2 | 3:112:A:LEU:CD2 | 3        | 1.11          |
| (1,569) | 3:95:A:PHE:CD2 | 3:112:A:LEU:CD2 | 5        | 1.11          |
| (1,336) | 3:18:A:TYR:CD2 | 3:24:A:LEU:CD2  | 10       | 1.11          |
| (1,322) | 3:18:A:TYR:CE1 | 3:23:A:HIS:CD2  | 15       | 1.11          |
| (1,561) | 3:95:A:PHE:CE1 | 3:108:A:ARG:CA  | 11       | 1.1           |
| (1,467) | 3:67:A:PHE:CD1 | 3:78:A:ARG:CA   | 9        | 1.1           |
| (1,375) | 3:37:A:TYR:CE2 | 3:51:A:SER:CA   | 8        | 1.1           |
| (1,271) | 3:7:A:PHE:CE2  | 3:20:A:LYS:CA   | 16       | 1.1           |
| (1,467) | 3:67:A:PHE:CD1 | 3:78:A:ARG:CA   | 13       | 1.09          |
| (1,408) | 3:41:A:PHE:CD2 | 3:44:A:CYS:CA   | 18       | 1.09          |
| (1,376) | 3:37:A:TYR:CE2 | 3:51:A:SER:CB   | 8        | 1.09          |
| (1,378) | 3:37:A:TYR:CD2 | 3:51:A:SER:CA   | 17       | 1.08          |
| (1,569) | 3:95:A:PHE:CD2 | 3:112:A:LEU:CD2 | 6        | 1.07          |
| (1,336) | 3:18:A:TYR:CD2 | 3:24:A:LEU:CD2  | 4        | 1.07          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,336) | 3:18:A:TYR:CD2 | 3:24:A:LEU:CD2  | 17       | 1.07          |
| (1,477) | 3:67:A:PHE:CD2 | 3:79:A:SER:CB   | 13       | 1.06          |
| (1,477) | 3:67:A:PHE:CD2 | 3:79:A:SER:CB   | 7        | 1.05          |
| (1,336) | 3:18:A:TYR:CD2 | 3:24:A:LEU:CD2  | 3        | 1.05          |
| (1,336) | 3:18:A:TYR:CD2 | 3:24:A:LEU:CD2  | 14       | 1.05          |
| (1,477) | 3:67:A:PHE:CD2 | 3:79:A:SER:CB   | 1        | 1.04          |
| (1,477) | 3:67:A:PHE:CD2 | 3:79:A:SER:CB   | 2        | 1.04          |
| (1,477) | 3:67:A:PHE:CD2 | 3:79:A:SER:CB   | 15       | 1.04          |
| (1,477) | 3:67:A:PHE:CD2 | 3:79:A:SER:CB   | 18       | 1.04          |
| (1,477) | 3:67:A:PHE:CD2 | 3:79:A:SER:CB   | 19       | 1.04          |
| (1,477) | 3:67:A:PHE:CD2 | 3:79:A:SER:CB   | 20       | 1.04          |
| (1,267) | 3:7:A:PHE:CD1  | 3:24:A:LEU:CD1  | 18       | 1.04          |
| (1,569) | 3:95:A:PHE:CD2 | 3:112:A:LEU:CD2 | 9        | 1.03          |
| (1,477) | 3:67:A:PHE:CD2 | 3:79:A:SER:CB   | 9        | 1.03          |
| (1,336) | 3:18:A:TYR:CD2 | 3:24:A:LEU:CD2  | 6        | 1.03          |
| (1,477) | 3:67:A:PHE:CD2 | 3:79:A:SER:CB   | 8        | 1.02          |
| (1,477) | 3:67:A:PHE:CD2 | 3:79:A:SER:CB   | 11       | 1.02          |
| (1,477) | 3:67:A:PHE:CD2 | 3:79:A:SER:CB   | 17       | 1.02          |
| (1,374) | 3:37:A:TYR:CE2 | 3:50:A:ARG:CA   | 12       | 1.02          |
| (1,569) | 3:95:A:PHE:CD2 | 3:112:A:LEU:CD2 | 11       | 1.01          |
| (1,569) | 3:95:A:PHE:CD2 | 3:112:A:LEU:CD2 | 12       | 1.0           |
| (1,336) | 3:18:A:TYR:CD2 | 3:24:A:LEU:CD2  | 7        | 1.0           |
| (1,336) | 3:18:A:TYR:CD2 | 3:24:A:LEU:CD2  | 9        | 1.0           |
| (1,477) | 3:67:A:PHE:CD2 | 3:79:A:SER:CB   | 14       | 0.99          |
| (1,378) | 3:37:A:TYR:CD2 | 3:51:A:SER:CA   | 7        | 0.99          |
| (1,336) | 3:18:A:TYR:CD2 | 3:24:A:LEU:CD2  | 11       | 0.99          |
| (4,1)   | 3:26:A:MET:HE3 | 1:134:B:DT:H72  | 8        | 0.98          |
| (1,426) | 3:48:A:PHE:CE2 | 3:54:A:LEU:CD1  | 19       | 0.98          |
| (1,425) | 3:48:A:PHE:CE2 | 3:54:A:LEU:CB   | 19       | 0.98          |
| (1,336) | 3:18:A:TYR:CD2 | 3:24:A:LEU:CD2  | 1        | 0.98          |
| (1,336) | 3:18:A:TYR:CD2 | 3:24:A:LEU:CD2  | 12       | 0.98          |
| (1,274) | 3:7:A:PHE:CD2  | 3:20:A:LYS:CA   | 16       | 0.98          |
| (1,336) | 3:18:A:TYR:CD2 | 3:24:A:LEU:CD2  | 13       | 0.97          |
| (1,336) | 3:18:A:TYR:CD2 | 3:24:A:LEU:CD2  | 19       | 0.97          |
| (1,336) | 3:18:A:TYR:CD2 | 3:24:A:LEU:CD2  | 20       | 0.96          |
| (1,336) | 3:18:A:TYR:CD2 | 3:24:A:LEU:CD2  | 2        | 0.93          |
| (1,475) | 3:67:A:PHE:CE2 | 3:79:A:SER:CB   | 19       | 0.92          |
| (1,377) | 3:37:A:TYR:CD2 | 3:50:A:ARG:CA   | 11       | 0.92          |
| (1,568) | 3:95:A:PHE:CD2 | 3:109:A:SER:CB  | 11       | 0.91          |
| (1,477) | 3:67:A:PHE:CD2 | 3:79:A:SER:CB   | 3        | 0.91          |
| (1,477) | 3:67:A:PHE:CD2 | 3:79:A:SER:CB   | 5        | 0.91          |
| (1,478) | 3:67:A:PHE:CD2 | 3:82:A:LEU:CD1  | 18       | 0.9           |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,474) | 3:67:A:PHE:CE2 | 3:79:A:SER:CA  | 19       | 0.9           |
| (1,378) | 3:37:A:TYR:CD2 | 3:51:A:SER:CA  | 2        | 0.9           |
| (1,568) | 3:95:A:PHE:CD2 | 3:109:A:SER:CB | 14       | 0.89          |
| (1,477) | 3:67:A:PHE:CD2 | 3:79:A:SER:CB  | 4        | 0.89          |
| (1,568) | 3:95:A:PHE:CD2 | 3:109:A:SER:CB | 12       | 0.88          |
| (1,568) | 3:95:A:PHE:CD2 | 3:109:A:SER:CB | 13       | 0.88          |
| (1,478) | 3:67:A:PHE:CD2 | 3:82:A:LEU:CD1 | 4        | 0.88          |
| (1,568) | 3:95:A:PHE:CD2 | 3:109:A:SER:CB | 4        | 0.87          |
| (1,568) | 3:95:A:PHE:CD2 | 3:109:A:SER:CB | 10       | 0.87          |
| (1,568) | 3:95:A:PHE:CD2 | 3:109:A:SER:CB | 1        | 0.86          |
| (1,568) | 3:95:A:PHE:CD2 | 3:109:A:SER:CB | 2        | 0.86          |
| (1,568) | 3:95:A:PHE:CD2 | 3:109:A:SER:CB | 6        | 0.86          |
| (1,568) | 3:95:A:PHE:CD2 | 3:109:A:SER:CB | 7        | 0.86          |
| (1,477) | 3:67:A:PHE:CD2 | 3:79:A:SER:CB  | 10       | 0.86          |
| (1,568) | 3:95:A:PHE:CD2 | 3:109:A:SER:CB | 3        | 0.85          |
| (1,568) | 3:95:A:PHE:CD2 | 3:109:A:SER:CB | 9        | 0.85          |
| (1,568) | 3:95:A:PHE:CD2 | 3:109:A:SER:CB | 15       | 0.85          |
| (1,478) | 3:67:A:PHE:CD2 | 3:82:A:LEU:CD1 | 8        | 0.85          |
| (1,568) | 3:95:A:PHE:CD2 | 3:109:A:SER:CB | 8        | 0.84          |
| (1,568) | 3:95:A:PHE:CD2 | 3:109:A:SER:CB | 18       | 0.84          |
| (1,478) | 3:67:A:PHE:CD2 | 3:82:A:LEU:CD1 | 1        | 0.84          |
| (1,478) | 3:67:A:PHE:CD2 | 3:82:A:LEU:CD1 | 19       | 0.84          |
| (1,568) | 3:95:A:PHE:CD2 | 3:109:A:SER:CB | 19       | 0.83          |
| (1,568) | 3:95:A:PHE:CD2 | 3:109:A:SER:CB | 20       | 0.83          |
| (1,478) | 3:67:A:PHE:CD2 | 3:82:A:LEU:CD1 | 9        | 0.82          |
| (1,478) | 3:67:A:PHE:CD2 | 3:82:A:LEU:CD1 | 15       | 0.82          |
| (1,379) | 3:37:A:TYR:CD2 | 3:51:A:SER:CB  | 8        | 0.82          |
| (1,378) | 3:37:A:TYR:CD2 | 3:51:A:SER:CA  | 9        | 0.82          |
| (1,267) | 3:7:A:PHE:CD1  | 3:24:A:LEU:CD1 | 4        | 0.82          |
| (4,1)   | 3:26:A:MET:HE1 | 1:136:B:DT:H71 | 15       | 0.81          |
| (1,478) | 3:67:A:PHE:CD2 | 3:82:A:LEU:CD1 | 13       | 0.81          |
| (4,1)   | 3:26:A:MET:HE3 | 1:136:B:DT:H72 | 14       | 0.8           |
| (1,568) | 3:95:A:PHE:CD2 | 3:109:A:SER:CB | 5        | 0.8           |
| (1,568) | 3:95:A:PHE:CD2 | 3:109:A:SER:CB | 17       | 0.8           |
| (1,478) | 3:67:A:PHE:CD2 | 3:82:A:LEU:CD1 | 2        | 0.8           |
| (1,478) | 3:67:A:PHE:CD2 | 3:82:A:LEU:CD1 | 7        | 0.8           |
| (1,478) | 3:67:A:PHE:CD2 | 3:82:A:LEU:CD1 | 14       | 0.8           |
| (1,330) | 3:18:A:TYR:CE2 | 3:24:A:LEU:CD2 | 5        | 0.8           |
| (1,477) | 3:67:A:PHE:CD2 | 3:79:A:SER:CB  | 12       | 0.79          |
| (1,401) | 3:41:A:PHE:CE1 | 3:61:A:HIS:CB  | 18       | 0.79          |
| (1,330) | 3:18:A:TYR:CE2 | 3:24:A:LEU:CD2 | 10       | 0.79          |
| (1,478) | 3:67:A:PHE:CD2 | 3:82:A:LEU:CD1 | 20       | 0.78          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,378) | 3:37:A:TYR:CD2 | 3:51:A:SER:CA  | 20       | 0.78          |
| (4,1)   | 3:26:A:MET:HE2 | 1:134:B:DT:H72 | 1        | 0.77          |
| (4,1)   | 3:26:A:MET:HE2 | 1:134:B:DT:H71 | 12       | 0.77          |
| (1,568) | 3:95:A:PHE:CD2 | 3:109:A:SER:CB | 16       | 0.77          |
| (1,478) | 3:67:A:PHE:CD2 | 3:82:A:LEU:CD1 | 10       | 0.77          |
| (1,478) | 3:67:A:PHE:CD2 | 3:82:A:LEU:CD1 | 17       | 0.77          |
| (1,378) | 3:37:A:TYR:CD2 | 3:51:A:SER:CA  | 18       | 0.76          |
| (4,1)   | 3:26:A:MET:HE1 | 1:136:B:DT:H71 | 10       | 0.75          |
| (1,478) | 3:67:A:PHE:CD2 | 3:82:A:LEU:CD1 | 11       | 0.75          |
| (1,330) | 3:18:A:TYR:CE2 | 3:24:A:LEU:CD2 | 4        | 0.75          |
| (1,294) | 3:11:A:TYR:CD1 | 3:31:A:HIS:CB  | 17       | 0.75          |
| (1,478) | 3:67:A:PHE:CD2 | 3:82:A:LEU:CD1 | 12       | 0.74          |
| (1,478) | 3:67:A:PHE:CD2 | 3:82:A:LEU:CD1 | 16       | 0.74          |
| (1,476) | 3:67:A:PHE:CD2 | 3:79:A:SER:CA  | 19       | 0.73          |
| (1,330) | 3:18:A:TYR:CE2 | 3:24:A:LEU:CD2 | 15       | 0.73          |
| (1,330) | 3:18:A:TYR:CE2 | 3:24:A:LEU:CD2 | 14       | 0.72          |
| (1,299) | 3:11:A:TYR:CE1 | 3:34:A:GLU:CA  | 18       | 0.72          |
| (1,375) | 3:37:A:TYR:CE2 | 3:51:A:SER:CA  | 7        | 0.71          |
| (1,478) | 3:67:A:PHE:CD2 | 3:82:A:LEU:CD1 | 3        | 0.7           |
| (1,375) | 3:37:A:TYR:CE2 | 3:51:A:SER:CA  | 2        | 0.7           |
| (1,333) | 3:18:A:TYR:CE2 | 3:27:A:HIS:CE1 | 15       | 0.7           |
| (1,330) | 3:18:A:TYR:CE2 | 3:24:A:LEU:CD2 | 17       | 0.7           |
| (1,477) | 3:67:A:PHE:CD2 | 3:79:A:SER:CB  | 16       | 0.69          |
| (1,417) | 3:48:A:PHE:CD1 | 3:53:A:GLN:CA  | 19       | 0.69          |
| (1,378) | 3:37:A:TYR:CD2 | 3:51:A:SER:CA  | 12       | 0.69          |
| (1,375) | 3:37:A:TYR:CE2 | 3:51:A:SER:CA  | 17       | 0.69          |
| (1,330) | 3:18:A:TYR:CE2 | 3:24:A:LEU:CD2 | 1        | 0.69          |
| (4,1)   | 3:26:A:MET:HE3 | 1:134:B:DT:H72 | 6        | 0.68          |
| (1,332) | 3:18:A:TYR:CE2 | 3:27:A:HIS:CD2 | 15       | 0.68          |
| (1,478) | 3:67:A:PHE:CD2 | 3:82:A:LEU:CD1 | 5        | 0.67          |
| (1,475) | 3:67:A:PHE:CE2 | 3:79:A:SER:CB  | 18       | 0.67          |
| (1,330) | 3:18:A:TYR:CE2 | 3:24:A:LEU:CD2 | 3        | 0.67          |
| (1,330) | 3:18:A:TYR:CE2 | 3:24:A:LEU:CD2 | 7        | 0.67          |
| (1,330) | 3:18:A:TYR:CE2 | 3:24:A:LEU:CD2 | 6        | 0.66          |
| (1,330) | 3:18:A:TYR:CE2 | 3:24:A:LEU:CD2 | 9        | 0.66          |
| (1,475) | 3:67:A:PHE:CE2 | 3:79:A:SER:CB  | 20       | 0.65          |
| (1,330) | 3:18:A:TYR:CE2 | 3:24:A:LEU:CD2 | 11       | 0.65          |
| (4,1)   | 3:26:A:MET:HE3 | 1:134:B:DT:H71 | 16       | 0.64          |
| (1,475) | 3:67:A:PHE:CE2 | 3:79:A:SER:CB  | 11       | 0.64          |
| (1,475) | 3:67:A:PHE:CE2 | 3:79:A:SER:CB  | 3        | 0.63          |
| (1,330) | 3:18:A:TYR:CE2 | 3:24:A:LEU:CD2 | 20       | 0.63          |
| (1,267) | 3:7:A:PHE:CD1  | 3:24:A:LEU:CD1 | 16       | 0.63          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,475) | 3:67:A:PHE:CE2 | 3:79:A:SER:CB  | 1        | 0.62          |
| (1,475) | 3:67:A:PHE:CE2 | 3:79:A:SER:CB  | 7        | 0.62          |
| (1,376) | 3:37:A:TYR:CE2 | 3:51:A:SER:CB  | 17       | 0.62          |
| (1,475) | 3:67:A:PHE:CE2 | 3:79:A:SER:CB  | 13       | 0.61          |
| (1,475) | 3:67:A:PHE:CE2 | 3:79:A:SER:CB  | 15       | 0.61          |
| (1,330) | 3:18:A:TYR:CE2 | 3:24:A:LEU:CD2 | 12       | 0.61          |
| (1,330) | 3:18:A:TYR:CE2 | 3:24:A:LEU:CD2 | 13       | 0.61          |
| (1,475) | 3:67:A:PHE:CE2 | 3:79:A:SER:CB  | 2        | 0.6           |
| (1,475) | 3:67:A:PHE:CE2 | 3:79:A:SER:CB  | 8        | 0.6           |
| (1,380) | 3:37:A:TYR:CD2 | 3:54:A:LEU:CB  | 7        | 0.6           |
| (1,374) | 3:37:A:TYR:CE2 | 3:50:A:ARG:CA  | 11       | 0.6           |
| (1,330) | 3:18:A:TYR:CE2 | 3:24:A:LEU:CD2 | 2        | 0.6           |
| (1,330) | 3:18:A:TYR:CE2 | 3:24:A:LEU:CD2 | 19       | 0.6           |
| (4,1)   | 3:26:A:MET:HE3 | 1:134:B:DT:H72 | 13       | 0.59          |
| (1,475) | 3:67:A:PHE:CE2 | 3:79:A:SER:CB  | 9        | 0.58          |
| (1,294) | 3:11:A:TYR:CD1 | 3:31:A:HIS:CB  | 18       | 0.58          |
| (1,318) | 3:18:A:TYR:CD1 | 3:24:A:LEU:CA  | 13       | 0.56          |
| (1,293) | 3:11:A:TYR:CD1 | 3:31:A:HIS:CA  | 17       | 0.56          |
| (4,2)   | 3:26:A:MET:HE1 | 1:135:B:DC:H5  | 8        | 0.55          |
| (1,434) | 3:48:A:PHE:CD2 | 3:57:A:HIS:CD2 | 19       | 0.55          |
| (1,318) | 3:18:A:TYR:CD1 | 3:24:A:LEU:CA  | 2        | 0.55          |
| (1,475) | 3:67:A:PHE:CE2 | 3:79:A:SER:CB  | 14       | 0.54          |
| (1,475) | 3:67:A:PHE:CE2 | 3:79:A:SER:CB  | 17       | 0.54          |
| (1,318) | 3:18:A:TYR:CD1 | 3:24:A:LEU:CA  | 1        | 0.54          |
| (1,318) | 3:18:A:TYR:CD1 | 3:24:A:LEU:CA  | 7        | 0.54          |
| (1,318) | 3:18:A:TYR:CD1 | 3:24:A:LEU:CA  | 9        | 0.54          |
| (1,476) | 3:67:A:PHE:CD2 | 3:79:A:SER:CA  | 18       | 0.53          |
| (1,475) | 3:67:A:PHE:CE2 | 3:79:A:SER:CB  | 4        | 0.53          |
| (1,474) | 3:67:A:PHE:CE2 | 3:79:A:SER:CA  | 18       | 0.53          |
| (1,380) | 3:37:A:TYR:CD2 | 3:54:A:LEU:CB  | 12       | 0.53          |
| (1,375) | 3:37:A:TYR:CE2 | 3:51:A:SER:CA  | 18       | 0.53          |
| (1,318) | 3:18:A:TYR:CD1 | 3:24:A:LEU:CA  | 4        | 0.53          |
| (1,318) | 3:18:A:TYR:CD1 | 3:24:A:LEU:CA  | 17       | 0.52          |
| (1,318) | 3:18:A:TYR:CD1 | 3:24:A:LEU:CA  | 20       | 0.52          |
| (1,476) | 3:67:A:PHE:CD2 | 3:79:A:SER:CA  | 15       | 0.51          |
| (1,411) | 3:41:A:PHE:CD2 | 3:61:A:HIS:CE1 | 18       | 0.51          |
| (1,380) | 3:37:A:TYR:CD2 | 3:54:A:LEU:CB  | 8        | 0.51          |
| (1,318) | 3:18:A:TYR:CD1 | 3:24:A:LEU:CA  | 14       | 0.51          |
| (1,476) | 3:67:A:PHE:CD2 | 3:79:A:SER:CA  | 20       | 0.5           |
| (1,475) | 3:67:A:PHE:CE2 | 3:79:A:SER:CB  | 10       | 0.5           |
| (1,376) | 3:37:A:TYR:CE2 | 3:51:A:SER:CB  | 7        | 0.5           |
| (1,318) | 3:18:A:TYR:CD1 | 3:24:A:LEU:CA  | 6        | 0.5           |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,318) | 3:18:A:TYR:CD1 | 3:24:A:LEU:CA  | 10       | 0.5           |
| (1,255) | 3:110:A:ASP:HA | 3:113:A:VAL:HB | 11       | 0.5           |
| (4,1)   | 3:26:A:MET:HE2 | 1:136:B:DT:H73 | 4        | 0.49          |
| (1,474) | 3:67:A:PHE:CE2 | 3:79:A:SER:CA  | 20       | 0.49          |
| (1,376) | 3:37:A:TYR:CE2 | 3:51:A:SER:CB  | 2        | 0.49          |
| (1,318) | 3:18:A:TYR:CD1 | 3:24:A:LEU:CA  | 15       | 0.49          |
| (1,307) | 3:11:A:TYR:CD2 | 3:31:A:HIS:CE1 | 17       | 0.49          |
| (1,476) | 3:67:A:PHE:CD2 | 3:79:A:SER:CA  | 2        | 0.48          |
| (1,318) | 3:18:A:TYR:CD1 | 3:24:A:LEU:CA  | 11       | 0.48          |
| (1,270) | 3:7:A:PHE:CE1  | 3:21:A:LEU:CD1 | 18       | 0.48          |
| (1,475) | 3:67:A:PHE:CE2 | 3:79:A:SER:CB  | 5        | 0.47          |
| (1,430) | 3:48:A:PHE:CD2 | 3:54:A:LEU:CA  | 19       | 0.47          |
| (1,476) | 3:67:A:PHE:CD2 | 3:79:A:SER:CA  | 13       | 0.46          |
| (1,380) | 3:37:A:TYR:CD2 | 3:54:A:LEU:CB  | 2        | 0.46          |
| (1,332) | 3:18:A:TYR:CE2 | 3:27:A:HIS:CD2 | 17       | 0.46          |
| (1,318) | 3:18:A:TYR:CD1 | 3:24:A:LEU:CA  | 12       | 0.46          |
| (1,474) | 3:67:A:PHE:CE2 | 3:79:A:SER:CA  | 15       | 0.45          |
| (1,375) | 3:37:A:TYR:CE2 | 3:51:A:SER:CA  | 9        | 0.45          |
| (1,318) | 3:18:A:TYR:CD1 | 3:24:A:LEU:CA  | 3        | 0.45          |
| (1,476) | 3:67:A:PHE:CD2 | 3:79:A:SER:CA  | 9        | 0.44          |
| (1,476) | 3:67:A:PHE:CD2 | 3:79:A:SER:CA  | 17       | 0.44          |
| (1,474) | 3:67:A:PHE:CE2 | 3:79:A:SER:CA  | 3        | 0.44          |
| (1,376) | 3:37:A:TYR:CE2 | 3:51:A:SER:CB  | 9        | 0.44          |
| (1,338) | 3:18:A:TYR:CD2 | 3:27:A:HIS:CD2 | 15       | 0.44          |
| (1,318) | 3:18:A:TYR:CD1 | 3:24:A:LEU:CA  | 19       | 0.44          |
| (1,476) | 3:67:A:PHE:CD2 | 3:79:A:SER:CA  | 1        | 0.43          |
| (1,476) | 3:67:A:PHE:CD2 | 3:79:A:SER:CA  | 7        | 0.42          |
| (1,476) | 3:67:A:PHE:CD2 | 3:79:A:SER:CA  | 8        | 0.42          |
| (1,318) | 3:18:A:TYR:CD1 | 3:24:A:LEU:CA  | 5        | 0.42          |
| (1,476) | 3:67:A:PHE:CD2 | 3:79:A:SER:CA  | 11       | 0.41          |
| (1,474) | 3:67:A:PHE:CE2 | 3:79:A:SER:CA  | 2        | 0.41          |
| (1,351) | 3:22:A:SER:CA  | 3:24:A:LEU:CA  | 17       | 0.41          |
| (1,293) | 3:11:A:TYR:CD1 | 3:31:A:HIS:CA  | 18       | 0.41          |
| (2,95)  | 3:27:A:HIS:N   | 3:23:A:HIS:O   | 16       | 0.4           |
| (1,379) | 3:37:A:TYR:CD2 | 3:51:A:SER:CB  | 17       | 0.4           |
| (2,125) | 3:112:A:LEU:N  | 3:108:A:ARG:O  | 3        | 0.39          |
| (2,125) | 3:112:A:LEU:N  | 3:108:A:ARG:O  | 7        | 0.39          |
| (2,125) | 3:112:A:LEU:N  | 3:108:A:ARG:O  | 13       | 0.39          |
| (2,125) | 3:112:A:LEU:N  | 3:108:A:ARG:O  | 17       | 0.39          |
| (2,103) | 3:54:A:LEU:N   | 3:50:A:ARG:O   | 19       | 0.39          |
| (1,476) | 3:67:A:PHE:CD2 | 3:79:A:SER:CA  | 3        | 0.39          |
| (1,475) | 3:67:A:PHE:CE2 | 3:79:A:SER:CB  | 12       | 0.39          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,474) | 3:67:A:PHE:CE2 | 3:79:A:SER:CA  | 13       | 0.39          |
| (2,125) | 3:112:A:LEU:N  | 3:108:A:ARG:O  | 4        | 0.38          |
| (2,125) | 3:112:A:LEU:N  | 3:108:A:ARG:O  | 6        | 0.38          |
| (2,125) | 3:112:A:LEU:N  | 3:108:A:ARG:O  | 11       | 0.38          |
| (2,125) | 3:112:A:LEU:N  | 3:108:A:ARG:O  | 12       | 0.38          |
| (2,125) | 3:112:A:LEU:N  | 3:108:A:ARG:O  | 15       | 0.38          |
| (2,125) | 3:112:A:LEU:N  | 3:108:A:ARG:O  | 16       | 0.38          |
| (2,125) | 3:112:A:LEU:N  | 3:108:A:ARG:O  | 19       | 0.38          |
| (2,125) | 3:112:A:LEU:N  | 3:108:A:ARG:O  | 20       | 0.38          |
| (2,119) | 3:87:A:ARG:N   | 3:84:A:THR:O   | 18       | 0.38          |
| (2,103) | 3:54:A:LEU:N   | 3:50:A:ARG:O   | 8        | 0.38          |
| (2,103) | 3:54:A:LEU:N   | 3:50:A:ARG:O   | 20       | 0.38          |
| (1,474) | 3:67:A:PHE:CE2 | 3:79:A:SER:CA  | 1        | 0.38          |
| (1,474) | 3:67:A:PHE:CE2 | 3:79:A:SER:CA  | 8        | 0.38          |
| (1,447) | 3:58:A:GLN:CA  | 3:61:A:HIS:CD2 | 12       | 0.38          |
| (1,375) | 3:37:A:TYR:CE2 | 3:51:A:SER:CA  | 12       | 0.38          |
| (1,307) | 3:11:A:TYR:CD2 | 3:31:A:HIS:CE1 | 18       | 0.38          |
| (2,125) | 3:112:A:LEU:N  | 3:108:A:ARG:O  | 5        | 0.37          |
| (2,125) | 3:112:A:LEU:N  | 3:108:A:ARG:O  | 8        | 0.37          |
| (2,125) | 3:112:A:LEU:N  | 3:108:A:ARG:O  | 10       | 0.37          |
| (2,125) | 3:112:A:LEU:N  | 3:108:A:ARG:O  | 14       | 0.37          |
| (2,103) | 3:54:A:LEU:N   | 3:50:A:ARG:O   | 3        | 0.37          |
| (2,103) | 3:54:A:LEU:N   | 3:50:A:ARG:O   | 12       | 0.37          |
| (2,103) | 3:54:A:LEU:N   | 3:50:A:ARG:O   | 14       | 0.37          |
| (2,98)  | 3:30:A:LYS:N   | 3:27:A:HIS:O   | 15       | 0.37          |
| (2,95)  | 3:27:A:HIS:N   | 3:23:A:HIS:O   | 3        | 0.37          |
| (2,95)  | 3:27:A:HIS:N   | 3:23:A:HIS:O   | 5        | 0.37          |
| (2,95)  | 3:27:A:HIS:N   | 3:23:A:HIS:O   | 7        | 0.37          |
| (2,90)  | 3:9:A:CYS:N    | 3:16:A:LYS:O   | 1        | 0.37          |
| (1,476) | 3:67:A:PHE:CD2 | 3:79:A:SER:CA  | 14       | 0.37          |
| (1,474) | 3:67:A:PHE:CE2 | 3:79:A:SER:CA  | 9        | 0.37          |
| (1,474) | 3:67:A:PHE:CE2 | 3:79:A:SER:CA  | 11       | 0.37          |
| (1,375) | 3:37:A:TYR:CE2 | 3:51:A:SER:CA  | 20       | 0.37          |
| (1,351) | 3:22:A:SER:CA  | 3:24:A:LEU:CA  | 20       | 0.37          |
| (1,332) | 3:18:A:TYR:CE2 | 3:27:A:HIS:CD2 | 19       | 0.37          |
| (2,132) | 3:119:A:HIS:N  | 3:116:A:HIS:O  | 8        | 0.36          |
| (2,132) | 3:119:A:HIS:N  | 3:116:A:HIS:O  | 9        | 0.36          |
| (2,132) | 3:119:A:HIS:N  | 3:116:A:HIS:O  | 12       | 0.36          |
| (2,132) | 3:119:A:HIS:N  | 3:116:A:HIS:O  | 16       | 0.36          |
| (2,132) | 3:119:A:HIS:N  | 3:116:A:HIS:O  | 17       | 0.36          |
| (2,125) | 3:112:A:LEU:N  | 3:108:A:ARG:O  | 1        | 0.36          |
| (2,125) | 3:112:A:LEU:N  | 3:108:A:ARG:O  | 2        | 0.36          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (2,125) | 3:112:A:LEU:N  | 3:108:A:ARG:O  | 9        | 0.36          |
| (2,125) | 3:112:A:LEU:N  | 3:108:A:ARG:O  | 18       | 0.36          |
| (2,119) | 3:87:A:ARG:N   | 3:84:A:THR:O   | 10       | 0.36          |
| (2,103) | 3:54:A:LEU:N   | 3:50:A:ARG:O   | 11       | 0.36          |
| (2,103) | 3:54:A:LEU:N   | 3:50:A:ARG:O   | 15       | 0.36          |
| (2,103) | 3:54:A:LEU:N   | 3:50:A:ARG:O   | 18       | 0.36          |
| (2,99)  | 3:31:A:HIS:N   | 3:28:A:SER:O   | 13       | 0.36          |
| (1,710) | 1:129:B:DG:C4' | 3:60:A:ARG:CZ  | 11       | 0.36          |
| (1,351) | 3:22:A:SER:CA  | 3:24:A:LEU:CA  | 9        | 0.36          |
| (1,279) | 3:8:A:MET:CB   | 3:16:A:LYS:CA  | 17       | 0.36          |
| (2,132) | 3:119:A:HIS:N  | 3:116:A:HIS:O  | 2        | 0.35          |
| (2,132) | 3:119:A:HIS:N  | 3:116:A:HIS:O  | 4        | 0.35          |
| (2,132) | 3:119:A:HIS:N  | 3:116:A:HIS:O  | 5        | 0.35          |
| (2,132) | 3:119:A:HIS:N  | 3:116:A:HIS:O  | 11       | 0.35          |
| (2,132) | 3:119:A:HIS:N  | 3:116:A:HIS:O  | 13       | 0.35          |
| (2,132) | 3:119:A:HIS:N  | 3:116:A:HIS:O  | 15       | 0.35          |
| (2,132) | 3:119:A:HIS:N  | 3:116:A:HIS:O  | 20       | 0.35          |
| (2,121) | 3:89:A:HIS:N   | 3:86:A:THR:O   | 10       | 0.35          |
| (2,103) | 3:54:A:LEU:N   | 3:50:A:ARG:O   | 5        | 0.35          |
| (2,103) | 3:54:A:LEU:N   | 3:50:A:ARG:O   | 6        | 0.35          |
| (2,103) | 3:54:A:LEU:N   | 3:50:A:ARG:O   | 16       | 0.35          |
| (1,474) | 3:67:A:PHE:CE2 | 3:79:A:SER:CA  | 7        | 0.35          |
| (1,351) | 3:22:A:SER:CA  | 3:24:A:LEU:CA  | 15       | 0.35          |
| (1,332) | 3:18:A:TYR:CE2 | 3:27:A:HIS:CD2 | 3        | 0.35          |
| (1,332) | 3:18:A:TYR:CE2 | 3:27:A:HIS:CD2 | 10       | 0.35          |
| (1,279) | 3:8:A:MET:CB   | 3:16:A:LYS:CA  | 3        | 0.35          |
| (1,279) | 3:8:A:MET:CB   | 3:16:A:LYS:CA  | 8        | 0.35          |
| (1,279) | 3:8:A:MET:CB   | 3:16:A:LYS:CA  | 16       | 0.35          |
| (1,4)   | 3:16:A:LYS:HA  | 3:17:A:ARG:H   | 1        | 0.35          |
| (2,132) | 3:119:A:HIS:N  | 3:116:A:HIS:O  | 1        | 0.34          |
| (2,132) | 3:119:A:HIS:N  | 3:116:A:HIS:O  | 14       | 0.34          |
| (2,126) | 3:113:A:VAL:N  | 3:109:A:SER:O  | 8        | 0.34          |
| (2,119) | 3:87:A:ARG:N   | 3:84:A:THR:O   | 3        | 0.34          |
| (2,114) | 3:82:A:LEU:N   | 3:78:A:ARG:O   | 13       | 0.34          |
| (2,97)  | 3:29:A:ARG:N   | 3:26:A:MET:O   | 13       | 0.34          |
| (2,95)  | 3:27:A:HIS:N   | 3:23:A:HIS:O   | 2        | 0.34          |
| (2,95)  | 3:27:A:HIS:N   | 3:23:A:HIS:O   | 10       | 0.34          |
| (2,95)  | 3:27:A:HIS:N   | 3:23:A:HIS:O   | 19       | 0.34          |
| (1,447) | 3:58:A:GLN:CA  | 3:61:A:HIS:CD2 | 15       | 0.34          |
| (1,429) | 3:48:A:PHE:CE2 | 3:57:A:HIS:CE1 | 19       | 0.34          |
| (1,279) | 3:8:A:MET:CB   | 3:16:A:LYS:CA  | 6        | 0.34          |
| (2,121) | 3:89:A:HIS:N   | 3:86:A:THR:O   | 13       | 0.33          |

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| Key     | Atom-1         | Atom-2        | Model ID | Violation (Å) |
|---------|----------------|---------------|----------|---------------|
| (2,121) | 3:89:A:HIS:N   | 3:86:A:THR:O  | 19       | 0.33          |
| (2,119) | 3:87:A:ARG:N   | 3:84:A:THR:O  | 2        | 0.33          |
| (2,119) | 3:87:A:ARG:N   | 3:84:A:THR:O  | 5        | 0.33          |
| (2,119) | 3:87:A:ARG:N   | 3:84:A:THR:O  | 6        | 0.33          |
| (2,119) | 3:87:A:ARG:N   | 3:84:A:THR:O  | 15       | 0.33          |
| (2,119) | 3:87:A:ARG:N   | 3:84:A:THR:O  | 19       | 0.33          |
| (2,114) | 3:82:A:LEU:N   | 3:78:A:ARG:O  | 11       | 0.33          |
| (2,114) | 3:82:A:LEU:N   | 3:78:A:ARG:O  | 18       | 0.33          |
| (2,108) | 3:59:A:ARG:N   | 3:56:A:ARG:O  | 5        | 0.33          |
| (2,108) | 3:59:A:ARG:N   | 3:56:A:ARG:O  | 7        | 0.33          |
| (2,108) | 3:59:A:ARG:N   | 3:56:A:ARG:O  | 15       | 0.33          |
| (2,108) | 3:59:A:ARG:N   | 3:56:A:ARG:O  | 20       | 0.33          |
| (2,103) | 3:54:A:LEU:N   | 3:50:A:ARG:O  | 4        | 0.33          |
| (2,98)  | 3:30:A:LYS:N   | 3:27:A:HIS:O  | 19       | 0.33          |
| (2,97)  | 3:29:A:ARG:N   | 3:26:A:MET:O  | 11       | 0.33          |
| (2,95)  | 3:27:A:HIS:N   | 3:23:A:HIS:O  | 11       | 0.33          |
| (2,95)  | 3:27:A:HIS:N   | 3:23:A:HIS:O  | 15       | 0.33          |
| (1,710) | 1:129:B:DG:C4' | 3:60:A:ARG:CZ | 5        | 0.33          |
| (1,475) | 3:67:A:PHE:CE2 | 3:79:A:SER:CB | 16       | 0.33          |
| (1,474) | 3:67:A:PHE:CE2 | 3:79:A:SER:CA | 17       | 0.33          |
| (1,378) | 3:37:A:TYR:CD2 | 3:51:A:SER:CA | 11       | 0.33          |
| (1,279) | 3:8:A:MET:CB   | 3:16:A:LYS:CA | 4        | 0.33          |
| (1,279) | 3:8:A:MET:CB   | 3:16:A:LYS:CA | 7        | 0.33          |
| (1,279) | 3:8:A:MET:CB   | 3:16:A:LYS:CA | 11       | 0.33          |
| (1,9)   | 3:17:A:ARG:HA  | 3:9:A:CYS:H   | 18       | 0.33          |
| (4,2)   | 3:26:A:MET:HE3 | 1:135:B:DC:H5 | 12       | 0.32          |
| (2,119) | 3:87:A:ARG:N   | 3:84:A:THR:O  | 1        | 0.32          |
| (2,119) | 3:87:A:ARG:N   | 3:84:A:THR:O  | 8        | 0.32          |
| (2,119) | 3:87:A:ARG:N   | 3:84:A:THR:O  | 13       | 0.32          |
| (2,119) | 3:87:A:ARG:N   | 3:84:A:THR:O  | 16       | 0.32          |
| (2,119) | 3:87:A:ARG:N   | 3:84:A:THR:O  | 17       | 0.32          |
| (2,119) | 3:87:A:ARG:N   | 3:84:A:THR:O  | 20       | 0.32          |
| (2,114) | 3:82:A:LEU:N   | 3:78:A:ARG:O  | 1        | 0.32          |
| (2,114) | 3:82:A:LEU:N   | 3:78:A:ARG:O  | 5        | 0.32          |
| (2,114) | 3:82:A:LEU:N   | 3:78:A:ARG:O  | 15       | 0.32          |
| (2,114) | 3:82:A:LEU:N   | 3:78:A:ARG:O  | 16       | 0.32          |
| (2,114) | 3:82:A:LEU:N   | 3:78:A:ARG:O  | 20       | 0.32          |
| (2,108) | 3:59:A:ARG:N   | 3:56:A:ARG:O  | 10       | 0.32          |
| (2,108) | 3:59:A:ARG:N   | 3:56:A:ARG:O  | 12       | 0.32          |
| (2,103) | 3:54:A:LEU:N   | 3:50:A:ARG:O  | 1        | 0.32          |
| (2,103) | 3:54:A:LEU:N   | 3:50:A:ARG:O  | 9        | 0.32          |
| (2,99)  | 3:31:A:HIS:N   | 3:28:A:SER:O  | 1        | 0.32          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (2,97)  | 3:29:A:ARG:N   | 3:26:A:MET:O   | 19       | 0.32          |
| (2,95)  | 3:27:A:HIS:N   | 3:23:A:HIS:O   | 12       | 0.32          |
| (2,95)  | 3:27:A:HIS:N   | 3:23:A:HIS:O   | 17       | 0.32          |
| (1,376) | 3:37:A:TYR:CE2 | 3:51:A:SER:CB  | 20       | 0.32          |
| (1,351) | 3:22:A:SER:CA  | 3:24:A:LEU:CA  | 13       | 0.32          |
| (1,351) | 3:22:A:SER:CA  | 3:24:A:LEU:CA  | 16       | 0.32          |
| (1,279) | 3:8:A:MET:CB   | 3:16:A:LYS:CA  | 20       | 0.32          |
| (1,267) | 3:7:A:PHE:CD1  | 3:24:A:LEU:CD1 | 8        | 0.32          |
| (1,11)  | 3:8:A:MET:HA   | 3:16:A:LYS:H   | 1        | 0.32          |
| (2,126) | 3:113:A:VAL:N  | 3:109:A:SER:O  | 4        | 0.31          |
| (2,119) | 3:87:A:ARG:N   | 3:84:A:THR:O   | 4        | 0.31          |
| (2,119) | 3:87:A:ARG:N   | 3:84:A:THR:O   | 12       | 0.31          |
| (2,114) | 3:82:A:LEU:N   | 3:78:A:ARG:O   | 2        | 0.31          |
| (2,114) | 3:82:A:LEU:N   | 3:78:A:ARG:O   | 7        | 0.31          |
| (2,114) | 3:82:A:LEU:N   | 3:78:A:ARG:O   | 9        | 0.31          |
| (2,114) | 3:82:A:LEU:N   | 3:78:A:ARG:O   | 17       | 0.31          |
| (2,108) | 3:59:A:ARG:N   | 3:56:A:ARG:O   | 16       | 0.31          |
| (2,103) | 3:54:A:LEU:N   | 3:50:A:ARG:O   | 7        | 0.31          |
| (2,98)  | 3:30:A:LYS:N   | 3:27:A:HIS:O   | 10       | 0.31          |
| (2,98)  | 3:30:A:LYS:N   | 3:27:A:HIS:O   | 11       | 0.31          |
| (2,97)  | 3:29:A:ARG:N   | 3:26:A:MET:O   | 2        | 0.31          |
| (2,97)  | 3:29:A:ARG:N   | 3:26:A:MET:O   | 10       | 0.31          |
| (2,97)  | 3:29:A:ARG:N   | 3:26:A:MET:O   | 12       | 0.31          |
| (2,97)  | 3:29:A:ARG:N   | 3:26:A:MET:O   | 16       | 0.31          |
| (1,407) | 3:41:A:PHE:CE2 | 3:61:A:HIS:CE1 | 18       | 0.31          |
| (1,351) | 3:22:A:SER:CA  | 3:24:A:LEU:CA  | 2        | 0.31          |
| (1,279) | 3:8:A:MET:CB   | 3:16:A:LYS:CA  | 9        | 0.31          |
| (1,143) | 3:68:A:GLN:HA  | 3:74:A:ARG:H   | 8        | 0.31          |
| (1,11)  | 3:8:A:MET:HA   | 3:16:A:LYS:H   | 18       | 0.31          |
| (1,9)   | 3:17:A:ARG:HA  | 3:9:A:CYS:H    | 9        | 0.31          |
| (2,119) | 3:87:A:ARG:N   | 3:84:A:THR:O   | 11       | 0.3           |
| (2,114) | 3:82:A:LEU:N   | 3:78:A:ARG:O   | 6        | 0.3           |
| (2,114) | 3:82:A:LEU:N   | 3:78:A:ARG:O   | 10       | 0.3           |
| (2,114) | 3:82:A:LEU:N   | 3:78:A:ARG:O   | 14       | 0.3           |
| (2,110) | 3:61:A:HIS:N   | 3:58:A:GLN:O   | 12       | 0.3           |
| (2,109) | 3:60:A:ARG:N   | 3:57:A:HIS:O   | 5        | 0.3           |
| (2,108) | 3:59:A:ARG:N   | 3:56:A:ARG:O   | 2        | 0.3           |
| (2,108) | 3:59:A:ARG:N   | 3:56:A:ARG:O   | 11       | 0.3           |
| (2,108) | 3:59:A:ARG:N   | 3:56:A:ARG:O   | 18       | 0.3           |
| (2,108) | 3:59:A:ARG:N   | 3:56:A:ARG:O   | 19       | 0.3           |
| (2,103) | 3:54:A:LEU:N   | 3:50:A:ARG:O   | 13       | 0.3           |
| (2,103) | 3:54:A:LEU:N   | 3:50:A:ARG:O   | 17       | 0.3           |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (2,98)  | 3:30:A:LYS:N   | 3:27:A:HIS:O   | 12       | 0.3           |
| (2,97)  | 3:29:A:ARG:N   | 3:26:A:MET:O   | 1        | 0.3           |
| (2,97)  | 3:29:A:ARG:N   | 3:26:A:MET:O   | 5        | 0.3           |
| (2,97)  | 3:29:A:ARG:N   | 3:26:A:MET:O   | 17       | 0.3           |
| (2,95)  | 3:27:A:HIS:N   | 3:23:A:HIS:O   | 18       | 0.3           |
| (2,92)  | 3:24:A:LEU:N   | 3:20:A:LYS:O   | 2        | 0.3           |
| (1,577) | 3:97:A:CYS:CB  | 3:99:A:TRP:CB  | 16       | 0.3           |
| (1,474) | 3:67:A:PHE:CE2 | 3:79:A:SER:CA  | 10       | 0.3           |
| (1,447) | 3:58:A:GLN:CA  | 3:61:A:HIS:CD2 | 18       | 0.3           |
| (1,351) | 3:22:A:SER:CA  | 3:24:A:LEU:CA  | 18       | 0.3           |
| (1,333) | 3:18:A:TYR:CE2 | 3:27:A:HIS:CE1 | 3        | 0.3           |
| (1,332) | 3:18:A:TYR:CE2 | 3:27:A:HIS:CD2 | 5        | 0.3           |
| (1,279) | 3:8:A:MET:CB   | 3:16:A:LYS:CA  | 12       | 0.3           |
| (1,279) | 3:8:A:MET:CB   | 3:16:A:LYS:CA  | 14       | 0.3           |
| (1,279) | 3:8:A:MET:CB   | 3:16:A:LYS:CA  | 15       | 0.3           |
| (1,11)  | 3:8:A:MET:HA   | 3:16:A:LYS:H   | 3        | 0.3           |
| (1,9)   | 3:17:A:ARG:HA  | 3:9:A:CYS:H    | 6        | 0.3           |
| (2,121) | 3:89:A:HIS:N   | 3:86:A:THR:O   | 17       | 0.29          |
| (2,121) | 3:89:A:HIS:N   | 3:86:A:THR:O   | 18       | 0.29          |
| (2,116) | 3:84:A:THR:N   | 3:80:A:ASP:O   | 8        | 0.29          |
| (2,116) | 3:84:A:THR:N   | 3:80:A:ASP:O   | 19       | 0.29          |
| (2,108) | 3:59:A:ARG:N   | 3:56:A:ARG:O   | 14       | 0.29          |
| (2,103) | 3:54:A:LEU:N   | 3:50:A:ARG:O   | 10       | 0.29          |
| (2,98)  | 3:30:A:LYS:N   | 3:27:A:HIS:O   | 16       | 0.29          |
| (2,98)  | 3:30:A:LYS:N   | 3:27:A:HIS:O   | 20       | 0.29          |
| (2,97)  | 3:29:A:ARG:N   | 3:26:A:MET:O   | 3        | 0.29          |
| (2,97)  | 3:29:A:ARG:N   | 3:26:A:MET:O   | 7        | 0.29          |
| (2,97)  | 3:29:A:ARG:N   | 3:26:A:MET:O   | 20       | 0.29          |
| (2,95)  | 3:27:A:HIS:N   | 3:23:A:HIS:O   | 9        | 0.29          |
| (2,92)  | 3:24:A:LEU:N   | 3:20:A:LYS:O   | 16       | 0.29          |
| (1,476) | 3:67:A:PHE:CD2 | 3:79:A:SER:CA  | 10       | 0.29          |
| (1,380) | 3:37:A:TYR:CD2 | 3:54:A:LEU:CB  | 17       | 0.29          |
| (1,351) | 3:22:A:SER:CA  | 3:24:A:LEU:CA  | 3        | 0.29          |
| (1,351) | 3:22:A:SER:CA  | 3:24:A:LEU:CA  | 5        | 0.29          |
| (1,351) | 3:22:A:SER:CA  | 3:24:A:LEU:CA  | 8        | 0.29          |
| (1,351) | 3:22:A:SER:CA  | 3:24:A:LEU:CA  | 11       | 0.29          |
| (1,351) | 3:22:A:SER:CA  | 3:24:A:LEU:CA  | 14       | 0.29          |
| (1,279) | 3:8:A:MET:CB   | 3:16:A:LYS:CA  | 2        | 0.29          |
| (1,279) | 3:8:A:MET:CB   | 3:16:A:LYS:CA  | 5        | 0.29          |
| (1,279) | 3:8:A:MET:CB   | 3:16:A:LYS:CA  | 13       | 0.29          |
| (1,279) | 3:8:A:MET:CB   | 3:16:A:LYS:CA  | 19       | 0.29          |
| (1,267) | 3:7:A:PHE:CD1  | 3:24:A:LEU:CD1 | 5        | 0.29          |

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| Key     | Atom-1         | Atom-2        | Model ID | Violation (Å) |
|---------|----------------|---------------|----------|---------------|
| (2,132) | 3:119:A:HIS:N  | 3:116:A:HIS:O | 7        | 0.28          |
| (2,119) | 3:87:A:ARG:N   | 3:84:A:THR:O  | 14       | 0.28          |
| (2,116) | 3:84:A:THR:N   | 3:80:A:ASP:O  | 7        | 0.28          |
| (2,114) | 3:82:A:LEU:N   | 3:78:A:ARG:O  | 12       | 0.28          |
| (2,114) | 3:82:A:LEU:N   | 3:78:A:ARG:O  | 19       | 0.28          |
| (2,108) | 3:59:A:ARG:N   | 3:56:A:ARG:O  | 6        | 0.28          |
| (2,108) | 3:59:A:ARG:N   | 3:56:A:ARG:O  | 13       | 0.28          |
| (2,99)  | 3:31:A:HIS:N   | 3:28:A:SER:O  | 17       | 0.28          |
| (2,97)  | 3:29:A:ARG:N   | 3:26:A:MET:O  | 15       | 0.28          |
| (2,96)  | 3:28:A:SER:N   | 3:24:A:LEU:O  | 6        | 0.28          |
| (1,351) | 3:22:A:SER:CA  | 3:24:A:LEU:CA | 1        | 0.28          |
| (1,351) | 3:22:A:SER:CA  | 3:24:A:LEU:CA | 6        | 0.28          |
| (1,351) | 3:22:A:SER:CA  | 3:24:A:LEU:CA | 12       | 0.28          |
| (1,14)  | 3:21:A:LEU:H   | 3:22:A:SER:H  | 7        | 0.28          |
| (2,132) | 3:119:A:HIS:N  | 3:116:A:HIS:O | 19       | 0.27          |
| (2,126) | 3:113:A:VAL:N  | 3:109:A:SER:O | 3        | 0.27          |
| (2,126) | 3:113:A:VAL:N  | 3:109:A:SER:O | 14       | 0.27          |
| (2,121) | 3:89:A:HIS:N   | 3:86:A:THR:O  | 1        | 0.27          |
| (2,121) | 3:89:A:HIS:N   | 3:86:A:THR:O  | 7        | 0.27          |
| (2,121) | 3:89:A:HIS:N   | 3:86:A:THR:O  | 8        | 0.27          |
| (2,121) | 3:89:A:HIS:N   | 3:86:A:THR:O  | 12       | 0.27          |
| (2,119) | 3:87:A:ARG:N   | 3:84:A:THR:O  | 7        | 0.27          |
| (2,114) | 3:82:A:LEU:N   | 3:78:A:ARG:O  | 8        | 0.27          |
| (2,112) | 3:69:A:CYS:N   | 3:74:A:ARG:O  | 7        | 0.27          |
| (2,112) | 3:69:A:CYS:N   | 3:74:A:ARG:O  | 15       | 0.27          |
| (2,112) | 3:69:A:CYS:N   | 3:74:A:ARG:O  | 17       | 0.27          |
| (2,98)  | 3:30:A:LYS:N   | 3:27:A:HIS:O  | 5        | 0.27          |
| (2,98)  | 3:30:A:LYS:N   | 3:27:A:HIS:O  | 6        | 0.27          |
| (2,94)  | 3:26:A:MET:N   | 3:22:A:SER:O  | 17       | 0.27          |
| (1,476) | 3:67:A:PHE:CD2 | 3:79:A:SER:CA | 5        | 0.27          |
| (1,474) | 3:67:A:PHE:CE2 | 3:79:A:SER:CA | 14       | 0.27          |
| (1,376) | 3:37:A:TYR:CE2 | 3:51:A:SER:CB | 18       | 0.27          |
| (1,351) | 3:22:A:SER:CA  | 3:24:A:LEU:CA | 10       | 0.27          |
| (1,347) | 3:20:A:LYS:CB  | 3:23:A:HIS:CB | 4        | 0.27          |
| (1,9)   | 3:17:A:ARG:HA  | 3:9:A:CYS:H   | 8        | 0.27          |
| (2,130) | 3:117:A:ASN:N  | 3:114:A:ARG:O | 3        | 0.26          |
| (2,121) | 3:89:A:HIS:N   | 3:86:A:THR:O  | 2        | 0.26          |
| (2,116) | 3:84:A:THR:N   | 3:80:A:ASP:O  | 18       | 0.26          |
| (2,110) | 3:61:A:HIS:N   | 3:58:A:GLN:O  | 18       | 0.26          |
| (2,109) | 3:60:A:ARG:N   | 3:57:A:HIS:O  | 3        | 0.26          |
| (2,108) | 3:59:A:ARG:N   | 3:56:A:ARG:O  | 4        | 0.26          |
| (2,108) | 3:59:A:ARG:N   | 3:56:A:ARG:O  | 17       | 0.26          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (2,98)  | 3:30:A:LYS:N    | 3:27:A:HIS:O    | 3        | 0.26          |
| (2,98)  | 3:30:A:LYS:N    | 3:27:A:HIS:O    | 4        | 0.26          |
| (2,94)  | 3:26:A:MET:N    | 3:22:A:SER:O    | 7        | 0.26          |
| (2,92)  | 3:24:A:LEU:N    | 3:20:A:LYS:O    | 18       | 0.26          |
| (2,61)  | 3:87:A:ARG:H    | 3:84:A:THR:O    | 18       | 0.26          |
| (1,707) | 1:129:B:DG:C5'  | 3:60:A:ARG:CZ   | 5        | 0.26          |
| (1,474) | 3:67:A:PHE:CE2  | 3:79:A:SER:CA   | 4        | 0.26          |
| (1,279) | 3:8:A:MET:CB    | 3:16:A:LYS:CA   | 18       | 0.26          |
| (1,210) | 3:107:A:ALA:HA  | 3:95:A:PHE:H    | 4        | 0.26          |
| (1,210) | 3:107:A:ALA:HA  | 3:95:A:PHE:H    | 10       | 0.26          |
| (1,210) | 3:107:A:ALA:HA  | 3:95:A:PHE:H    | 14       | 0.26          |
| (1,143) | 3:68:A:GLN:HA   | 3:74:A:ARG:H    | 4        | 0.26          |
| (1,9)   | 3:17:A:ARG:HA   | 3:9:A:CYS:H     | 4        | 0.26          |
| (2,132) | 3:119:A:HIS:N   | 3:116:A:HIS:O   | 3        | 0.25          |
| (2,126) | 3:113:A:VAL:N   | 3:109:A:SER:O   | 10       | 0.25          |
| (2,121) | 3:89:A:HIS:N    | 3:86:A:THR:O    | 14       | 0.25          |
| (2,112) | 3:69:A:CYS:N    | 3:74:A:ARG:O    | 2        | 0.25          |
| (2,109) | 3:60:A:ARG:N    | 3:57:A:HIS:O    | 18       | 0.25          |
| (2,103) | 3:54:A:LEU:N    | 3:50:A:ARG:O    | 2        | 0.25          |
| (2,99)  | 3:31:A:HIS:N    | 3:28:A:SER:O    | 14       | 0.25          |
| (2,99)  | 3:31:A:HIS:N    | 3:28:A:SER:O    | 18       | 0.25          |
| (2,98)  | 3:30:A:LYS:N    | 3:27:A:HIS:O    | 9        | 0.25          |
| (2,98)  | 3:30:A:LYS:N    | 3:27:A:HIS:O    | 13       | 0.25          |
| (2,97)  | 3:29:A:ARG:N    | 3:26:A:MET:O    | 9        | 0.25          |
| (2,92)  | 3:24:A:LEU:N    | 3:20:A:LYS:O    | 10       | 0.25          |
| (2,17)  | 3:29:A:ARG:H    | 3:26:A:MET:O    | 2        | 0.25          |
| (1,709) | 1:129:B:DG:C4'  | 3:60:A:ARG:CD   | 5        | 0.25          |
| (1,707) | 1:129:B:DG:C5'  | 3:60:A:ARG:CZ   | 11       | 0.25          |
| (1,694) | 1:128:B:DG:C5   | 3:81:A:HIS:CD2  | 5        | 0.25          |
| (1,652) | 3:115:A:HIS:CD2 | 3:119:A:HIS:CE1 | 1        | 0.25          |
| (1,351) | 3:22:A:SER:CA   | 3:24:A:LEU:CA   | 4        | 0.25          |
| (1,347) | 3:20:A:LYS:CB   | 3:23:A:HIS:CB   | 3        | 0.25          |
| (1,347) | 3:20:A:LYS:CB   | 3:23:A:HIS:CB   | 5        | 0.25          |
| (1,347) | 3:20:A:LYS:CB   | 3:23:A:HIS:CB   | 18       | 0.25          |
| (1,333) | 3:18:A:TYR:CE2  | 3:27:A:HIS:CE1  | 5        | 0.25          |
| (1,332) | 3:18:A:TYR:CE2  | 3:27:A:HIS:CD2  | 6        | 0.25          |
| (1,327) | 3:18:A:TYR:CE1  | 3:27:A:HIS:CB   | 1        | 0.25          |
| (1,299) | 3:11:A:TYR:CE1  | 3:34:A:GLU:CA   | 19       | 0.25          |
| (1,210) | 3:107:A:ALA:HA  | 3:95:A:PHE:H    | 17       | 0.25          |
| (1,9)   | 3:17:A:ARG:HA   | 3:9:A:CYS:H     | 7        | 0.25          |
| (1,9)   | 3:17:A:ARG:HA   | 3:9:A:CYS:H     | 12       | 0.25          |
| (2,126) | 3:113:A:VAL:N   | 3:109:A:SER:O   | 2        | 0.24          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (2,126) | 3:113:A:VAL:N   | 3:109:A:SER:O   | 6        | 0.24          |
| (2,126) | 3:113:A:VAL:N   | 3:109:A:SER:O   | 20       | 0.24          |
| (2,119) | 3:87:A:ARG:N    | 3:84:A:THR:O    | 9        | 0.24          |
| (2,110) | 3:61:A:HIS:N    | 3:58:A:GLN:O    | 2        | 0.24          |
| (2,109) | 3:60:A:ARG:N    | 3:57:A:HIS:O    | 16       | 0.24          |
| (2,108) | 3:59:A:ARG:N    | 3:56:A:ARG:O    | 8        | 0.24          |
| (2,108) | 3:59:A:ARG:N    | 3:56:A:ARG:O    | 9        | 0.24          |
| (2,97)  | 3:29:A:ARG:N    | 3:26:A:MET:O    | 6        | 0.24          |
| (2,95)  | 3:27:A:HIS:N    | 3:23:A:HIS:O    | 13       | 0.24          |
| (2,61)  | 3:87:A:ARG:H    | 3:84:A:THR:O    | 7        | 0.24          |
| (1,694) | 1:128:B:DG:C5   | 3:81:A:HIS:CD2  | 11       | 0.24          |
| (1,652) | 3:115:A:HIS:CD2 | 3:119:A:HIS:CE1 | 4        | 0.24          |
| (1,476) | 3:67:A:PHE:CD2  | 3:79:A:SER:CA   | 4        | 0.24          |
| (1,465) | 3:67:A:PHE:CB   | 3:82:A:LEU:CD1  | 13       | 0.24          |
| (1,465) | 3:67:A:PHE:CB   | 3:82:A:LEU:CD1  | 18       | 0.24          |
| (1,388) | 3:39:A:CYS:CB   | 3:41:A:PHE:CB   | 9        | 0.24          |
| (1,380) | 3:37:A:TYR:CD2  | 3:54:A:LEU:CB   | 11       | 0.24          |
| (1,347) | 3:20:A:LYS:CB   | 3:23:A:HIS:CB   | 12       | 0.24          |
| (1,347) | 3:20:A:LYS:CB   | 3:23:A:HIS:CB   | 17       | 0.24          |
| (1,347) | 3:20:A:LYS:CB   | 3:23:A:HIS:CB   | 20       | 0.24          |
| (1,332) | 3:18:A:TYR:CE2  | 3:27:A:HIS:CD2  | 12       | 0.24          |
| (1,327) | 3:18:A:TYR:CE1  | 3:27:A:HIS:CB   | 4        | 0.24          |
| (1,210) | 3:107:A:ALA:HA  | 3:95:A:PHE:H    | 3        | 0.24          |
| (1,210) | 3:107:A:ALA:HA  | 3:95:A:PHE:H    | 18       | 0.24          |
| (1,143) | 3:68:A:GLN:HA   | 3:74:A:ARG:H    | 6        | 0.24          |
| (1,77)  | 3:38:A:GLN:HA   | 3:46:A:ARG:H    | 16       | 0.24          |
| (1,9)   | 3:17:A:ARG:HA   | 3:9:A:CYS:H     | 2        | 0.24          |
| (1,9)   | 3:17:A:ARG:HA   | 3:9:A:CYS:H     | 5        | 0.24          |
| (1,9)   | 3:17:A:ARG:HA   | 3:9:A:CYS:H     | 14       | 0.24          |
| (2,129) | 3:116:A:HIS:N   | 3:112:A:LEU:O   | 8        | 0.23          |
| (2,126) | 3:113:A:VAL:N   | 3:109:A:SER:O   | 1        | 0.23          |
| (2,121) | 3:89:A:HIS:N    | 3:86:A:THR:O    | 9        | 0.23          |
| (2,121) | 3:89:A:HIS:N    | 3:86:A:THR:O    | 20       | 0.23          |
| (2,116) | 3:84:A:THR:N    | 3:80:A:ASP:O    | 10       | 0.23          |
| (2,114) | 3:82:A:LEU:N    | 3:78:A:ARG:O    | 3        | 0.23          |
| (2,109) | 3:60:A:ARG:N    | 3:57:A:HIS:O    | 13       | 0.23          |
| (2,99)  | 3:31:A:HIS:N    | 3:28:A:SER:O    | 4        | 0.23          |
| (2,98)  | 3:30:A:LYS:N    | 3:27:A:HIS:O    | 14       | 0.23          |
| (2,83)  | 3:117:A:ASN:H   | 3:114:A:ARG:O   | 3        | 0.23          |
| (2,17)  | 3:29:A:ARG:H    | 3:26:A:MET:O    | 1        | 0.23          |
| (1,715) | 1:129:B:DG:C2'  | 3:78:A:ARG:CZ   | 11       | 0.23          |
| (1,694) | 1:128:B:DG:C5   | 3:81:A:HIS:CD2  | 6        | 0.23          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,687) | 1:128:B:DG:C2'  | 3:81:A:HIS:CE1  | 5        | 0.23          |
| (1,652) | 3:115:A:HIS:CD2 | 3:119:A:HIS:CE1 | 12       | 0.23          |
| (1,652) | 3:115:A:HIS:CD2 | 3:119:A:HIS:CE1 | 15       | 0.23          |
| (1,465) | 3:67:A:PHE:CB   | 3:82:A:LEU:CD1  | 20       | 0.23          |
| (1,356) | 3:24:A:LEU:CD2  | 3:27:A:HIS:CB   | 5        | 0.23          |
| (1,351) | 3:22:A:SER:CA   | 3:24:A:LEU:CA   | 7        | 0.23          |
| (1,332) | 3:18:A:TYR:CE2  | 3:27:A:HIS:CD2  | 7        | 0.23          |
| (1,327) | 3:18:A:TYR:CE1  | 3:27:A:HIS:CB   | 14       | 0.23          |
| (1,210) | 3:107:A:ALA:HA  | 3:95:A:PHE:H    | 2        | 0.23          |
| (1,210) | 3:107:A:ALA:HA  | 3:95:A:PHE:H    | 8        | 0.23          |
| (1,210) | 3:107:A:ALA:HA  | 3:95:A:PHE:H    | 9        | 0.23          |
| (1,210) | 3:107:A:ALA:HA  | 3:95:A:PHE:H    | 13       | 0.23          |
| (1,210) | 3:107:A:ALA:HA  | 3:95:A:PHE:H    | 15       | 0.23          |
| (1,210) | 3:107:A:ALA:HA  | 3:95:A:PHE:H    | 19       | 0.23          |
| (1,11)  | 3:8:A:MET:HA    | 3:16:A:LYS:H    | 10       | 0.23          |
| (1,9)   | 3:17:A:ARG:HA   | 3:9:A:CYS:H     | 11       | 0.23          |
| (1,9)   | 3:17:A:ARG:HA   | 3:9:A:CYS:H     | 13       | 0.23          |
| (2,131) | 3:118:A:MET:N   | 3:115:A:HIS:O   | 5        | 0.22          |
| (2,131) | 3:118:A:MET:N   | 3:115:A:HIS:O   | 20       | 0.22          |
| (2,129) | 3:116:A:HIS:N   | 3:112:A:LEU:O   | 9        | 0.22          |
| (2,129) | 3:116:A:HIS:N   | 3:112:A:LEU:O   | 12       | 0.22          |
| (2,128) | 3:115:A:HIS:N   | 3:111:A:GLU:O   | 11       | 0.22          |
| (2,126) | 3:113:A:VAL:N   | 3:109:A:SER:O   | 9        | 0.22          |
| (2,126) | 3:113:A:VAL:N   | 3:109:A:SER:O   | 18       | 0.22          |
| (2,121) | 3:89:A:HIS:N    | 3:86:A:THR:O    | 4        | 0.22          |
| (2,120) | 3:88:A:THR:N    | 3:85:A:HIS:O    | 6        | 0.22          |
| (2,116) | 3:84:A:THR:N    | 3:80:A:ASP:O    | 1        | 0.22          |
| (2,116) | 3:84:A:THR:N    | 3:80:A:ASP:O    | 2        | 0.22          |
| (2,116) | 3:84:A:THR:N    | 3:80:A:ASP:O    | 3        | 0.22          |
| (2,116) | 3:84:A:THR:N    | 3:80:A:ASP:O    | 5        | 0.22          |
| (2,116) | 3:84:A:THR:N    | 3:80:A:ASP:O    | 6        | 0.22          |
| (2,112) | 3:69:A:CYS:N    | 3:74:A:ARG:O    | 13       | 0.22          |
| (2,110) | 3:61:A:HIS:N    | 3:58:A:GLN:O    | 15       | 0.22          |
| (2,109) | 3:60:A:ARG:N    | 3:57:A:HIS:O    | 12       | 0.22          |
| (2,109) | 3:60:A:ARG:N    | 3:57:A:HIS:O    | 19       | 0.22          |
| (2,108) | 3:59:A:ARG:N    | 3:56:A:ARG:O    | 1        | 0.22          |
| (2,107) | 3:58:A:GLN:N    | 3:54:A:LEU:O    | 4        | 0.22          |
| (2,107) | 3:58:A:GLN:N    | 3:54:A:LEU:O    | 17       | 0.22          |
| (2,106) | 3:57:A:HIS:N    | 3:53:A:GLN:O    | 6        | 0.22          |
| (2,106) | 3:57:A:HIS:N    | 3:53:A:GLN:O    | 20       | 0.22          |
| (2,98)  | 3:30:A:LYS:N    | 3:27:A:HIS:O    | 7        | 0.22          |
| (2,98)  | 3:30:A:LYS:N    | 3:27:A:HIS:O    | 8        | 0.22          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (2,98)  | 3:30:A:LYS:N    | 3:27:A:HIS:O    | 17       | 0.22          |
| (2,97)  | 3:29:A:ARG:N    | 3:26:A:MET:O    | 4        | 0.22          |
| (2,97)  | 3:29:A:ARG:N    | 3:26:A:MET:O    | 18       | 0.22          |
| (2,95)  | 3:27:A:HIS:N    | 3:23:A:HIS:O    | 4        | 0.22          |
| (2,94)  | 3:26:A:MET:N    | 3:22:A:SER:O    | 10       | 0.22          |
| (2,83)  | 3:117:A:ASN:H   | 3:114:A:ARG:O   | 12       | 0.22          |
| (2,39)  | 3:59:A:ARG:H    | 3:56:A:ARG:O    | 3        | 0.22          |
| (1,739) | 1:133:B:DG:C6   | 3:50:A:ARG:CZ   | 15       | 0.22          |
| (1,709) | 1:129:B:DG:C4'  | 3:60:A:ARG:CD   | 11       | 0.22          |
| (1,694) | 1:128:B:DG:C5   | 3:81:A:HIS:CD2  | 8        | 0.22          |
| (1,687) | 1:128:B:DG:C2'  | 3:81:A:HIS:CE1  | 11       | 0.22          |
| (1,652) | 3:115:A:HIS:CD2 | 3:119:A:HIS:CE1 | 9        | 0.22          |
| (1,652) | 3:115:A:HIS:CD2 | 3:119:A:HIS:CE1 | 11       | 0.22          |
| (1,652) | 3:115:A:HIS:CD2 | 3:119:A:HIS:CE1 | 17       | 0.22          |
| (1,537) | 3:87:A:ARG:CB   | 3:90:A:THR:CB   | 15       | 0.22          |
| (1,465) | 3:67:A:PHE:CB   | 3:82:A:LEU:CD1  | 1        | 0.22          |
| (1,465) | 3:67:A:PHE:CB   | 3:82:A:LEU:CD1  | 9        | 0.22          |
| (1,465) | 3:67:A:PHE:CB   | 3:82:A:LEU:CD1  | 19       | 0.22          |
| (1,388) | 3:39:A:CYS:CB   | 3:41:A:PHE:CB   | 18       | 0.22          |
| (1,347) | 3:20:A:LYS:CB   | 3:23:A:HIS:CB   | 1        | 0.22          |
| (1,347) | 3:20:A:LYS:CB   | 3:23:A:HIS:CB   | 8        | 0.22          |
| (1,327) | 3:18:A:TYR:CE1  | 3:27:A:HIS:CB   | 6        | 0.22          |
| (1,327) | 3:18:A:TYR:CE1  | 3:27:A:HIS:CB   | 9        | 0.22          |
| (1,210) | 3:107:A:ALA:HA  | 3:95:A:PHE:H    | 11       | 0.22          |
| (1,210) | 3:107:A:ALA:HA  | 3:95:A:PHE:H    | 12       | 0.22          |
| (1,143) | 3:68:A:GLN:HA   | 3:74:A:ARG:H    | 7        | 0.22          |
| (1,77)  | 3:38:A:GLN:HA   | 3:46:A:ARG:H    | 1        | 0.22          |
| (1,77)  | 3:38:A:GLN:HA   | 3:46:A:ARG:H    | 13       | 0.22          |
| (1,11)  | 3:8:A:MET:HA    | 3:16:A:LYS:H    | 7        | 0.22          |
| (1,9)   | 3:17:A:ARG:HA   | 3:9:A:CYS:H     | 3        | 0.22          |
| (2,132) | 3:119:A:HIS:N   | 3:116:A:HIS:O   | 6        | 0.21          |
| (2,131) | 3:118:A:MET:N   | 3:115:A:HIS:O   | 2        | 0.21          |
| (2,131) | 3:118:A:MET:N   | 3:115:A:HIS:O   | 4        | 0.21          |
| (2,131) | 3:118:A:MET:N   | 3:115:A:HIS:O   | 11       | 0.21          |
| (2,131) | 3:118:A:MET:N   | 3:115:A:HIS:O   | 12       | 0.21          |
| (2,131) | 3:118:A:MET:N   | 3:115:A:HIS:O   | 13       | 0.21          |
| (2,131) | 3:118:A:MET:N   | 3:115:A:HIS:O   | 17       | 0.21          |
| (2,130) | 3:117:A:ASN:N   | 3:114:A:ARG:O   | 6        | 0.21          |
| (2,130) | 3:117:A:ASN:N   | 3:114:A:ARG:O   | 10       | 0.21          |
| (2,129) | 3:116:A:HIS:N   | 3:112:A:LEU:O   | 4        | 0.21          |
| (2,126) | 3:113:A:VAL:N   | 3:109:A:SER:O   | 7        | 0.21          |
| (2,126) | 3:113:A:VAL:N   | 3:109:A:SER:O   | 15       | 0.21          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (2,126) | 3:113:A:VAL:N   | 3:109:A:SER:O   | 19       | 0.21          |
| (2,121) | 3:89:A:HIS:N    | 3:86:A:THR:O    | 11       | 0.21          |
| (2,121) | 3:89:A:HIS:N    | 3:86:A:THR:O    | 16       | 0.21          |
| (2,120) | 3:88:A:THR:N    | 3:85:A:HIS:O    | 3        | 0.21          |
| (2,116) | 3:84:A:THR:N    | 3:80:A:ASP:O    | 11       | 0.21          |
| (2,116) | 3:84:A:THR:N    | 3:80:A:ASP:O    | 20       | 0.21          |
| (2,114) | 3:82:A:LEU:N    | 3:78:A:ARG:O    | 4        | 0.21          |
| (2,109) | 3:60:A:ARG:N    | 3:57:A:HIS:O    | 1        | 0.21          |
| (2,106) | 3:57:A:HIS:N    | 3:53:A:GLN:O    | 11       | 0.21          |
| (2,99)  | 3:31:A:HIS:N    | 3:28:A:SER:O    | 2        | 0.21          |
| (2,99)  | 3:31:A:HIS:N    | 3:28:A:SER:O    | 16       | 0.21          |
| (2,98)  | 3:30:A:LYS:N    | 3:27:A:HIS:O    | 1        | 0.21          |
| (2,97)  | 3:29:A:ARG:N    | 3:26:A:MET:O    | 8        | 0.21          |
| (2,97)  | 3:29:A:ARG:N    | 3:26:A:MET:O    | 14       | 0.21          |
| (2,96)  | 3:28:A:SER:N    | 3:24:A:LEU:O    | 17       | 0.21          |
| (2,94)  | 3:26:A:MET:N    | 3:22:A:SER:O    | 2        | 0.21          |
| (2,83)  | 3:117:A:ASN:H   | 3:114:A:ARG:O   | 4        | 0.21          |
| (2,83)  | 3:117:A:ASN:H   | 3:114:A:ARG:O   | 5        | 0.21          |
| (2,83)  | 3:117:A:ASN:H   | 3:114:A:ARG:O   | 8        | 0.21          |
| (2,83)  | 3:117:A:ASN:H   | 3:114:A:ARG:O   | 9        | 0.21          |
| (2,83)  | 3:117:A:ASN:H   | 3:114:A:ARG:O   | 14       | 0.21          |
| (2,61)  | 3:87:A:ARG:H    | 3:84:A:THR:O    | 11       | 0.21          |
| (2,17)  | 3:29:A:ARG:H    | 3:26:A:MET:O    | 13       | 0.21          |
| (1,694) | 1:128:B:DG:C5   | 3:81:A:HIS:CD2  | 1        | 0.21          |
| (1,694) | 1:128:B:DG:C5   | 3:81:A:HIS:CD2  | 7        | 0.21          |
| (1,694) | 1:128:B:DG:C5   | 3:81:A:HIS:CD2  | 13       | 0.21          |
| (1,687) | 1:128:B:DG:C2'  | 3:81:A:HIS:CE1  | 1        | 0.21          |
| (1,687) | 1:128:B:DG:C2'  | 3:81:A:HIS:CE1  | 10       | 0.21          |
| (1,652) | 3:115:A:HIS:CD2 | 3:119:A:HIS:CE1 | 2        | 0.21          |
| (1,652) | 3:115:A:HIS:CD2 | 3:119:A:HIS:CE1 | 5        | 0.21          |
| (1,537) | 3:87:A:ARG:CB   | 3:90:A:THR:CB   | 6        | 0.21          |
| (1,498) | 3:72:A:CYS:CB   | 3:89:A:HIS:CE1  | 1        | 0.21          |
| (1,379) | 3:37:A:TYR:CD2  | 3:51:A:SER:CB   | 9        | 0.21          |
| (1,351) | 3:22:A:SER:CA   | 3:24:A:LEU:CA   | 19       | 0.21          |
| (1,347) | 3:20:A:LYS:CB   | 3:23:A:HIS:CB   | 10       | 0.21          |
| (1,347) | 3:20:A:LYS:CB   | 3:23:A:HIS:CB   | 11       | 0.21          |
| (1,327) | 3:18:A:TYR:CE1  | 3:27:A:HIS:CB   | 13       | 0.21          |
| (1,319) | 3:18:A:TYR:CD1  | 3:24:A:LEU:CB   | 13       | 0.21          |
| (1,299) | 3:11:A:TYR:CE1  | 3:34:A:GLU:CA   | 17       | 0.21          |
| (1,274) | 3:7:A:PHE:CD2   | 3:20:A:LYS:CA   | 5        | 0.21          |
| (1,210) | 3:107:A:ALA:HA  | 3:95:A:PHE:H    | 1        | 0.21          |
| (1,210) | 3:107:A:ALA:HA  | 3:95:A:PHE:H    | 6        | 0.21          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,143) | 3:68:A:GLN:HA   | 3:74:A:ARG:H    | 13       | 0.21          |
| (1,77)  | 3:38:A:GLN:HA   | 3:46:A:ARG:H    | 18       | 0.21          |
| (1,76)  | 3:49:A:SER:HA   | 3:37:A:TYR:H    | 5        | 0.21          |
| (1,76)  | 3:49:A:SER:HA   | 3:37:A:TYR:H    | 10       | 0.21          |
| (1,9)   | 3:17:A:ARG:HA   | 3:9:A:CYS:H     | 1        | 0.21          |
| (1,9)   | 3:17:A:ARG:HA   | 3:9:A:CYS:H     | 20       | 0.21          |
| (2,131) | 3:118:A:MET:N   | 3:115:A:HIS:O   | 1        | 0.2           |
| (2,131) | 3:118:A:MET:N   | 3:115:A:HIS:O   | 10       | 0.2           |
| (2,131) | 3:118:A:MET:N   | 3:115:A:HIS:O   | 14       | 0.2           |
| (2,131) | 3:118:A:MET:N   | 3:115:A:HIS:O   | 15       | 0.2           |
| (2,126) | 3:113:A:VAL:N   | 3:109:A:SER:O   | 12       | 0.2           |
| (2,121) | 3:89:A:HIS:N    | 3:86:A:THR:O    | 6        | 0.2           |
| (2,120) | 3:88:A:THR:N    | 3:85:A:HIS:O    | 14       | 0.2           |
| (2,110) | 3:61:A:HIS:N    | 3:58:A:GLN:O    | 1        | 0.2           |
| (2,109) | 3:60:A:ARG:N    | 3:57:A:HIS:O    | 8        | 0.2           |
| (2,109) | 3:60:A:ARG:N    | 3:57:A:HIS:O    | 14       | 0.2           |
| (2,109) | 3:60:A:ARG:N    | 3:57:A:HIS:O    | 15       | 0.2           |
| (2,108) | 3:59:A:ARG:N    | 3:56:A:ARG:O    | 3        | 0.2           |
| (2,95)  | 3:27:A:HIS:N    | 3:23:A:HIS:O    | 1        | 0.2           |
| (2,95)  | 3:27:A:HIS:N    | 3:23:A:HIS:O    | 8        | 0.2           |
| (2,95)  | 3:27:A:HIS:N    | 3:23:A:HIS:O    | 14       | 0.2           |
| (2,90)  | 3:9:A:CYS:N     | 3:16:A:LYS:O    | 15       | 0.2           |
| (2,83)  | 3:117:A:ASN:H   | 3:114:A:ARG:O   | 2        | 0.2           |
| (2,83)  | 3:117:A:ASN:H   | 3:114:A:ARG:O   | 11       | 0.2           |
| (2,83)  | 3:117:A:ASN:H   | 3:114:A:ARG:O   | 13       | 0.2           |
| (2,83)  | 3:117:A:ASN:H   | 3:114:A:ARG:O   | 15       | 0.2           |
| (2,83)  | 3:117:A:ASN:H   | 3:114:A:ARG:O   | 16       | 0.2           |
| (2,83)  | 3:117:A:ASN:H   | 3:114:A:ARG:O   | 17       | 0.2           |
| (2,61)  | 3:87:A:ARG:H    | 3:84:A:THR:O    | 8        | 0.2           |
| (2,61)  | 3:87:A:ARG:H    | 3:84:A:THR:O    | 9        | 0.2           |
| (1,694) | 1:128:B:DG:C5   | 3:81:A:HIS:CD2  | 2        | 0.2           |
| (1,687) | 1:128:B:DG:C2'  | 3:81:A:HIS:CE1  | 2        | 0.2           |
| (1,687) | 1:128:B:DG:C2'  | 3:81:A:HIS:CE1  | 6        | 0.2           |
| (1,687) | 1:128:B:DG:C2'  | 3:81:A:HIS:CE1  | 7        | 0.2           |
| (1,687) | 1:128:B:DG:C2'  | 3:81:A:HIS:CE1  | 8        | 0.2           |
| (1,687) | 1:128:B:DG:C2'  | 3:81:A:HIS:CE1  | 15       | 0.2           |
| (1,687) | 1:128:B:DG:C2'  | 3:81:A:HIS:CE1  | 18       | 0.2           |
| (1,652) | 3:115:A:HIS:CD2 | 3:119:A:HIS:CE1 | 8        | 0.2           |
| (1,652) | 3:115:A:HIS:CD2 | 3:119:A:HIS:CE1 | 16       | 0.2           |
| (1,484) | 3:69:A:CYS:CA   | 3:74:A:ARG:CA   | 4        | 0.2           |
| (1,476) | 3:67:A:PHE:CD2  | 3:79:A:SER:CA   | 12       | 0.2           |
| (1,465) | 3:67:A:PHE:CB   | 3:82:A:LEU:CD1  | 2        | 0.2           |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,465) | 3:67:A:PHE:CB  | 3:82:A:LEU:CD1 | 15       | 0.2           |
| (1,408) | 3:41:A:PHE:CD2 | 3:44:A:CYS:CA  | 11       | 0.2           |
| (1,347) | 3:20:A:LYS:CB  | 3:23:A:HIS:CB  | 19       | 0.2           |
| (1,333) | 3:18:A:TYR:CE2 | 3:27:A:HIS:CE1 | 17       | 0.2           |
| (1,333) | 3:18:A:TYR:CE2 | 3:27:A:HIS:CE1 | 19       | 0.2           |
| (1,327) | 3:18:A:TYR:CE1 | 3:27:A:HIS:CB  | 2        | 0.2           |
| (1,308) | 3:11:A:TYR:CD2 | 3:34:A:GLU:CB  | 7        | 0.2           |
| (1,210) | 3:107:A:ALA:HA | 3:95:A:PHE:H   | 16       | 0.2           |
| (1,210) | 3:107:A:ALA:HA | 3:95:A:PHE:H   | 20       | 0.2           |
| (1,142) | 3:77:A:SER:HA  | 3:67:A:PHE:H   | 4        | 0.2           |
| (1,77)  | 3:38:A:GLN:HA  | 3:46:A:ARG:H   | 7        | 0.2           |
| (1,77)  | 3:38:A:GLN:HA  | 3:46:A:ARG:H   | 12       | 0.2           |
| (1,75)  | 3:47:A:ARG:HA  | 3:39:A:CYS:H   | 12       | 0.2           |
| (2,132) | 3:119:A:HIS:N  | 3:116:A:HIS:O  | 18       | 0.19          |
| (2,131) | 3:118:A:MET:N  | 3:115:A:HIS:O  | 8        | 0.19          |
| (2,131) | 3:118:A:MET:N  | 3:115:A:HIS:O  | 9        | 0.19          |
| (2,131) | 3:118:A:MET:N  | 3:115:A:HIS:O  | 16       | 0.19          |
| (2,130) | 3:117:A:ASN:N  | 3:114:A:ARG:O  | 9        | 0.19          |
| (2,130) | 3:117:A:ASN:N  | 3:114:A:ARG:O  | 14       | 0.19          |
| (2,129) | 3:116:A:HIS:N  | 3:112:A:LEU:O  | 3        | 0.19          |
| (2,129) | 3:116:A:HIS:N  | 3:112:A:LEU:O  | 11       | 0.19          |
| (2,129) | 3:116:A:HIS:N  | 3:112:A:LEU:O  | 16       | 0.19          |
| (2,128) | 3:115:A:HIS:N  | 3:111:A:GLU:O  | 6        | 0.19          |
| (2,128) | 3:115:A:HIS:N  | 3:111:A:GLU:O  | 10       | 0.19          |
| (2,121) | 3:89:A:HIS:N   | 3:86:A:THR:O   | 5        | 0.19          |
| (2,120) | 3:88:A:THR:N   | 3:85:A:HIS:O   | 1        | 0.19          |
| (2,120) | 3:88:A:THR:N   | 3:85:A:HIS:O   | 10       | 0.19          |
| (2,116) | 3:84:A:THR:N   | 3:80:A:ASP:O   | 9        | 0.19          |
| (2,116) | 3:84:A:THR:N   | 3:80:A:ASP:O   | 13       | 0.19          |
| (2,110) | 3:61:A:HIS:N   | 3:58:A:GLN:O   | 14       | 0.19          |
| (2,109) | 3:60:A:ARG:N   | 3:57:A:HIS:O   | 11       | 0.19          |
| (2,107) | 3:58:A:GLN:N   | 3:54:A:LEU:O   | 8        | 0.19          |
| (2,96)  | 3:28:A:SER:N   | 3:24:A:LEU:O   | 14       | 0.19          |
| (2,95)  | 3:27:A:HIS:N   | 3:23:A:HIS:O   | 6        | 0.19          |
| (2,94)  | 3:26:A:MET:N   | 3:22:A:SER:O   | 18       | 0.19          |
| (2,92)  | 3:24:A:LEU:N   | 3:20:A:LYS:O   | 6        | 0.19          |
| (2,83)  | 3:117:A:ASN:H  | 3:114:A:ARG:O  | 1        | 0.19          |
| (2,83)  | 3:117:A:ASN:H  | 3:114:A:ARG:O  | 10       | 0.19          |
| (2,83)  | 3:117:A:ASN:H  | 3:114:A:ARG:O  | 20       | 0.19          |
| (2,65)  | 3:89:A:HIS:H   | 3:86:A:THR:O   | 7        | 0.19          |
| (2,63)  | 3:88:A:THR:H   | 3:85:A:HIS:O   | 16       | 0.19          |
| (2,61)  | 3:87:A:ARG:H   | 3:84:A:THR:O   | 5        | 0.19          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (2,61)  | 3:87:A:ARG:H    | 3:84:A:THR:O    | 10       | 0.19          |
| (2,61)  | 3:87:A:ARG:H    | 3:84:A:THR:O    | 20       | 0.19          |
| (2,39)  | 3:59:A:ARG:H    | 3:56:A:ARG:O    | 10       | 0.19          |
| (2,17)  | 3:29:A:ARG:H    | 3:26:A:MET:O    | 7        | 0.19          |
| (1,719) | 1:129:B:DG:C6   | 3:81:A:HIS:CE1  | 19       | 0.19          |
| (1,694) | 1:128:B:DG:C5   | 3:81:A:HIS:CD2  | 3        | 0.19          |
| (1,687) | 1:128:B:DG:C2'  | 3:81:A:HIS:CE1  | 3        | 0.19          |
| (1,687) | 1:128:B:DG:C2'  | 3:81:A:HIS:CE1  | 12       | 0.19          |
| (1,687) | 1:128:B:DG:C2'  | 3:81:A:HIS:CE1  | 13       | 0.19          |
| (1,652) | 3:115:A:HIS:CD2 | 3:119:A:HIS:CE1 | 20       | 0.19          |
| (1,577) | 3:97:A:CYS:CB   | 3:99:A:TRP:CB   | 9        | 0.19          |
| (1,535) | 3:87:A:ARG:CA   | 3:90:A:THR:CB   | 3        | 0.19          |
| (1,535) | 3:87:A:ARG:CA   | 3:90:A:THR:CB   | 6        | 0.19          |
| (1,474) | 3:67:A:PHE:CE2  | 3:79:A:SER:CA   | 5        | 0.19          |
| (1,380) | 3:37:A:TYR:CD2  | 3:54:A:LEU:CB   | 20       | 0.19          |
| (1,356) | 3:24:A:LEU:CD2  | 3:27:A:HIS:CB   | 12       | 0.19          |
| (1,347) | 3:20:A:LYS:CB   | 3:23:A:HIS:CB   | 7        | 0.19          |
| (1,319) | 3:18:A:TYR:CD1  | 3:24:A:LEU:CB   | 2        | 0.19          |
| (1,319) | 3:18:A:TYR:CD1  | 3:24:A:LEU:CB   | 4        | 0.19          |
| (1,300) | 3:11:A:TYR:CE1  | 3:34:A:GLU:CB   | 18       | 0.19          |
| (1,298) | 3:11:A:TYR:CE1  | 3:31:A:HIS:CB   | 17       | 0.19          |
| (1,271) | 3:7:A:PHE:CE2   | 3:20:A:LYS:CA   | 5        | 0.19          |
| (1,262) | 3:7:A:PHE:CB    | 3:18:A:TYR:CB   | 19       | 0.19          |
| (1,210) | 3:107:A:ALA:HA  | 3:95:A:PHE:H    | 5        | 0.19          |
| (1,142) | 3:77:A:SER:HA   | 3:67:A:PHE:H    | 1        | 0.19          |
| (1,142) | 3:77:A:SER:HA   | 3:67:A:PHE:H    | 3        | 0.19          |
| (1,142) | 3:77:A:SER:HA   | 3:67:A:PHE:H    | 5        | 0.19          |
| (1,142) | 3:77:A:SER:HA   | 3:67:A:PHE:H    | 9        | 0.19          |
| (1,142) | 3:77:A:SER:HA   | 3:67:A:PHE:H    | 12       | 0.19          |
| (1,142) | 3:77:A:SER:HA   | 3:67:A:PHE:H    | 13       | 0.19          |
| (1,77)  | 3:38:A:GLN:HA   | 3:46:A:ARG:H    | 3        | 0.19          |
| (1,77)  | 3:38:A:GLN:HA   | 3:46:A:ARG:H    | 4        | 0.19          |
| (1,77)  | 3:38:A:GLN:HA   | 3:46:A:ARG:H    | 6        | 0.19          |
| (1,77)  | 3:38:A:GLN:HA   | 3:46:A:ARG:H    | 10       | 0.19          |
| (1,77)  | 3:38:A:GLN:HA   | 3:46:A:ARG:H    | 20       | 0.19          |
| (1,76)  | 3:49:A:SER:HA   | 3:37:A:TYR:H    | 1        | 0.19          |
| (1,76)  | 3:49:A:SER:HA   | 3:37:A:TYR:H    | 4        | 0.19          |
| (1,11)  | 3:8:A:MET:HA    | 3:16:A:LYS:H    | 13       | 0.19          |
| (1,9)   | 3:17:A:ARG:HA   | 3:9:A:CYS:H     | 10       | 0.19          |
| (1,9)   | 3:17:A:ARG:HA   | 3:9:A:CYS:H     | 16       | 0.19          |
| (2,130) | 3:117:A:ASN:N   | 3:114:A:ARG:O   | 18       | 0.18          |
| (2,129) | 3:116:A:HIS:N   | 3:112:A:LEU:O   | 1        | 0.18          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (2,129) | 3:116:A:HIS:N   | 3:112:A:LEU:O   | 14       | 0.18          |
| (2,129) | 3:116:A:HIS:N   | 3:112:A:LEU:O   | 20       | 0.18          |
| (2,128) | 3:115:A:HIS:N   | 3:111:A:GLU:O   | 12       | 0.18          |
| (2,126) | 3:113:A:VAL:N   | 3:109:A:SER:O   | 5        | 0.18          |
| (2,126) | 3:113:A:VAL:N   | 3:109:A:SER:O   | 16       | 0.18          |
| (2,121) | 3:89:A:HIS:N    | 3:86:A:THR:O    | 3        | 0.18          |
| (2,120) | 3:88:A:THR:N    | 3:85:A:HIS:O    | 11       | 0.18          |
| (2,116) | 3:84:A:THR:N    | 3:80:A:ASP:O    | 4        | 0.18          |
| (2,116) | 3:84:A:THR:N    | 3:80:A:ASP:O    | 14       | 0.18          |
| (2,112) | 3:69:A:CYS:N    | 3:74:A:ARG:O    | 20       | 0.18          |
| (2,110) | 3:61:A:HIS:N    | 3:58:A:GLN:O    | 7        | 0.18          |
| (2,109) | 3:60:A:ARG:N    | 3:57:A:HIS:O    | 4        | 0.18          |
| (2,109) | 3:60:A:ARG:N    | 3:57:A:HIS:O    | 10       | 0.18          |
| (2,106) | 3:57:A:HIS:N    | 3:53:A:GLN:O    | 7        | 0.18          |
| (2,101) | 3:39:A:CYS:N    | 3:46:A:ARG:O    | 16       | 0.18          |
| (2,99)  | 3:31:A:HIS:N    | 3:28:A:SER:O    | 7        | 0.18          |
| (2,99)  | 3:31:A:HIS:N    | 3:28:A:SER:O    | 8        | 0.18          |
| (2,99)  | 3:31:A:HIS:N    | 3:28:A:SER:O    | 9        | 0.18          |
| (2,94)  | 3:26:A:MET:N    | 3:22:A:SER:O    | 8        | 0.18          |
| (2,61)  | 3:87:A:ARG:H    | 3:84:A:THR:O    | 1        | 0.18          |
| (2,61)  | 3:87:A:ARG:H    | 3:84:A:THR:O    | 2        | 0.18          |
| (2,61)  | 3:87:A:ARG:H    | 3:84:A:THR:O    | 3        | 0.18          |
| (2,61)  | 3:87:A:ARG:H    | 3:84:A:THR:O    | 12       | 0.18          |
| (2,61)  | 3:87:A:ARG:H    | 3:84:A:THR:O    | 16       | 0.18          |
| (2,39)  | 3:59:A:ARG:H    | 3:56:A:ARG:O    | 7        | 0.18          |
| (2,21)  | 3:31:A:HIS:H    | 3:28:A:SER:O    | 1        | 0.18          |
| (2,17)  | 3:29:A:ARG:H    | 3:26:A:MET:O    | 5        | 0.18          |
| (2,17)  | 3:29:A:ARG:H    | 3:26:A:MET:O    | 8        | 0.18          |
| (2,17)  | 3:29:A:ARG:H    | 3:26:A:MET:O    | 18       | 0.18          |
| (1,719) | 1:129:B:DG:C6   | 3:81:A:HIS:CE1  | 16       | 0.18          |
| (1,715) | 1:129:B:DG:C2'  | 3:78:A:ARG:CZ   | 5        | 0.18          |
| (1,694) | 1:128:B:DG:C5   | 3:81:A:HIS:CD2  | 12       | 0.18          |
| (1,694) | 1:128:B:DG:C5   | 3:81:A:HIS:CD2  | 15       | 0.18          |
| (1,688) | 1:128:B:DG:C1'  | 3:81:A:HIS:CE1  | 2        | 0.18          |
| (1,651) | 3:115:A:HIS:CD2 | 3:119:A:HIS:CD2 | 7        | 0.18          |
| (1,535) | 3:87:A:ARG:CA   | 3:90:A:THR:CB   | 15       | 0.18          |
| (1,465) | 3:67:A:PHE:CB   | 3:82:A:LEU:CD1  | 8        | 0.18          |
| (1,465) | 3:67:A:PHE:CB   | 3:82:A:LEU:CD1  | 17       | 0.18          |
| (1,452) | 3:59:A:ARG:CA   | 3:62:A:THR:CG2  | 11       | 0.18          |
| (1,408) | 3:41:A:PHE:CD2  | 3:44:A:CYS:CA   | 9        | 0.18          |
| (1,356) | 3:24:A:LEU:CD2  | 3:27:A:HIS:CB   | 11       | 0.18          |
| (1,356) | 3:24:A:LEU:CD2  | 3:27:A:HIS:CB   | 13       | 0.18          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,356) | 3:24:A:LEU:CD2 | 3:27:A:HIS:CB  | 14       | 0.18          |
| (1,356) | 3:24:A:LEU:CD2 | 3:27:A:HIS:CB  | 19       | 0.18          |
| (1,356) | 3:24:A:LEU:CD2 | 3:27:A:HIS:CB  | 20       | 0.18          |
| (1,347) | 3:20:A:LYS:CB  | 3:23:A:HIS:CB  | 2        | 0.18          |
| (1,347) | 3:20:A:LYS:CB  | 3:23:A:HIS:CB  | 9        | 0.18          |
| (1,319) | 3:18:A:TYR:CD1 | 3:24:A:LEU:CB  | 9        | 0.18          |
| (1,319) | 3:18:A:TYR:CD1 | 3:24:A:LEU:CB  | 17       | 0.18          |
| (1,319) | 3:18:A:TYR:CD1 | 3:24:A:LEU:CB  | 20       | 0.18          |
| (1,308) | 3:11:A:TYR:CD2 | 3:34:A:GLU:CB  | 6        | 0.18          |
| (1,308) | 3:11:A:TYR:CD2 | 3:34:A:GLU:CB  | 20       | 0.18          |
| (1,288) | 3:11:A:TYR:CA  | 3:31:A:HIS:CE1 | 2        | 0.18          |
| (1,282) | 3:9:A:CYS:CA   | 3:27:A:HIS:CD2 | 1        | 0.18          |
| (1,211) | 3:96:A:SER:HA  | 3:104:A:LYS:H  | 4        | 0.18          |
| (1,209) | 3:105:A:LYS:HA | 3:97:A:CYS:H   | 10       | 0.18          |
| (1,143) | 3:68:A:GLN:HA  | 3:74:A:ARG:H   | 14       | 0.18          |
| (1,142) | 3:77:A:SER:HA  | 3:67:A:PHE:H   | 10       | 0.18          |
| (1,142) | 3:77:A:SER:HA  | 3:67:A:PHE:H   | 11       | 0.18          |
| (1,142) | 3:77:A:SER:HA  | 3:67:A:PHE:H   | 16       | 0.18          |
| (1,77)  | 3:38:A:GLN:HA  | 3:46:A:ARG:H   | 8        | 0.18          |
| (1,77)  | 3:38:A:GLN:HA  | 3:46:A:ARG:H   | 9        | 0.18          |
| (1,77)  | 3:38:A:GLN:HA  | 3:46:A:ARG:H   | 15       | 0.18          |
| (1,76)  | 3:49:A:SER:HA  | 3:37:A:TYR:H   | 9        | 0.18          |
| (1,76)  | 3:49:A:SER:HA  | 3:37:A:TYR:H   | 17       | 0.18          |
| (1,25)  | 3:32:A:THR:H   | 3:33:A:GLY:H   | 7        | 0.18          |
| (1,11)  | 3:8:A:MET:HA   | 3:16:A:LYS:H   | 9        | 0.18          |
| (1,10)  | 3:19:A:PHE:HA  | 3:7:A:PHE:H    | 12       | 0.18          |
| (1,9)   | 3:17:A:ARG:HA  | 3:9:A:CYS:H    | 17       | 0.18          |
| (4,1)   | 3:26:A:MET:HE2 | 1:136:B:DT:H71 | 20       | 0.17          |
| (2,129) | 3:116:A:HIS:N  | 3:112:A:LEU:O  | 13       | 0.17          |
| (2,128) | 3:115:A:HIS:N  | 3:111:A:GLU:O  | 18       | 0.17          |
| (2,126) | 3:113:A:VAL:N  | 3:109:A:SER:O  | 13       | 0.17          |
| (2,126) | 3:113:A:VAL:N  | 3:109:A:SER:O  | 17       | 0.17          |
| (2,120) | 3:88:A:THR:N   | 3:85:A:HIS:O   | 2        | 0.17          |
| (2,120) | 3:88:A:THR:N   | 3:85:A:HIS:O   | 5        | 0.17          |
| (2,120) | 3:88:A:THR:N   | 3:85:A:HIS:O   | 13       | 0.17          |
| (2,120) | 3:88:A:THR:N   | 3:85:A:HIS:O   | 15       | 0.17          |
| (2,120) | 3:88:A:THR:N   | 3:85:A:HIS:O   | 19       | 0.17          |
| (2,116) | 3:84:A:THR:N   | 3:80:A:ASP:O   | 12       | 0.17          |
| (2,116) | 3:84:A:THR:N   | 3:80:A:ASP:O   | 15       | 0.17          |
| (2,112) | 3:69:A:CYS:N   | 3:74:A:ARG:O   | 1        | 0.17          |
| (2,112) | 3:69:A:CYS:N   | 3:74:A:ARG:O   | 14       | 0.17          |
| (2,110) | 3:61:A:HIS:N   | 3:58:A:GLN:O   | 6        | 0.17          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (2,110) | 3:61:A:HIS:N    | 3:58:A:GLN:O    | 9        | 0.17          |
| (2,110) | 3:61:A:HIS:N    | 3:58:A:GLN:O    | 17       | 0.17          |
| (2,109) | 3:60:A:ARG:N    | 3:57:A:HIS:O    | 6        | 0.17          |
| (2,109) | 3:60:A:ARG:N    | 3:57:A:HIS:O    | 7        | 0.17          |
| (2,109) | 3:60:A:ARG:N    | 3:57:A:HIS:O    | 20       | 0.17          |
| (2,106) | 3:57:A:HIS:N    | 3:53:A:GLN:O    | 14       | 0.17          |
| (2,106) | 3:57:A:HIS:N    | 3:53:A:GLN:O    | 19       | 0.17          |
| (2,101) | 3:39:A:CYS:N    | 3:46:A:ARG:O    | 10       | 0.17          |
| (2,94)  | 3:26:A:MET:N    | 3:22:A:SER:O    | 9        | 0.17          |
| (2,93)  | 3:25:A:GLN:N    | 3:21:A:LEU:O    | 6        | 0.17          |
| (2,83)  | 3:117:A:ASN:H   | 3:114:A:ARG:O   | 6        | 0.17          |
| (2,61)  | 3:87:A:ARG:H    | 3:84:A:THR:O    | 6        | 0.17          |
| (2,61)  | 3:87:A:ARG:H    | 3:84:A:THR:O    | 15       | 0.17          |
| (2,61)  | 3:87:A:ARG:H    | 3:84:A:THR:O    | 19       | 0.17          |
| (2,39)  | 3:59:A:ARG:H    | 3:56:A:ARG:O    | 12       | 0.17          |
| (2,17)  | 3:29:A:ARG:H    | 3:26:A:MET:O    | 11       | 0.17          |
| (2,17)  | 3:29:A:ARG:H    | 3:26:A:MET:O    | 20       | 0.17          |
| (1,739) | 1:133:B:DG:C6   | 3:50:A:ARG:CZ   | 12       | 0.17          |
| (1,719) | 1:129:B:DG:C6   | 3:81:A:HIS:CE1  | 14       | 0.17          |
| (1,719) | 1:129:B:DG:C6   | 3:81:A:HIS:CE1  | 20       | 0.17          |
| (1,694) | 1:128:B:DG:C5   | 3:81:A:HIS:CD2  | 10       | 0.17          |
| (1,652) | 3:115:A:HIS:CD2 | 3:119:A:HIS:CE1 | 13       | 0.17          |
| (1,652) | 3:115:A:HIS:CD2 | 3:119:A:HIS:CE1 | 14       | 0.17          |
| (1,502) | 3:76:A:PHE:CB   | 3:82:A:LEU:CD1  | 2        | 0.17          |
| (1,474) | 3:67:A:PHE:CE2  | 3:79:A:SER:CA   | 12       | 0.17          |
| (1,474) | 3:67:A:PHE:CE2  | 3:79:A:SER:CA   | 16       | 0.17          |
| (1,465) | 3:67:A:PHE:CB   | 3:82:A:LEU:CD1  | 4        | 0.17          |
| (1,465) | 3:67:A:PHE:CB   | 3:82:A:LEU:CD1  | 11       | 0.17          |
| (1,452) | 3:59:A:ARG:CA   | 3:62:A:THR:CG2  | 7        | 0.17          |
| (1,382) | 3:38:A:GLN:CA   | 3:47:A:ARG:CA   | 12       | 0.17          |
| (1,368) | 3:31:A:HIS:CB   | 3:34:A:GLU:CB   | 3        | 0.17          |
| (1,356) | 3:24:A:LEU:CD2  | 3:27:A:HIS:CB   | 2        | 0.17          |
| (1,356) | 3:24:A:LEU:CD2  | 3:27:A:HIS:CB   | 10       | 0.17          |
| (1,347) | 3:20:A:LYS:CB   | 3:23:A:HIS:CB   | 6        | 0.17          |
| (1,347) | 3:20:A:LYS:CB   | 3:23:A:HIS:CB   | 14       | 0.17          |
| (1,333) | 3:18:A:TYR:CE2  | 3:27:A:HIS:CE1  | 10       | 0.17          |
| (1,333) | 3:18:A:TYR:CE2  | 3:27:A:HIS:CE1  | 12       | 0.17          |
| (1,332) | 3:18:A:TYR:CE2  | 3:27:A:HIS:CD2  | 20       | 0.17          |
| (1,319) | 3:18:A:TYR:CD1  | 3:24:A:LEU:CB   | 7        | 0.17          |
| (1,319) | 3:18:A:TYR:CD1  | 3:24:A:LEU:CB   | 11       | 0.17          |
| (1,288) | 3:11:A:TYR:CA   | 3:31:A:HIS:CE1  | 4        | 0.17          |
| (1,288) | 3:11:A:TYR:CA   | 3:31:A:HIS:CE1  | 12       | 0.17          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,211) | 3:96:A:SER:HA  | 3:104:A:LYS:H  | 2        | 0.17          |
| (1,211) | 3:96:A:SER:HA  | 3:104:A:LYS:H  | 7        | 0.17          |
| (1,211) | 3:96:A:SER:HA  | 3:104:A:LYS:H  | 11       | 0.17          |
| (1,210) | 3:107:A:ALA:HA | 3:95:A:PHE:H   | 7        | 0.17          |
| (1,142) | 3:77:A:SER:HA  | 3:67:A:PHE:H   | 20       | 0.17          |
| (1,77)  | 3:38:A:GLN:HA  | 3:46:A:ARG:H   | 2        | 0.17          |
| (1,77)  | 3:38:A:GLN:HA  | 3:46:A:ARG:H   | 17       | 0.17          |
| (1,76)  | 3:49:A:SER:HA  | 3:37:A:TYR:H   | 11       | 0.17          |
| (1,76)  | 3:49:A:SER:HA  | 3:37:A:TYR:H   | 19       | 0.17          |
| (1,76)  | 3:49:A:SER:HA  | 3:37:A:TYR:H   | 20       | 0.17          |
| (1,75)  | 3:47:A:ARG:HA  | 3:39:A:CYS:H   | 15       | 0.17          |
| (2,130) | 3:117:A:ASN:N  | 3:114:A:ARG:O  | 7        | 0.16          |
| (2,130) | 3:117:A:ASN:N  | 3:114:A:ARG:O  | 13       | 0.16          |
| (2,130) | 3:117:A:ASN:N  | 3:114:A:ARG:O  | 20       | 0.16          |
| (2,129) | 3:116:A:HIS:N  | 3:112:A:LEU:O  | 2        | 0.16          |
| (2,129) | 3:116:A:HIS:N  | 3:112:A:LEU:O  | 7        | 0.16          |
| (2,129) | 3:116:A:HIS:N  | 3:112:A:LEU:O  | 15       | 0.16          |
| (2,128) | 3:115:A:HIS:N  | 3:111:A:GLU:O  | 2        | 0.16          |
| (2,128) | 3:115:A:HIS:N  | 3:111:A:GLU:O  | 14       | 0.16          |
| (2,128) | 3:115:A:HIS:N  | 3:111:A:GLU:O  | 20       | 0.16          |
| (2,120) | 3:88:A:THR:N   | 3:85:A:HIS:O   | 17       | 0.16          |
| (2,120) | 3:88:A:THR:N   | 3:85:A:HIS:O   | 18       | 0.16          |
| (2,112) | 3:69:A:CYS:N   | 3:74:A:ARG:O   | 18       | 0.16          |
| (2,110) | 3:61:A:HIS:N   | 3:58:A:GLN:O   | 4        | 0.16          |
| (2,110) | 3:61:A:HIS:N   | 3:58:A:GLN:O   | 10       | 0.16          |
| (2,110) | 3:61:A:HIS:N   | 3:58:A:GLN:O   | 11       | 0.16          |
| (2,107) | 3:58:A:GLN:N   | 3:54:A:LEU:O   | 1        | 0.16          |
| (2,106) | 3:57:A:HIS:N   | 3:53:A:GLN:O   | 9        | 0.16          |
| (2,106) | 3:57:A:HIS:N   | 3:53:A:GLN:O   | 15       | 0.16          |
| (2,101) | 3:39:A:CYS:N   | 3:46:A:ARG:O   | 7        | 0.16          |
| (2,99)  | 3:31:A:HIS:N   | 3:28:A:SER:O   | 20       | 0.16          |
| (2,98)  | 3:30:A:LYS:N   | 3:27:A:HIS:O   | 2        | 0.16          |
| (2,92)  | 3:24:A:LEU:N   | 3:20:A:LYS:O   | 4        | 0.16          |
| (2,92)  | 3:24:A:LEU:N   | 3:20:A:LYS:O   | 9        | 0.16          |
| (2,39)  | 3:59:A:ARG:H   | 3:56:A:ARG:O   | 2        | 0.16          |
| (2,39)  | 3:59:A:ARG:H   | 3:56:A:ARG:O   | 11       | 0.16          |
| (2,39)  | 3:59:A:ARG:H   | 3:56:A:ARG:O   | 15       | 0.16          |
| (2,21)  | 3:31:A:HIS:H   | 3:28:A:SER:O   | 13       | 0.16          |
| (2,21)  | 3:31:A:HIS:H   | 3:28:A:SER:O   | 18       | 0.16          |
| (2,17)  | 3:29:A:ARG:H   | 3:26:A:MET:O   | 3        | 0.16          |
| (2,5)   | 3:7:A:PHE:H    | 3:18:A:TYR:O   | 12       | 0.16          |
| (1,791) | 3:109:A:SER:CB | 2:150:C:DC:C3' | 10       | 0.16          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,763) | 2:149:C:DG:N7  | 3:80:A:ASP:CG  | 5        | 0.16          |
| (1,739) | 1:133:B:DG:C6  | 3:50:A:ARG:CZ  | 2        | 0.16          |
| (1,739) | 1:133:B:DG:C6  | 3:50:A:ARG:CZ  | 6        | 0.16          |
| (1,691) | 1:128:B:DG:C6  | 3:81:A:HIS:CE1 | 4        | 0.16          |
| (1,688) | 1:128:B:DG:C1' | 3:81:A:HIS:CE1 | 6        | 0.16          |
| (1,688) | 1:128:B:DG:C1' | 3:81:A:HIS:CE1 | 10       | 0.16          |
| (1,688) | 1:128:B:DG:C1' | 3:81:A:HIS:CE1 | 12       | 0.16          |
| (1,537) | 3:87:A:ARG:CB  | 3:90:A:THR:CB  | 3        | 0.16          |
| (1,465) | 3:67:A:PHE:CB  | 3:82:A:LEU:CD1 | 5        | 0.16          |
| (1,448) | 3:58:A:GLN:CA  | 3:62:A:THR:CG2 | 15       | 0.16          |
| (1,440) | 3:54:A:LEU:CA  | 3:57:A:HIS:CB  | 3        | 0.16          |
| (1,440) | 3:54:A:LEU:CA  | 3:57:A:HIS:CB  | 5        | 0.16          |
| (1,440) | 3:54:A:LEU:CA  | 3:57:A:HIS:CB  | 9        | 0.16          |
| (1,440) | 3:54:A:LEU:CA  | 3:57:A:HIS:CB  | 10       | 0.16          |
| (1,440) | 3:54:A:LEU:CA  | 3:57:A:HIS:CB  | 13       | 0.16          |
| (1,440) | 3:54:A:LEU:CA  | 3:57:A:HIS:CB  | 16       | 0.16          |
| (1,388) | 3:39:A:CYS:CB  | 3:41:A:PHE:CB  | 12       | 0.16          |
| (1,380) | 3:37:A:TYR:CD2 | 3:54:A:LEU:CB  | 9        | 0.16          |
| (1,379) | 3:37:A:TYR:CD2 | 3:51:A:SER:CB  | 7        | 0.16          |
| (1,356) | 3:24:A:LEU:CD2 | 3:27:A:HIS:CB  | 4        | 0.16          |
| (1,347) | 3:20:A:LYS:CB  | 3:23:A:HIS:CB  | 13       | 0.16          |
| (1,347) | 3:20:A:LYS:CB  | 3:23:A:HIS:CB  | 15       | 0.16          |
| (1,347) | 3:20:A:LYS:CB  | 3:23:A:HIS:CB  | 16       | 0.16          |
| (1,341) | 3:19:A:PHE:CB  | 3:23:A:HIS:CD2 | 7        | 0.16          |
| (1,341) | 3:19:A:PHE:CB  | 3:23:A:HIS:CD2 | 16       | 0.16          |
| (1,332) | 3:18:A:TYR:CE2 | 3:27:A:HIS:CD2 | 11       | 0.16          |
| (1,319) | 3:18:A:TYR:CD1 | 3:24:A:LEU:CB  | 1        | 0.16          |
| (1,319) | 3:18:A:TYR:CD1 | 3:24:A:LEU:CB  | 12       | 0.16          |
| (1,319) | 3:18:A:TYR:CD1 | 3:24:A:LEU:CB  | 14       | 0.16          |
| (1,319) | 3:18:A:TYR:CD1 | 3:24:A:LEU:CB  | 15       | 0.16          |
| (1,308) | 3:11:A:TYR:CD2 | 3:34:A:GLU:CB  | 13       | 0.16          |
| (1,270) | 3:7:A:PHE:CE1  | 3:21:A:LEU:CD1 | 5        | 0.16          |
| (1,211) | 3:96:A:SER:HA  | 3:104:A:LYS:H  | 6        | 0.16          |
| (1,211) | 3:96:A:SER:HA  | 3:104:A:LYS:H  | 19       | 0.16          |
| (1,209) | 3:105:A:LYS:HA | 3:97:A:CYS:H   | 17       | 0.16          |
| (1,208) | 3:96:A:SER:HA  | 3:106:A:PHE:H  | 1        | 0.16          |
| (1,143) | 3:68:A:GLN:HA  | 3:74:A:ARG:H   | 9        | 0.16          |
| (1,143) | 3:68:A:GLN:HA  | 3:74:A:ARG:H   | 10       | 0.16          |
| (1,143) | 3:68:A:GLN:HA  | 3:74:A:ARG:H   | 11       | 0.16          |
| (1,142) | 3:77:A:SER:HA  | 3:67:A:PHE:H   | 6        | 0.16          |
| (1,77)  | 3:38:A:GLN:HA  | 3:46:A:ARG:H   | 11       | 0.16          |
| (1,76)  | 3:49:A:SER:HA  | 3:37:A:TYR:H   | 2        | 0.16          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,76)  | 3:49:A:SER:HA  | 3:37:A:TYR:H   | 6        | 0.16          |
| (1,11)  | 3:8:A:MET:HA   | 3:16:A:LYS:H   | 5        | 0.16          |
| (1,10)  | 3:19:A:PHE:HA  | 3:7:A:PHE:H    | 3        | 0.16          |
| (2,132) | 3:119:A:HIS:N  | 3:116:A:HIS:O  | 10       | 0.15          |
| (2,131) | 3:118:A:MET:N  | 3:115:A:HIS:O  | 7        | 0.15          |
| (2,130) | 3:117:A:ASN:N  | 3:114:A:ARG:O  | 4        | 0.15          |
| (2,130) | 3:117:A:ASN:N  | 3:114:A:ARG:O  | 5        | 0.15          |
| (2,130) | 3:117:A:ASN:N  | 3:114:A:ARG:O  | 12       | 0.15          |
| (2,129) | 3:116:A:HIS:N  | 3:112:A:LEU:O  | 5        | 0.15          |
| (2,129) | 3:116:A:HIS:N  | 3:112:A:LEU:O  | 17       | 0.15          |
| (2,128) | 3:115:A:HIS:N  | 3:111:A:GLU:O  | 5        | 0.15          |
| (2,128) | 3:115:A:HIS:N  | 3:111:A:GLU:O  | 16       | 0.15          |
| (2,120) | 3:88:A:THR:N   | 3:85:A:HIS:O   | 20       | 0.15          |
| (2,110) | 3:61:A:HIS:N   | 3:58:A:GLN:O   | 20       | 0.15          |
| (2,109) | 3:60:A:ARG:N   | 3:57:A:HIS:O   | 9        | 0.15          |
| (2,107) | 3:58:A:GLN:N   | 3:54:A:LEU:O   | 9        | 0.15          |
| (2,106) | 3:57:A:HIS:N   | 3:53:A:GLN:O   | 3        | 0.15          |
| (2,105) | 3:56:A:ARG:N   | 3:52:A:ASP:O   | 2        | 0.15          |
| (2,101) | 3:39:A:CYS:N   | 3:46:A:ARG:O   | 4        | 0.15          |
| (2,101) | 3:39:A:CYS:N   | 3:46:A:ARG:O   | 13       | 0.15          |
| (2,94)  | 3:26:A:MET:N   | 3:22:A:SER:O   | 16       | 0.15          |
| (2,93)  | 3:25:A:GLN:N   | 3:21:A:LEU:O   | 19       | 0.15          |
| (2,92)  | 3:24:A:LEU:N   | 3:20:A:LYS:O   | 17       | 0.15          |
| (2,90)  | 3:9:A:CYS:N    | 3:16:A:LYS:O   | 10       | 0.15          |
| (2,65)  | 3:89:A:HIS:H   | 3:86:A:THR:O   | 12       | 0.15          |
| (2,65)  | 3:89:A:HIS:H   | 3:86:A:THR:O   | 19       | 0.15          |
| (2,61)  | 3:87:A:ARG:H   | 3:84:A:THR:O   | 4        | 0.15          |
| (2,61)  | 3:87:A:ARG:H   | 3:84:A:THR:O   | 13       | 0.15          |
| (2,61)  | 3:87:A:ARG:H   | 3:84:A:THR:O   | 17       | 0.15          |
| (2,39)  | 3:59:A:ARG:H   | 3:56:A:ARG:O   | 1        | 0.15          |
| (2,39)  | 3:59:A:ARG:H   | 3:56:A:ARG:O   | 13       | 0.15          |
| (2,39)  | 3:59:A:ARG:H   | 3:56:A:ARG:O   | 14       | 0.15          |
| (2,39)  | 3:59:A:ARG:H   | 3:56:A:ARG:O   | 16       | 0.15          |
| (2,39)  | 3:59:A:ARG:H   | 3:56:A:ARG:O   | 18       | 0.15          |
| (2,19)  | 3:30:A:LYS:H   | 3:27:A:HIS:O   | 16       | 0.15          |
| (2,17)  | 3:29:A:ARG:H   | 3:26:A:MET:O   | 9        | 0.15          |
| (2,17)  | 3:29:A:ARG:H   | 3:26:A:MET:O   | 16       | 0.15          |
| (2,17)  | 3:29:A:ARG:H   | 3:26:A:MET:O   | 17       | 0.15          |
| (1,791) | 3:109:A:SER:CB | 2:150:C:DC:C3' | 15       | 0.15          |
| (1,758) | 2:147:C:DA:C8  | 3:52:A:ASP:CB  | 1        | 0.15          |
| (1,752) | 2:147:C:DA:N6  | 3:52:A:ASP:CG  | 2        | 0.15          |
| (1,739) | 1:133:B:DG:C6  | 3:50:A:ARG:CZ  | 18       | 0.15          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,719) | 1:129:B:DG:C6  | 3:81:A:HIS:CE1 | 4        | 0.15          |
| (1,719) | 1:129:B:DG:C6  | 3:81:A:HIS:CE1 | 17       | 0.15          |
| (1,706) | 1:129:B:DG:C5' | 3:60:A:ARG:CD  | 20       | 0.15          |
| (1,704) | 1:129:B:DG:C5' | 3:60:A:ARG:CB  | 11       | 0.15          |
| (1,696) | 1:128:B:DG:N7  | 3:81:A:HIS:CB  | 1        | 0.15          |
| (1,694) | 1:128:B:DG:C5  | 3:81:A:HIS:CD2 | 18       | 0.15          |
| (1,688) | 1:128:B:DG:C1' | 3:81:A:HIS:CE1 | 1        | 0.15          |
| (1,670) | 1:126:B:DC:N4  | 3:108:A:ARG:CZ | 5        | 0.15          |
| (1,577) | 3:97:A:CYS:CB  | 3:99:A:TRP:CB  | 3        | 0.15          |
| (1,577) | 3:97:A:CYS:CB  | 3:99:A:TRP:CB  | 10       | 0.15          |
| (1,484) | 3:69:A:CYS:CA  | 3:74:A:ARG:CA  | 18       | 0.15          |
| (1,476) | 3:67:A:PHE:CD2 | 3:79:A:SER:CA  | 16       | 0.15          |
| (1,465) | 3:67:A:PHE:CB  | 3:82:A:LEU:CD1 | 7        | 0.15          |
| (1,465) | 3:67:A:PHE:CB  | 3:82:A:LEU:CD1 | 14       | 0.15          |
| (1,440) | 3:54:A:LEU:CA  | 3:57:A:HIS:CB  | 1        | 0.15          |
| (1,440) | 3:54:A:LEU:CA  | 3:57:A:HIS:CB  | 18       | 0.15          |
| (1,388) | 3:39:A:CYS:CB  | 3:41:A:PHE:CB  | 15       | 0.15          |
| (1,356) | 3:24:A:LEU:CD2 | 3:27:A:HIS:CB  | 1        | 0.15          |
| (1,345) | 3:20:A:LYS:CA  | 3:23:A:HIS:CE1 | 16       | 0.15          |
| (1,341) | 3:19:A:PHE:CB  | 3:23:A:HIS:CD2 | 15       | 0.15          |
| (1,338) | 3:18:A:TYR:CD2 | 3:27:A:HIS:CD2 | 17       | 0.15          |
| (1,332) | 3:18:A:TYR:CE2 | 3:27:A:HIS:CD2 | 13       | 0.15          |
| (1,327) | 3:18:A:TYR:CE1 | 3:27:A:HIS:CB  | 12       | 0.15          |
| (1,308) | 3:11:A:TYR:CD2 | 3:34:A:GLU:CB  | 16       | 0.15          |
| (1,301) | 3:11:A:TYR:CE2 | 3:31:A:HIS:CB  | 2        | 0.15          |
| (1,301) | 3:11:A:TYR:CE2 | 3:31:A:HIS:CB  | 9        | 0.15          |
| (1,288) | 3:11:A:TYR:CA  | 3:31:A:HIS:CE1 | 13       | 0.15          |
| (1,262) | 3:7:A:PHE:CB   | 3:18:A:TYR:CB  | 8        | 0.15          |
| (1,262) | 3:7:A:PHE:CB   | 3:18:A:TYR:CB  | 17       | 0.15          |
| (1,211) | 3:96:A:SER:HA  | 3:104:A:LYS:H  | 20       | 0.15          |
| (1,142) | 3:77:A:SER:HA  | 3:67:A:PHE:H   | 14       | 0.15          |
| (1,142) | 3:77:A:SER:HA  | 3:67:A:PHE:H   | 18       | 0.15          |
| (1,142) | 3:77:A:SER:HA  | 3:67:A:PHE:H   | 19       | 0.15          |
| (1,140) | 3:68:A:GLN:HA  | 3:76:A:PHE:H   | 14       | 0.15          |
| (1,77)  | 3:38:A:GLN:HA  | 3:46:A:ARG:H   | 19       | 0.15          |
| (1,76)  | 3:49:A:SER:HA  | 3:37:A:TYR:H   | 8        | 0.15          |
| (1,76)  | 3:49:A:SER:HA  | 3:37:A:TYR:H   | 18       | 0.15          |
| (1,75)  | 3:47:A:ARG:HA  | 3:39:A:CYS:H   | 3        | 0.15          |
| (1,75)  | 3:47:A:ARG:HA  | 3:39:A:CYS:H   | 19       | 0.15          |
| (1,9)   | 3:17:A:ARG:HA  | 3:9:A:CYS:H    | 19       | 0.15          |
| (2,130) | 3:117:A:ASN:N  | 3:114:A:ARG:O  | 1        | 0.14          |
| (2,130) | 3:117:A:ASN:N  | 3:114:A:ARG:O  | 8        | 0.14          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (2,130) | 3:117:A:ASN:N  | 3:114:A:ARG:O  | 15       | 0.14          |
| (2,130) | 3:117:A:ASN:N  | 3:114:A:ARG:O  | 16       | 0.14          |
| (2,130) | 3:117:A:ASN:N  | 3:114:A:ARG:O  | 17       | 0.14          |
| (2,128) | 3:115:A:HIS:N  | 3:111:A:GLU:O  | 13       | 0.14          |
| (2,128) | 3:115:A:HIS:N  | 3:111:A:GLU:O  | 15       | 0.14          |
| (2,120) | 3:88:A:THR:N   | 3:85:A:HIS:O   | 4        | 0.14          |
| (2,120) | 3:88:A:THR:N   | 3:85:A:HIS:O   | 12       | 0.14          |
| (2,112) | 3:69:A:CYS:N   | 3:74:A:ARG:O   | 11       | 0.14          |
| (2,112) | 3:69:A:CYS:N   | 3:74:A:ARG:O   | 12       | 0.14          |
| (2,110) | 3:61:A:HIS:N   | 3:58:A:GLN:O   | 5        | 0.14          |
| (2,110) | 3:61:A:HIS:N   | 3:58:A:GLN:O   | 8        | 0.14          |
| (2,109) | 3:60:A:ARG:N   | 3:57:A:HIS:O   | 2        | 0.14          |
| (2,109) | 3:60:A:ARG:N   | 3:57:A:HIS:O   | 17       | 0.14          |
| (2,107) | 3:58:A:GLN:N   | 3:54:A:LEU:O   | 19       | 0.14          |
| (2,106) | 3:57:A:HIS:N   | 3:53:A:GLN:O   | 5        | 0.14          |
| (2,101) | 3:39:A:CYS:N   | 3:46:A:ARG:O   | 19       | 0.14          |
| (2,96)  | 3:28:A:SER:N   | 3:24:A:LEU:O   | 4        | 0.14          |
| (2,95)  | 3:27:A:HIS:N   | 3:23:A:HIS:O   | 20       | 0.14          |
| (2,93)  | 3:25:A:GLN:N   | 3:21:A:LEU:O   | 12       | 0.14          |
| (2,92)  | 3:24:A:LEU:N   | 3:20:A:LYS:O   | 3        | 0.14          |
| (2,92)  | 3:24:A:LEU:N   | 3:20:A:LYS:O   | 13       | 0.14          |
| (2,83)  | 3:117:A:ASN:H  | 3:114:A:ARG:O  | 18       | 0.14          |
| (2,65)  | 3:89:A:HIS:H   | 3:86:A:THR:O   | 11       | 0.14          |
| (2,61)  | 3:87:A:ARG:H   | 3:84:A:THR:O   | 14       | 0.14          |
| (2,49)  | 3:67:A:PHE:H   | 3:76:A:PHE:O   | 12       | 0.14          |
| (2,39)  | 3:59:A:ARG:H   | 3:56:A:ARG:O   | 4        | 0.14          |
| (2,39)  | 3:59:A:ARG:H   | 3:56:A:ARG:O   | 6        | 0.14          |
| (2,39)  | 3:59:A:ARG:H   | 3:56:A:ARG:O   | 17       | 0.14          |
| (2,39)  | 3:59:A:ARG:H   | 3:56:A:ARG:O   | 19       | 0.14          |
| (2,39)  | 3:59:A:ARG:H   | 3:56:A:ARG:O   | 20       | 0.14          |
| (1,791) | 3:109:A:SER:CB | 2:150:C:DC:C3' | 5        | 0.14          |
| (1,791) | 3:109:A:SER:CB | 2:150:C:DC:C3' | 19       | 0.14          |
| (1,791) | 3:109:A:SER:CB | 2:150:C:DC:C3' | 20       | 0.14          |
| (1,767) | 2:150:C:DC:N4  | 3:80:A:ASP:CB  | 20       | 0.14          |
| (1,764) | 2:149:C:DG:C8  | 3:80:A:ASP:CB  | 5        | 0.14          |
| (1,762) | 2:149:C:DG:N7  | 3:80:A:ASP:CB  | 7        | 0.14          |
| (1,752) | 2:147:C:DA:N6  | 3:52:A:ASP:CG  | 1        | 0.14          |
| (1,752) | 2:147:C:DA:N6  | 3:52:A:ASP:CG  | 4        | 0.14          |
| (1,739) | 1:133:B:DG:C6  | 3:50:A:ARG:CZ  | 14       | 0.14          |
| (1,737) | 1:132:B:DC:C5  | 3:50:A:ARG:CZ  | 11       | 0.14          |
| (1,727) | 1:130:B:DG:C6  | 3:78:A:ARG:CZ  | 20       | 0.14          |
| (1,704) | 1:129:B:DG:C5' | 3:60:A:ARG:CB  | 5        | 0.14          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,696) | 1:128:B:DG:N7   | 3:81:A:HIS:CB   | 2        | 0.14          |
| (1,691) | 1:128:B:DG:C6   | 3:81:A:HIS:CE1  | 9        | 0.14          |
| (1,688) | 1:128:B:DG:C1'  | 3:81:A:HIS:CE1  | 8        | 0.14          |
| (1,688) | 1:128:B:DG:C1'  | 3:81:A:HIS:CE1  | 13       | 0.14          |
| (1,688) | 1:128:B:DG:C1'  | 3:81:A:HIS:CE1  | 15       | 0.14          |
| (1,680) | 1:127:B:DG:C4'  | 3:74:A:ARG:CZ   | 15       | 0.14          |
| (1,670) | 1:126:B:DC:N4   | 3:108:A:ARG:CZ  | 8        | 0.14          |
| (1,660) | 3:84:A:THR:HG21 | 1:126:B:DC:H6   | 18       | 0.14          |
| (1,660) | 3:84:A:THR:HG22 | 1:126:B:DC:H6   | 18       | 0.14          |
| (1,660) | 3:84:A:THR:HG23 | 1:126:B:DC:H6   | 18       | 0.14          |
| (1,659) | 3:80:A:ASP:HA   | 2:150:C:DC:H6   | 13       | 0.14          |
| (1,651) | 3:115:A:HIS:CD2 | 3:119:A:HIS:CD2 | 18       | 0.14          |
| (1,638) | 3:110:A:ASP:CB  | 3:113:A:VAL:CG2 | 15       | 0.14          |
| (1,638) | 3:110:A:ASP:CB  | 3:113:A:VAL:CG2 | 17       | 0.14          |
| (1,583) | 3:97:A:CYS:CB   | 3:116:A:HIS:CE1 | 6        | 0.14          |
| (1,535) | 3:87:A:ARG:CA   | 3:90:A:THR:CB   | 18       | 0.14          |
| (1,502) | 3:76:A:PHE:CB   | 3:82:A:LEU:CD1  | 15       | 0.14          |
| (1,497) | 3:72:A:CYS:CB   | 3:74:A:ARG:CB   | 7        | 0.14          |
| (1,484) | 3:69:A:CYS:CA   | 3:74:A:ARG:CA   | 12       | 0.14          |
| (1,465) | 3:67:A:PHE:CB   | 3:82:A:LEU:CD1  | 3        | 0.14          |
| (1,465) | 3:67:A:PHE:CB   | 3:82:A:LEU:CD1  | 10       | 0.14          |
| (1,440) | 3:54:A:LEU:CA   | 3:57:A:HIS:CB   | 4        | 0.14          |
| (1,440) | 3:54:A:LEU:CA   | 3:57:A:HIS:CB   | 6        | 0.14          |
| (1,440) | 3:54:A:LEU:CA   | 3:57:A:HIS:CB   | 8        | 0.14          |
| (1,440) | 3:54:A:LEU:CA   | 3:57:A:HIS:CB   | 17       | 0.14          |
| (1,382) | 3:38:A:GLN:CA   | 3:47:A:ARG:CA   | 2        | 0.14          |
| (1,377) | 3:37:A:TYR:CD2  | 3:50:A:ARG:CA   | 13       | 0.14          |
| (1,373) | 3:37:A:TYR:CD1  | 3:54:A:LEU:CD2  | 13       | 0.14          |
| (1,356) | 3:24:A:LEU:CD2  | 3:27:A:HIS:CB   | 7        | 0.14          |
| (1,356) | 3:24:A:LEU:CD2  | 3:27:A:HIS:CB   | 16       | 0.14          |
| (1,354) | 3:22:A:SER:CB   | 3:25:A:GLN:CB   | 12       | 0.14          |
| (1,341) | 3:19:A:PHE:CB   | 3:23:A:HIS:CD2  | 14       | 0.14          |
| (1,341) | 3:19:A:PHE:CB   | 3:23:A:HIS:CD2  | 20       | 0.14          |
| (1,333) | 3:18:A:TYR:CE2  | 3:27:A:HIS:CE1  | 11       | 0.14          |
| (1,319) | 3:18:A:TYR:CD1  | 3:24:A:LEU:CB   | 3        | 0.14          |
| (1,319) | 3:18:A:TYR:CD1  | 3:24:A:LEU:CB   | 5        | 0.14          |
| (1,319) | 3:18:A:TYR:CD1  | 3:24:A:LEU:CB   | 6        | 0.14          |
| (1,319) | 3:18:A:TYR:CD1  | 3:24:A:LEU:CB   | 10       | 0.14          |
| (1,308) | 3:11:A:TYR:CD2  | 3:34:A:GLU:CB   | 4        | 0.14          |
| (1,299) | 3:11:A:TYR:CE1  | 3:34:A:GLU:CA   | 13       | 0.14          |
| (1,299) | 3:11:A:TYR:CE1  | 3:34:A:GLU:CA   | 15       | 0.14          |
| (1,298) | 3:11:A:TYR:CE1  | 3:31:A:HIS:CB   | 18       | 0.14          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,288) | 3:11:A:TYR:CA  | 3:31:A:HIS:CE1 | 3        | 0.14          |
| (1,272) | 3:7:A:PHE:CE2  | 3:21:A:LEU:CA  | 4        | 0.14          |
| (1,269) | 3:7:A:PHE:CE1  | 3:21:A:LEU:CB  | 5        | 0.14          |
| (1,262) | 3:7:A:PHE:CB   | 3:18:A:TYR:CB  | 15       | 0.14          |
| (1,262) | 3:7:A:PHE:CB   | 3:18:A:TYR:CB  | 18       | 0.14          |
| (1,211) | 3:96:A:SER:HA  | 3:104:A:LYS:H  | 1        | 0.14          |
| (1,211) | 3:96:A:SER:HA  | 3:104:A:LYS:H  | 9        | 0.14          |
| (1,211) | 3:96:A:SER:HA  | 3:104:A:LYS:H  | 15       | 0.14          |
| (1,208) | 3:96:A:SER:HA  | 3:106:A:PHE:H  | 4        | 0.14          |
| (1,143) | 3:68:A:GLN:HA  | 3:74:A:ARG:H   | 5        | 0.14          |
| (1,142) | 3:77:A:SER:HA  | 3:67:A:PHE:H   | 2        | 0.14          |
| (1,142) | 3:77:A:SER:HA  | 3:67:A:PHE:H   | 7        | 0.14          |
| (1,142) | 3:77:A:SER:HA  | 3:67:A:PHE:H   | 8        | 0.14          |
| (1,141) | 3:75:A:LYS:HA  | 3:69:A:CYS:H   | 6        | 0.14          |
| (1,140) | 3:68:A:GLN:HA  | 3:76:A:PHE:H   | 5        | 0.14          |
| (1,77)  | 3:38:A:GLN:HA  | 3:46:A:ARG:H   | 14       | 0.14          |
| (1,76)  | 3:49:A:SER:HA  | 3:37:A:TYR:H   | 12       | 0.14          |
| (1,76)  | 3:49:A:SER:HA  | 3:37:A:TYR:H   | 16       | 0.14          |
| (1,75)  | 3:47:A:ARG:HA  | 3:39:A:CYS:H   | 8        | 0.14          |
| (1,75)  | 3:47:A:ARG:HA  | 3:39:A:CYS:H   | 9        | 0.14          |
| (1,75)  | 3:47:A:ARG:HA  | 3:39:A:CYS:H   | 18       | 0.14          |
| (1,13)  | 3:7:A:PHE:H    | 3:18:A:TYR:H   | 6        | 0.14          |
| (1,11)  | 3:8:A:MET:HA   | 3:16:A:LYS:H   | 2        | 0.14          |
| (4,2)   | 3:26:A:MET:HE3 | 1:135:B:DC:H6  | 14       | 0.13          |
| (2,130) | 3:117:A:ASN:N  | 3:114:A:ARG:O  | 2        | 0.13          |
| (2,130) | 3:117:A:ASN:N  | 3:114:A:ARG:O  | 19       | 0.13          |
| (2,128) | 3:115:A:HIS:N  | 3:111:A:GLU:O  | 1        | 0.13          |
| (2,128) | 3:115:A:HIS:N  | 3:111:A:GLU:O  | 4        | 0.13          |
| (2,128) | 3:115:A:HIS:N  | 3:111:A:GLU:O  | 9        | 0.13          |
| (2,128) | 3:115:A:HIS:N  | 3:111:A:GLU:O  | 19       | 0.13          |
| (2,123) | 3:97:A:CYS:N   | 3:104:A:LYS:O  | 2        | 0.13          |
| (2,123) | 3:97:A:CYS:N   | 3:104:A:LYS:O  | 14       | 0.13          |
| (2,121) | 3:89:A:HIS:N   | 3:86:A:THR:O   | 15       | 0.13          |
| (2,120) | 3:88:A:THR:N   | 3:85:A:HIS:O   | 7        | 0.13          |
| (2,120) | 3:88:A:THR:N   | 3:85:A:HIS:O   | 8        | 0.13          |
| (2,112) | 3:69:A:CYS:N   | 3:74:A:ARG:O   | 9        | 0.13          |
| (2,112) | 3:69:A:CYS:N   | 3:74:A:ARG:O   | 10       | 0.13          |
| (2,110) | 3:61:A:HIS:N   | 3:58:A:GLN:O   | 16       | 0.13          |
| (2,107) | 3:58:A:GLN:N   | 3:54:A:LEU:O   | 6        | 0.13          |
| (2,107) | 3:58:A:GLN:N   | 3:54:A:LEU:O   | 20       | 0.13          |
| (2,106) | 3:57:A:HIS:N   | 3:53:A:GLN:O   | 8        | 0.13          |
| (2,106) | 3:57:A:HIS:N   | 3:53:A:GLN:O   | 10       | 0.13          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (2,105) | 3:56:A:ARG:N   | 3:52:A:ASP:O   | 3        | 0.13          |
| (2,101) | 3:39:A:CYS:N   | 3:46:A:ARG:O   | 11       | 0.13          |
| (2,101) | 3:39:A:CYS:N   | 3:46:A:ARG:O   | 14       | 0.13          |
| (2,101) | 3:39:A:CYS:N   | 3:46:A:ARG:O   | 20       | 0.13          |
| (2,99)  | 3:31:A:HIS:N   | 3:28:A:SER:O   | 6        | 0.13          |
| (2,94)  | 3:26:A:MET:N   | 3:22:A:SER:O   | 20       | 0.13          |
| (2,92)  | 3:24:A:LEU:N   | 3:20:A:LYS:O   | 5        | 0.13          |
| (2,92)  | 3:24:A:LEU:N   | 3:20:A:LYS:O   | 8        | 0.13          |
| (2,92)  | 3:24:A:LEU:N   | 3:20:A:LYS:O   | 15       | 0.13          |
| (2,87)  | 3:119:A:HIS:H  | 3:116:A:HIS:O  | 10       | 0.13          |
| (2,65)  | 3:89:A:HIS:H   | 3:86:A:THR:O   | 5        | 0.13          |
| (2,65)  | 3:89:A:HIS:H   | 3:86:A:THR:O   | 13       | 0.13          |
| (2,65)  | 3:89:A:HIS:H   | 3:86:A:THR:O   | 20       | 0.13          |
| (2,49)  | 3:67:A:PHE:H   | 3:76:A:PHE:O   | 10       | 0.13          |
| (2,43)  | 3:61:A:HIS:H   | 3:58:A:GLN:O   | 4        | 0.13          |
| (2,43)  | 3:61:A:HIS:H   | 3:58:A:GLN:O   | 8        | 0.13          |
| (2,39)  | 3:59:A:ARG:H   | 3:56:A:ARG:O   | 8        | 0.13          |
| (2,21)  | 3:31:A:HIS:H   | 3:28:A:SER:O   | 4        | 0.13          |
| (2,19)  | 3:30:A:LYS:H   | 3:27:A:HIS:O   | 1        | 0.13          |
| (2,19)  | 3:30:A:LYS:H   | 3:27:A:HIS:O   | 2        | 0.13          |
| (2,19)  | 3:30:A:LYS:H   | 3:27:A:HIS:O   | 5        | 0.13          |
| (2,19)  | 3:30:A:LYS:H   | 3:27:A:HIS:O   | 6        | 0.13          |
| (2,19)  | 3:30:A:LYS:H   | 3:27:A:HIS:O   | 11       | 0.13          |
| (2,19)  | 3:30:A:LYS:H   | 3:27:A:HIS:O   | 15       | 0.13          |
| (2,5)   | 3:7:A:PHE:H    | 3:18:A:TYR:O   | 6        | 0.13          |
| (1,791) | 3:109:A:SER:CB | 2:150:C:DC:C3' | 1        | 0.13          |
| (1,791) | 3:109:A:SER:CB | 2:150:C:DC:C3' | 2        | 0.13          |
| (1,791) | 3:109:A:SER:CB | 2:150:C:DC:C3' | 4        | 0.13          |
| (1,791) | 3:109:A:SER:CB | 2:150:C:DC:C3' | 8        | 0.13          |
| (1,791) | 3:109:A:SER:CB | 2:150:C:DC:C3' | 12       | 0.13          |
| (1,767) | 2:150:C:DC:N4  | 3:80:A:ASP:CB  | 17       | 0.13          |
| (1,762) | 2:149:C:DG:N7  | 3:80:A:ASP:CB  | 17       | 0.13          |
| (1,740) | 1:133:B:DG:C5  | 3:50:A:ARG:CZ  | 15       | 0.13          |
| (1,739) | 1:133:B:DG:C6  | 3:50:A:ARG:CZ  | 9        | 0.13          |
| (1,737) | 1:132:B:DC:C5  | 3:50:A:ARG:CZ  | 13       | 0.13          |
| (1,719) | 1:129:B:DG:C6  | 3:81:A:HIS:CE1 | 9        | 0.13          |
| (1,696) | 1:128:B:DG:N7  | 3:81:A:HIS:CB  | 7        | 0.13          |
| (1,696) | 1:128:B:DG:N7  | 3:81:A:HIS:CB  | 13       | 0.13          |
| (1,688) | 1:128:B:DG:C1' | 3:81:A:HIS:CE1 | 3        | 0.13          |
| (1,688) | 1:128:B:DG:C1' | 3:81:A:HIS:CE1 | 5        | 0.13          |
| (1,688) | 1:128:B:DG:C1' | 3:81:A:HIS:CE1 | 11       | 0.13          |
| (1,688) | 1:128:B:DG:C1' | 3:81:A:HIS:CE1 | 18       | 0.13          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,659) | 3:80:A:ASP:HA  | 2:150:C:DC:H6   | 18       | 0.13          |
| (1,638) | 3:110:A:ASP:CB | 3:113:A:VAL:CG2 | 1        | 0.13          |
| (1,638) | 3:110:A:ASP:CB | 3:113:A:VAL:CG2 | 3        | 0.13          |
| (1,638) | 3:110:A:ASP:CB | 3:113:A:VAL:CG2 | 5        | 0.13          |
| (1,638) | 3:110:A:ASP:CB | 3:113:A:VAL:CG2 | 7        | 0.13          |
| (1,638) | 3:110:A:ASP:CB | 3:113:A:VAL:CG2 | 9        | 0.13          |
| (1,638) | 3:110:A:ASP:CB | 3:113:A:VAL:CG2 | 12       | 0.13          |
| (1,577) | 3:97:A:CYS:CB  | 3:99:A:TRP:CB   | 18       | 0.13          |
| (1,577) | 3:97:A:CYS:CB  | 3:99:A:TRP:CB   | 19       | 0.13          |
| (1,502) | 3:76:A:PHE:CB  | 3:82:A:LEU:CD1  | 8        | 0.13          |
| (1,484) | 3:69:A:CYS:CA  | 3:74:A:ARG:CA   | 3        | 0.13          |
| (1,484) | 3:69:A:CYS:CA  | 3:74:A:ARG:CA   | 10       | 0.13          |
| (1,465) | 3:67:A:PHE:CB  | 3:82:A:LEU:CD1  | 6        | 0.13          |
| (1,465) | 3:67:A:PHE:CB  | 3:82:A:LEU:CD1  | 12       | 0.13          |
| (1,452) | 3:59:A:ARG:CA  | 3:62:A:THR:CG2  | 1        | 0.13          |
| (1,452) | 3:59:A:ARG:CA  | 3:62:A:THR:CG2  | 10       | 0.13          |
| (1,452) | 3:59:A:ARG:CA  | 3:62:A:THR:CG2  | 12       | 0.13          |
| (1,440) | 3:54:A:LEU:CA  | 3:57:A:HIS:CB   | 14       | 0.13          |
| (1,440) | 3:54:A:LEU:CA  | 3:57:A:HIS:CB   | 19       | 0.13          |
| (1,404) | 3:41:A:PHE:CE2 | 3:44:A:CYS:CB   | 15       | 0.13          |
| (1,396) | 3:41:A:PHE:CB  | 3:61:A:HIS:CE1  | 12       | 0.13          |
| (1,395) | 3:41:A:PHE:CB  | 3:61:A:HIS:CD2  | 11       | 0.13          |
| (1,386) | 3:38:A:GLN:CB  | 3:47:A:ARG:CB   | 14       | 0.13          |
| (1,380) | 3:37:A:TYR:CD2 | 3:54:A:LEU:CB   | 15       | 0.13          |
| (1,379) | 3:37:A:TYR:CD2 | 3:51:A:SER:CB   | 20       | 0.13          |
| (1,376) | 3:37:A:TYR:CE2 | 3:51:A:SER:CB   | 12       | 0.13          |
| (1,366) | 3:29:A:ARG:CB  | 3:32:A:THR:CG2  | 6        | 0.13          |
| (1,356) | 3:24:A:LEU:CD2 | 3:27:A:HIS:CB   | 9        | 0.13          |
| (1,331) | 3:18:A:TYR:CE2 | 3:27:A:HIS:CB   | 8        | 0.13          |
| (1,329) | 3:18:A:TYR:CE2 | 3:24:A:LEU:CB   | 1        | 0.13          |
| (1,328) | 3:18:A:TYR:CE2 | 3:24:A:LEU:CA   | 18       | 0.13          |
| (1,327) | 3:18:A:TYR:CE1 | 3:27:A:HIS:CB   | 20       | 0.13          |
| (1,311) | 3:18:A:TYR:CA  | 3:24:A:LEU:CB   | 16       | 0.13          |
| (1,308) | 3:11:A:TYR:CD2 | 3:34:A:GLU:CB   | 14       | 0.13          |
| (1,301) | 3:11:A:TYR:CE2 | 3:31:A:HIS:CB   | 13       | 0.13          |
| (1,268) | 3:7:A:PHE:CE1  | 3:21:A:LEU:CA   | 10       | 0.13          |
| (1,211) | 3:96:A:SER:HA  | 3:104:A:LYS:H   | 3        | 0.13          |
| (1,211) | 3:96:A:SER:HA  | 3:104:A:LYS:H   | 18       | 0.13          |
| (1,208) | 3:96:A:SER:HA  | 3:106:A:PHE:H   | 11       | 0.13          |
| (1,208) | 3:96:A:SER:HA  | 3:106:A:PHE:H   | 18       | 0.13          |
| (1,208) | 3:96:A:SER:HA  | 3:106:A:PHE:H   | 19       | 0.13          |
| (1,197) | 3:81:A:HIS:HA  | 3:84:A:THR:HG21 | 1        | 0.13          |

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| Key     | Atom-1        | Atom-2          | Model ID | Violation (Å) |
|---------|---------------|-----------------|----------|---------------|
| (1,197) | 3:81:A:HIS:HA | 3:84:A:THR:HG22 | 1        | 0.13          |
| (1,197) | 3:81:A:HIS:HA | 3:84:A:THR:HG23 | 1        | 0.13          |
| (1,197) | 3:81:A:HIS:HA | 3:84:A:THR:HG21 | 10       | 0.13          |
| (1,197) | 3:81:A:HIS:HA | 3:84:A:THR:HG22 | 10       | 0.13          |
| (1,197) | 3:81:A:HIS:HA | 3:84:A:THR:HG23 | 10       | 0.13          |
| (1,197) | 3:81:A:HIS:HA | 3:84:A:THR:HG21 | 13       | 0.13          |
| (1,197) | 3:81:A:HIS:HA | 3:84:A:THR:HG22 | 13       | 0.13          |
| (1,197) | 3:81:A:HIS:HA | 3:84:A:THR:HG23 | 13       | 0.13          |
| (1,197) | 3:81:A:HIS:HA | 3:84:A:THR:HG21 | 15       | 0.13          |
| (1,197) | 3:81:A:HIS:HA | 3:84:A:THR:HG22 | 15       | 0.13          |
| (1,197) | 3:81:A:HIS:HA | 3:84:A:THR:HG23 | 15       | 0.13          |
| (1,142) | 3:77:A:SER:HA | 3:67:A:PHE:H    | 15       | 0.13          |
| (1,10)  | 3:19:A:PHE:HA | 3:7:A:PHE:H     | 13       | 0.13          |
| (1,10)  | 3:19:A:PHE:HA | 3:7:A:PHE:H     | 20       | 0.13          |
| (2,131) | 3:118:A:MET:N | 3:115:A:HIS:O   | 19       | 0.12          |
| (2,130) | 3:117:A:ASN:N | 3:114:A:ARG:O   | 11       | 0.12          |
| (2,128) | 3:115:A:HIS:N | 3:111:A:GLU:O   | 7        | 0.12          |
| (2,123) | 3:97:A:CYS:N  | 3:104:A:LYS:O   | 8        | 0.12          |
| (2,123) | 3:97:A:CYS:N  | 3:104:A:LYS:O   | 10       | 0.12          |
| (2,123) | 3:97:A:CYS:N  | 3:104:A:LYS:O   | 17       | 0.12          |
| (2,123) | 3:97:A:CYS:N  | 3:104:A:LYS:O   | 20       | 0.12          |
| (2,120) | 3:88:A:THR:N  | 3:85:A:HIS:O    | 16       | 0.12          |
| (2,116) | 3:84:A:THR:N  | 3:80:A:ASP:O    | 17       | 0.12          |
| (2,115) | 3:83:A:LYS:N  | 3:79:A:SER:O    | 19       | 0.12          |
| (2,112) | 3:69:A:CYS:N  | 3:74:A:ARG:O    | 6        | 0.12          |
| (2,110) | 3:61:A:HIS:N  | 3:58:A:GLN:O    | 3        | 0.12          |
| (2,106) | 3:57:A:HIS:N  | 3:53:A:GLN:O    | 12       | 0.12          |
| (2,101) | 3:39:A:CYS:N  | 3:46:A:ARG:O    | 5        | 0.12          |
| (2,101) | 3:39:A:CYS:N  | 3:46:A:ARG:O    | 15       | 0.12          |
| (2,99)  | 3:31:A:HIS:N  | 3:28:A:SER:O    | 11       | 0.12          |
| (2,98)  | 3:30:A:LYS:N  | 3:27:A:HIS:O    | 18       | 0.12          |
| (2,96)  | 3:28:A:SER:N  | 3:24:A:LEU:O    | 3        | 0.12          |
| (2,96)  | 3:28:A:SER:N  | 3:24:A:LEU:O    | 12       | 0.12          |
| (2,96)  | 3:28:A:SER:N  | 3:24:A:LEU:O    | 13       | 0.12          |
| (2,94)  | 3:26:A:MET:N  | 3:22:A:SER:O    | 1        | 0.12          |
| (2,94)  | 3:26:A:MET:N  | 3:22:A:SER:O    | 15       | 0.12          |
| (2,92)  | 3:24:A:LEU:N  | 3:20:A:LYS:O    | 14       | 0.12          |
| (2,87)  | 3:119:A:HIS:H | 3:116:A:HIS:O   | 14       | 0.12          |
| (2,83)  | 3:117:A:ASN:H | 3:114:A:ARG:O   | 7        | 0.12          |
| (2,73)  | 3:112:A:LEU:H | 3:108:A:ARG:O   | 4        | 0.12          |
| (2,73)  | 3:112:A:LEU:H | 3:108:A:ARG:O   | 7        | 0.12          |
| (2,73)  | 3:112:A:LEU:H | 3:108:A:ARG:O   | 13       | 0.12          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (2,73)  | 3:112:A:LEU:H  | 3:108:A:ARG:O   | 14       | 0.12          |
| (2,65)  | 3:89:A:HIS:H   | 3:86:A:THR:O    | 8        | 0.12          |
| (2,65)  | 3:89:A:HIS:H   | 3:86:A:THR:O    | 9        | 0.12          |
| (2,65)  | 3:89:A:HIS:H   | 3:86:A:THR:O    | 10       | 0.12          |
| (2,65)  | 3:89:A:HIS:H   | 3:86:A:THR:O    | 16       | 0.12          |
| (2,65)  | 3:89:A:HIS:H   | 3:86:A:THR:O    | 17       | 0.12          |
| (2,49)  | 3:67:A:PHE:H   | 3:76:A:PHE:O    | 7        | 0.12          |
| (2,49)  | 3:67:A:PHE:H   | 3:76:A:PHE:O    | 14       | 0.12          |
| (2,49)  | 3:67:A:PHE:H   | 3:76:A:PHE:O    | 16       | 0.12          |
| (2,39)  | 3:59:A:ARG:H   | 3:56:A:ARG:O    | 9        | 0.12          |
| (2,21)  | 3:31:A:HIS:H   | 3:28:A:SER:O    | 2        | 0.12          |
| (2,21)  | 3:31:A:HIS:H   | 3:28:A:SER:O    | 17       | 0.12          |
| (2,19)  | 3:30:A:LYS:H   | 3:27:A:HIS:O    | 4        | 0.12          |
| (2,17)  | 3:29:A:ARG:H   | 3:26:A:MET:O    | 10       | 0.12          |
| (2,17)  | 3:29:A:ARG:H   | 3:26:A:MET:O    | 12       | 0.12          |
| (2,17)  | 3:29:A:ARG:H   | 3:26:A:MET:O    | 19       | 0.12          |
| (2,7)   | 3:24:A:LEU:H   | 3:20:A:LYS:O    | 5        | 0.12          |
| (2,5)   | 3:7:A:PHE:H    | 3:18:A:TYR:O    | 13       | 0.12          |
| (2,3)   | 3:9:A:CYS:H    | 3:16:A:LYS:O    | 1        | 0.12          |
| (1,791) | 3:109:A:SER:CB | 2:150:C:DC:C3'  | 17       | 0.12          |
| (1,791) | 3:109:A:SER:CB | 2:150:C:DC:C3'  | 18       | 0.12          |
| (1,783) | 3:108:A:ARG:CD | 1:126:B:DC:C2'  | 18       | 0.12          |
| (1,762) | 2:149:C:DG:N7  | 3:80:A:ASP:CB   | 2        | 0.12          |
| (1,743) | 1:134:B:DT:C4  | 3:50:A:ARG:CZ   | 11       | 0.12          |
| (1,739) | 1:133:B:DG:C6  | 3:50:A:ARG:CZ   | 16       | 0.12          |
| (1,739) | 1:133:B:DG:C6  | 3:50:A:ARG:CZ   | 20       | 0.12          |
| (1,738) | 1:132:B:DC:C6  | 3:50:A:ARG:CZ   | 4        | 0.12          |
| (1,738) | 1:132:B:DC:C6  | 3:50:A:ARG:CZ   | 17       | 0.12          |
| (1,737) | 1:132:B:DC:C5  | 3:50:A:ARG:CZ   | 1        | 0.12          |
| (1,688) | 1:128:B:DG:C1' | 3:81:A:HIS:CE1  | 7        | 0.12          |
| (1,688) | 1:128:B:DG:C1' | 3:81:A:HIS:CE1  | 19       | 0.12          |
| (1,659) | 3:80:A:ASP:HA  | 2:150:C:DC:H6   | 10       | 0.12          |
| (1,638) | 3:110:A:ASP:CB | 3:113:A:VAL:CG2 | 2        | 0.12          |
| (1,638) | 3:110:A:ASP:CB | 3:113:A:VAL:CG2 | 4        | 0.12          |
| (1,638) | 3:110:A:ASP:CB | 3:113:A:VAL:CG2 | 6        | 0.12          |
| (1,638) | 3:110:A:ASP:CB | 3:113:A:VAL:CG2 | 8        | 0.12          |
| (1,638) | 3:110:A:ASP:CB | 3:113:A:VAL:CG2 | 10       | 0.12          |
| (1,638) | 3:110:A:ASP:CB | 3:113:A:VAL:CG2 | 13       | 0.12          |
| (1,638) | 3:110:A:ASP:CB | 3:113:A:VAL:CG2 | 16       | 0.12          |
| (1,638) | 3:110:A:ASP:CB | 3:113:A:VAL:CG2 | 18       | 0.12          |
| (1,583) | 3:97:A:CYS:CB  | 3:116:A:HIS:CE1 | 3        | 0.12          |
| (1,577) | 3:97:A:CYS:CB  | 3:99:A:TRP:CB   | 8        | 0.12          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,577) | 3:97:A:CYS:CB  | 3:99:A:TRP:CB   | 15       | 0.12          |
| (1,577) | 3:97:A:CYS:CB  | 3:99:A:TRP:CB   | 17       | 0.12          |
| (1,536) | 3:87:A:ARG:CA  | 3:90:A:THR:CG2  | 10       | 0.12          |
| (1,533) | 3:85:A:HIS:CE1 | 3:88:A:THR:CG2  | 11       | 0.12          |
| (1,533) | 3:85:A:HIS:CE1 | 3:88:A:THR:CG2  | 18       | 0.12          |
| (1,533) | 3:85:A:HIS:CE1 | 3:88:A:THR:CG2  | 20       | 0.12          |
| (1,502) | 3:76:A:PHE:CB  | 3:82:A:LEU:CD1  | 9        | 0.12          |
| (1,502) | 3:76:A:PHE:CB  | 3:82:A:LEU:CD1  | 17       | 0.12          |
| (1,502) | 3:76:A:PHE:CB  | 3:82:A:LEU:CD1  | 20       | 0.12          |
| (1,484) | 3:69:A:CYS:CA  | 3:74:A:ARG:CA   | 8        | 0.12          |
| (1,452) | 3:59:A:ARG:CA  | 3:62:A:THR:CG2  | 16       | 0.12          |
| (1,442) | 3:55:A:LYS:CA  | 3:58:A:GLN:CA   | 17       | 0.12          |
| (1,404) | 3:41:A:PHE:CE2 | 3:44:A:CYS:CB   | 20       | 0.12          |
| (1,382) | 3:38:A:GLN:CA  | 3:47:A:ARG:CA   | 11       | 0.12          |
| (1,356) | 3:24:A:LEU:CD2 | 3:27:A:HIS:CB   | 6        | 0.12          |
| (1,356) | 3:24:A:LEU:CD2 | 3:27:A:HIS:CB   | 18       | 0.12          |
| (1,331) | 3:18:A:TYR:CE2 | 3:27:A:HIS:CB   | 18       | 0.12          |
| (1,327) | 3:18:A:TYR:CE1 | 3:27:A:HIS:CB   | 7        | 0.12          |
| (1,327) | 3:18:A:TYR:CE1 | 3:27:A:HIS:CB   | 11       | 0.12          |
| (1,327) | 3:18:A:TYR:CE1 | 3:27:A:HIS:CB   | 17       | 0.12          |
| (1,319) | 3:18:A:TYR:CD1 | 3:24:A:LEU:CB   | 8        | 0.12          |
| (1,308) | 3:11:A:TYR:CD2 | 3:34:A:GLU:CB   | 11       | 0.12          |
| (1,308) | 3:11:A:TYR:CD2 | 3:34:A:GLU:CB   | 12       | 0.12          |
| (1,308) | 3:11:A:TYR:CD2 | 3:34:A:GLU:CB   | 15       | 0.12          |
| (1,304) | 3:11:A:TYR:CD2 | 3:14:A:CYS:CB   | 8        | 0.12          |
| (1,273) | 3:7:A:PHE:CE2  | 3:21:A:LEU:CB   | 10       | 0.12          |
| (1,211) | 3:96:A:SER:HA  | 3:104:A:LYS:H   | 10       | 0.12          |
| (1,211) | 3:96:A:SER:HA  | 3:104:A:LYS:H   | 14       | 0.12          |
| (1,208) | 3:96:A:SER:HA  | 3:106:A:PHE:H   | 13       | 0.12          |
| (1,200) | 3:83:A:LYS:HA  | 3:86:A:THR:HG21 | 13       | 0.12          |
| (1,200) | 3:83:A:LYS:HA  | 3:86:A:THR:HG22 | 13       | 0.12          |
| (1,200) | 3:83:A:LYS:HA  | 3:86:A:THR:HG23 | 13       | 0.12          |
| (1,197) | 3:81:A:HIS:HA  | 3:84:A:THR:HG21 | 6        | 0.12          |
| (1,197) | 3:81:A:HIS:HA  | 3:84:A:THR:HG22 | 6        | 0.12          |
| (1,197) | 3:81:A:HIS:HA  | 3:84:A:THR:HG23 | 6        | 0.12          |
| (1,197) | 3:81:A:HIS:HA  | 3:84:A:THR:HG21 | 18       | 0.12          |
| (1,197) | 3:81:A:HIS:HA  | 3:84:A:THR:HG22 | 18       | 0.12          |
| (1,197) | 3:81:A:HIS:HA  | 3:84:A:THR:HG23 | 18       | 0.12          |
| (1,143) | 3:68:A:GLN:HA  | 3:74:A:ARG:H    | 12       | 0.12          |
| (1,141) | 3:75:A:LYS:HA  | 3:69:A:CYS:H    | 16       | 0.12          |
| (1,140) | 3:68:A:GLN:HA  | 3:76:A:PHE:H    | 6        | 0.12          |
| (1,76)  | 3:49:A:SER:HA  | 3:37:A:TYR:H    | 13       | 0.12          |

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| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,13)  | 3:7:A:PHE:H   | 3:18:A:TYR:H  | 4        | 0.12          |
| (1,10)  | 3:19:A:PHE:HA | 3:7:A:PHE:H   | 17       | 0.12          |
| (2,131) | 3:118:A:MET:N | 3:115:A:HIS:O | 3        | 0.11          |
| (2,131) | 3:118:A:MET:N | 3:115:A:HIS:O | 18       | 0.11          |
| (2,128) | 3:115:A:HIS:N | 3:111:A:GLU:O | 8        | 0.11          |
| (2,128) | 3:115:A:HIS:N | 3:111:A:GLU:O | 17       | 0.11          |
| (2,127) | 3:114:A:ARG:N | 3:110:A:ASP:O | 7        | 0.11          |
| (2,120) | 3:88:A:THR:N  | 3:85:A:HIS:O  | 9        | 0.11          |
| (2,112) | 3:69:A:CYS:N  | 3:74:A:ARG:O  | 19       | 0.11          |
| (2,110) | 3:61:A:HIS:N  | 3:58:A:GLN:O  | 13       | 0.11          |
| (2,110) | 3:61:A:HIS:N  | 3:58:A:GLN:O  | 19       | 0.11          |
| (2,107) | 3:58:A:GLN:N  | 3:54:A:LEU:O  | 5        | 0.11          |
| (2,107) | 3:58:A:GLN:N  | 3:54:A:LEU:O  | 10       | 0.11          |
| (2,107) | 3:58:A:GLN:N  | 3:54:A:LEU:O  | 14       | 0.11          |
| (2,106) | 3:57:A:HIS:N  | 3:53:A:GLN:O  | 2        | 0.11          |
| (2,106) | 3:57:A:HIS:N  | 3:53:A:GLN:O  | 16       | 0.11          |
| (2,105) | 3:56:A:ARG:N  | 3:52:A:ASP:O  | 1        | 0.11          |
| (2,105) | 3:56:A:ARG:N  | 3:52:A:ASP:O  | 15       | 0.11          |
| (2,105) | 3:56:A:ARG:N  | 3:52:A:ASP:O  | 18       | 0.11          |
| (2,104) | 3:55:A:LYS:N  | 3:51:A:SER:O  | 5        | 0.11          |
| (2,99)  | 3:31:A:HIS:N  | 3:28:A:SER:O  | 12       | 0.11          |
| (2,96)  | 3:28:A:SER:N  | 3:24:A:LEU:O  | 9        | 0.11          |
| (2,94)  | 3:26:A:MET:N  | 3:22:A:SER:O  | 13       | 0.11          |
| (2,92)  | 3:24:A:LEU:N  | 3:20:A:LYS:O  | 1        | 0.11          |
| (2,92)  | 3:24:A:LEU:N  | 3:20:A:LYS:O  | 12       | 0.11          |
| (2,83)  | 3:117:A:ASN:H | 3:114:A:ARG:O | 19       | 0.11          |
| (2,79)  | 3:115:A:HIS:H | 3:111:A:GLU:O | 3        | 0.11          |
| (2,73)  | 3:112:A:LEU:H | 3:108:A:ARG:O | 3        | 0.11          |
| (2,73)  | 3:112:A:LEU:H | 3:108:A:ARG:O | 6        | 0.11          |
| (2,73)  | 3:112:A:LEU:H | 3:108:A:ARG:O | 8        | 0.11          |
| (2,73)  | 3:112:A:LEU:H | 3:108:A:ARG:O | 11       | 0.11          |
| (2,73)  | 3:112:A:LEU:H | 3:108:A:ARG:O | 12       | 0.11          |
| (2,73)  | 3:112:A:LEU:H | 3:108:A:ARG:O | 15       | 0.11          |
| (2,73)  | 3:112:A:LEU:H | 3:108:A:ARG:O | 16       | 0.11          |
| (2,73)  | 3:112:A:LEU:H | 3:108:A:ARG:O | 17       | 0.11          |
| (2,73)  | 3:112:A:LEU:H | 3:108:A:ARG:O | 19       | 0.11          |
| (2,73)  | 3:112:A:LEU:H | 3:108:A:ARG:O | 20       | 0.11          |
| (2,65)  | 3:89:A:HIS:H  | 3:86:A:THR:O  | 18       | 0.11          |
| (2,49)  | 3:67:A:PHE:H  | 3:76:A:PHE:O  | 3        | 0.11          |
| (2,43)  | 3:61:A:HIS:H  | 3:58:A:GLN:O  | 1        | 0.11          |
| (2,43)  | 3:61:A:HIS:H  | 3:58:A:GLN:O  | 17       | 0.11          |
| (2,39)  | 3:59:A:ARG:H  | 3:56:A:ARG:O  | 5        | 0.11          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (2,21)  | 3:31:A:HIS:H   | 3:28:A:SER:O    | 9        | 0.11          |
| (2,19)  | 3:30:A:LYS:H   | 3:27:A:HIS:O    | 3        | 0.11          |
| (2,19)  | 3:30:A:LYS:H   | 3:27:A:HIS:O    | 9        | 0.11          |
| (2,19)  | 3:30:A:LYS:H   | 3:27:A:HIS:O    | 13       | 0.11          |
| (2,19)  | 3:30:A:LYS:H   | 3:27:A:HIS:O    | 19       | 0.11          |
| (2,17)  | 3:29:A:ARG:H   | 3:26:A:MET:O    | 6        | 0.11          |
| (2,17)  | 3:29:A:ARG:H   | 3:26:A:MET:O    | 14       | 0.11          |
| (2,17)  | 3:29:A:ARG:H   | 3:26:A:MET:O    | 15       | 0.11          |
| (2,15)  | 3:28:A:SER:H   | 3:24:A:LEU:O    | 16       | 0.11          |
| (2,5)   | 3:7:A:PHE:H    | 3:18:A:TYR:O    | 11       | 0.11          |
| (2,5)   | 3:7:A:PHE:H    | 3:18:A:TYR:O    | 20       | 0.11          |
| (1,791) | 3:109:A:SER:CB | 2:150:C:DC:C3'  | 6        | 0.11          |
| (1,791) | 3:109:A:SER:CB | 2:150:C:DC:C3'  | 13       | 0.11          |
| (1,791) | 3:109:A:SER:CB | 2:150:C:DC:C3'  | 14       | 0.11          |
| (1,781) | 2:154:C:DC:N4  | 3:114:A:ARG:CZ  | 14       | 0.11          |
| (1,768) | 2:150:C:DC:N4  | 3:80:A:ASP:CG   | 8        | 0.11          |
| (1,764) | 2:149:C:DG:C8  | 3:80:A:ASP:CB   | 1        | 0.11          |
| (1,763) | 2:149:C:DG:N7  | 3:80:A:ASP:CG   | 8        | 0.11          |
| (1,762) | 2:149:C:DG:N7  | 3:80:A:ASP:CB   | 11       | 0.11          |
| (1,752) | 2:147:C:DA:N6  | 3:52:A:ASP:CG   | 17       | 0.11          |
| (1,740) | 1:133:B:DG:C5  | 3:50:A:ARG:CZ   | 2        | 0.11          |
| (1,739) | 1:133:B:DG:C6  | 3:50:A:ARG:CZ   | 5        | 0.11          |
| (1,739) | 1:133:B:DG:C6  | 3:50:A:ARG:CZ   | 13       | 0.11          |
| (1,738) | 1:132:B:DC:C6  | 3:50:A:ARG:CZ   | 1        | 0.11          |
| (1,738) | 1:132:B:DC:C6  | 3:50:A:ARG:CZ   | 3        | 0.11          |
| (1,737) | 1:132:B:DC:C5  | 3:50:A:ARG:CZ   | 16       | 0.11          |
| (1,715) | 1:129:B:DG:C2' | 3:78:A:ARG:CZ   | 1        | 0.11          |
| (1,715) | 1:129:B:DG:C2' | 3:78:A:ARG:CZ   | 9        | 0.11          |
| (1,706) | 1:129:B:DG:C5' | 3:60:A:ARG:CD   | 1        | 0.11          |
| (1,706) | 1:129:B:DG:C5' | 3:60:A:ARG:CD   | 7        | 0.11          |
| (1,706) | 1:129:B:DG:C5' | 3:60:A:ARG:CD   | 14       | 0.11          |
| (1,706) | 1:129:B:DG:C5' | 3:60:A:ARG:CD   | 18       | 0.11          |
| (1,696) | 1:128:B:DG:N7  | 3:81:A:HIS:CB   | 9        | 0.11          |
| (1,683) | 1:127:B:DG:C6  | 3:108:A:ARG:CZ  | 4        | 0.11          |
| (1,680) | 1:127:B:DG:C4' | 3:74:A:ARG:CZ   | 6        | 0.11          |
| (1,670) | 1:126:B:DC:N4  | 3:108:A:ARG:CZ  | 20       | 0.11          |
| (1,659) | 3:80:A:ASP:HA  | 2:150:C:DC:H6   | 4        | 0.11          |
| (1,659) | 3:80:A:ASP:HA  | 2:150:C:DC:H6   | 7        | 0.11          |
| (1,638) | 3:110:A:ASP:CB | 3:113:A:VAL:CG2 | 20       | 0.11          |
| (1,585) | 3:98:A:ARG:CB  | 3:116:A:HIS:CE1 | 16       | 0.11          |
| (1,577) | 3:97:A:CYS:CB  | 3:99:A:TRP:CB   | 1        | 0.11          |
| (1,545) | 3:93:A:LYS:CB  | 3:106:A:PHE:CA  | 10       | 0.11          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,509) | 3:76:A:PHE:CE2 | 3:85:A:HIS:CD2 | 16       | 0.11          |
| (1,502) | 3:76:A:PHE:CB  | 3:82:A:LEU:CD1 | 1        | 0.11          |
| (1,502) | 3:76:A:PHE:CB  | 3:82:A:LEU:CD1 | 18       | 0.11          |
| (1,498) | 3:72:A:CYS:CB  | 3:89:A:HIS:CE1 | 13       | 0.11          |
| (1,487) | 3:69:A:CYS:CB  | 3:72:A:CYS:CB  | 20       | 0.11          |
| (1,465) | 3:67:A:PHE:CB  | 3:82:A:LEU:CD1 | 16       | 0.11          |
| (1,458) | 3:65:A:LYS:CB  | 3:76:A:PHE:CA  | 1        | 0.11          |
| (1,452) | 3:59:A:ARG:CA  | 3:62:A:THR:CG2 | 6        | 0.11          |
| (1,442) | 3:55:A:LYS:CA  | 3:58:A:GLN:CA  | 1        | 0.11          |
| (1,442) | 3:55:A:LYS:CA  | 3:58:A:GLN:CA  | 14       | 0.11          |
| (1,440) | 3:54:A:LEU:CA  | 3:57:A:HIS:CB  | 15       | 0.11          |
| (1,440) | 3:54:A:LEU:CA  | 3:57:A:HIS:CB  | 20       | 0.11          |
| (1,428) | 3:48:A:PHE:CE2 | 3:57:A:HIS:CD2 | 11       | 0.11          |
| (1,404) | 3:41:A:PHE:CE2 | 3:44:A:CYS:CB  | 12       | 0.11          |
| (1,404) | 3:41:A:PHE:CE2 | 3:44:A:CYS:CB  | 19       | 0.11          |
| (1,388) | 3:39:A:CYS:CB  | 3:41:A:PHE:CB  | 11       | 0.11          |
| (1,386) | 3:38:A:GLN:CB  | 3:47:A:ARG:CB  | 1        | 0.11          |
| (1,382) | 3:38:A:GLN:CA  | 3:47:A:ARG:CA  | 4        | 0.11          |
| (1,376) | 3:37:A:TYR:CE2 | 3:51:A:SER:CB  | 16       | 0.11          |
| (1,370) | 3:37:A:TYR:CB  | 3:48:A:PHE:CB  | 5        | 0.11          |
| (1,365) | 3:29:A:ARG:CA  | 3:32:A:THR:CG2 | 2        | 0.11          |
| (1,356) | 3:24:A:LEU:CD2 | 3:27:A:HIS:CB  | 3        | 0.11          |
| (1,356) | 3:24:A:LEU:CD2 | 3:27:A:HIS:CB  | 8        | 0.11          |
| (1,356) | 3:24:A:LEU:CD2 | 3:27:A:HIS:CB  | 15       | 0.11          |
| (1,356) | 3:24:A:LEU:CD2 | 3:27:A:HIS:CB  | 17       | 0.11          |
| (1,341) | 3:19:A:PHE:CB  | 3:23:A:HIS:CD2 | 9        | 0.11          |
| (1,338) | 3:18:A:TYR:CD2 | 3:27:A:HIS:CD2 | 3        | 0.11          |
| (1,338) | 3:18:A:TYR:CD2 | 3:27:A:HIS:CD2 | 6        | 0.11          |
| (1,333) | 3:18:A:TYR:CE2 | 3:27:A:HIS:CE1 | 7        | 0.11          |
| (1,332) | 3:18:A:TYR:CE2 | 3:27:A:HIS:CD2 | 9        | 0.11          |
| (1,331) | 3:18:A:TYR:CE2 | 3:27:A:HIS:CB  | 16       | 0.11          |
| (1,327) | 3:18:A:TYR:CE1 | 3:27:A:HIS:CB  | 19       | 0.11          |
| (1,324) | 3:18:A:TYR:CE1 | 3:24:A:LEU:CA  | 1        | 0.11          |
| (1,319) | 3:18:A:TYR:CD1 | 3:24:A:LEU:CB  | 16       | 0.11          |
| (1,304) | 3:11:A:TYR:CD2 | 3:14:A:CYS:CB  | 10       | 0.11          |
| (1,304) | 3:11:A:TYR:CD2 | 3:14:A:CYS:CB  | 11       | 0.11          |
| (1,301) | 3:11:A:TYR:CE2 | 3:31:A:HIS:CB  | 16       | 0.11          |
| (1,299) | 3:11:A:TYR:CE1 | 3:34:A:GLU:CA  | 3        | 0.11          |
| (1,294) | 3:11:A:TYR:CD1 | 3:31:A:HIS:CB  | 7        | 0.11          |
| (1,288) | 3:11:A:TYR:CA  | 3:31:A:HIS:CE1 | 20       | 0.11          |
| (1,282) | 3:9:A:CYS:CA   | 3:27:A:HIS:CD2 | 10       | 0.11          |
| (1,211) | 3:96:A:SER:HA  | 3:104:A:LYS:H  | 5        | 0.11          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,211) | 3:96:A:SER:HA  | 3:104:A:LYS:H   | 12       | 0.11          |
| (1,209) | 3:105:A:LYS:HA | 3:97:A:CYS:H    | 5        | 0.11          |
| (1,209) | 3:105:A:LYS:HA | 3:97:A:CYS:H    | 15       | 0.11          |
| (1,209) | 3:105:A:LYS:HA | 3:97:A:CYS:H    | 18       | 0.11          |
| (1,208) | 3:96:A:SER:HA  | 3:106:A:PHE:H   | 9        | 0.11          |
| (1,200) | 3:83:A:LYS:HA  | 3:86:A:THR:HG21 | 8        | 0.11          |
| (1,200) | 3:83:A:LYS:HA  | 3:86:A:THR:HG22 | 8        | 0.11          |
| (1,200) | 3:83:A:LYS:HA  | 3:86:A:THR:HG23 | 8        | 0.11          |
| (1,197) | 3:81:A:HIS:HA  | 3:84:A:THR:HG21 | 2        | 0.11          |
| (1,197) | 3:81:A:HIS:HA  | 3:84:A:THR:HG22 | 2        | 0.11          |
| (1,197) | 3:81:A:HIS:HA  | 3:84:A:THR:HG23 | 2        | 0.11          |
| (1,197) | 3:81:A:HIS:HA  | 3:84:A:THR:HG21 | 3        | 0.11          |
| (1,197) | 3:81:A:HIS:HA  | 3:84:A:THR:HG22 | 3        | 0.11          |
| (1,197) | 3:81:A:HIS:HA  | 3:84:A:THR:HG23 | 3        | 0.11          |
| (1,197) | 3:81:A:HIS:HA  | 3:84:A:THR:HG21 | 7        | 0.11          |
| (1,197) | 3:81:A:HIS:HA  | 3:84:A:THR:HG22 | 7        | 0.11          |
| (1,197) | 3:81:A:HIS:HA  | 3:84:A:THR:HG23 | 7        | 0.11          |
| (1,197) | 3:81:A:HIS:HA  | 3:84:A:THR:HG21 | 8        | 0.11          |
| (1,197) | 3:81:A:HIS:HA  | 3:84:A:THR:HG22 | 8        | 0.11          |
| (1,197) | 3:81:A:HIS:HA  | 3:84:A:THR:HG23 | 8        | 0.11          |
| (1,197) | 3:81:A:HIS:HA  | 3:84:A:THR:HG21 | 11       | 0.11          |
| (1,197) | 3:81:A:HIS:HA  | 3:84:A:THR:HG22 | 11       | 0.11          |
| (1,197) | 3:81:A:HIS:HA  | 3:84:A:THR:HG23 | 11       | 0.11          |
| (1,143) | 3:68:A:GLN:HA  | 3:74:A:ARG:H    | 15       | 0.11          |
| (1,142) | 3:77:A:SER:HA  | 3:67:A:PHE:H    | 17       | 0.11          |
| (1,141) | 3:75:A:LYS:HA  | 3:69:A:CYS:H    | 8        | 0.11          |
| (1,141) | 3:75:A:LYS:HA  | 3:69:A:CYS:H    | 9        | 0.11          |
| (1,141) | 3:75:A:LYS:HA  | 3:69:A:CYS:H    | 17       | 0.11          |
| (1,76)  | 3:49:A:SER:HA  | 3:37:A:TYR:H    | 7        | 0.11          |
| (1,75)  | 3:47:A:ARG:HA  | 3:39:A:CYS:H    | 13       | 0.11          |
| (1,13)  | 3:7:A:PHE:H    | 3:18:A:TYR:H    | 12       | 0.11          |
| (1,11)  | 3:8:A:MET:HA   | 3:16:A:LYS:H    | 16       | 0.11          |
| (1,10)  | 3:19:A:PHE:HA  | 3:7:A:PHE:H     | 5        | 0.11          |
| (1,10)  | 3:19:A:PHE:HA  | 3:7:A:PHE:H     | 6        | 0.11          |
| (1,10)  | 3:19:A:PHE:HA  | 3:7:A:PHE:H     | 11       | 0.11          |
| (1,10)  | 3:19:A:PHE:HA  | 3:7:A:PHE:H     | 16       | 0.11          |
| (1,10)  | 3:19:A:PHE:HA  | 3:7:A:PHE:H     | 18       | 0.11          |
| (1,9)   | 3:17:A:ARG:HA  | 3:9:A:CYS:H     | 15       | 0.11          |
| (2,131) | 3:118:A:MET:N  | 3:115:A:HIS:O   | 6        | 0.1           |
| (2,127) | 3:114:A:ARG:N  | 3:110:A:ASP:O   | 18       | 0.1           |
| (2,123) | 3:97:A:CYS:N   | 3:104:A:LYS:O   | 18       | 0.1           |
| (2,107) | 3:58:A:GLN:N   | 3:54:A:LEU:O    | 13       | 0.1           |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (2,101) | 3:39:A:CYS:N   | 3:46:A:ARG:O    | 17       | 0.1           |
| (2,99)  | 3:31:A:HIS:N   | 3:28:A:SER:O    | 3        | 0.1           |
| (2,94)  | 3:26:A:MET:N   | 3:22:A:SER:O    | 14       | 0.1           |
| (2,87)  | 3:119:A:HIS:H  | 3:116:A:HIS:O   | 9        | 0.1           |
| (2,87)  | 3:119:A:HIS:H  | 3:116:A:HIS:O   | 16       | 0.1           |
| (2,73)  | 3:112:A:LEU:H  | 3:108:A:ARG:O   | 1        | 0.1           |
| (2,73)  | 3:112:A:LEU:H  | 3:108:A:ARG:O   | 2        | 0.1           |
| (2,73)  | 3:112:A:LEU:H  | 3:108:A:ARG:O   | 10       | 0.1           |
| (2,55)  | 3:84:A:THR:H   | 3:80:A:ASP:O    | 7        | 0.1           |
| (2,29)  | 3:54:A:LEU:H   | 3:50:A:ARG:O    | 16       | 0.1           |
| (2,21)  | 3:31:A:HIS:H   | 3:28:A:SER:O    | 8        | 0.1           |
| (2,19)  | 3:30:A:LYS:H   | 3:27:A:HIS:O    | 8        | 0.1           |
| (2,17)  | 3:29:A:ARG:H   | 3:26:A:MET:O    | 4        | 0.1           |
| (2,13)  | 3:27:A:HIS:H   | 3:23:A:HIS:O    | 3        | 0.1           |
| (2,13)  | 3:27:A:HIS:H   | 3:23:A:HIS:O    | 5        | 0.1           |
| (1,791) | 3:109:A:SER:CB | 2:150:C:DC:C3'  | 11       | 0.1           |
| (1,764) | 2:149:C:DG:C8  | 3:80:A:ASP:CB   | 8        | 0.1           |
| (1,764) | 2:149:C:DG:C8  | 3:80:A:ASP:CB   | 18       | 0.1           |
| (1,762) | 2:149:C:DG:N7  | 3:80:A:ASP:CB   | 9        | 0.1           |
| (1,744) | 1:134:B:DT:C5  | 3:50:A:ARG:CZ   | 13       | 0.1           |
| (1,739) | 1:133:B:DG:C6  | 3:50:A:ARG:CZ   | 3        | 0.1           |
| (1,726) | 1:129:B:DG:C8  | 3:81:A:HIS:CE1  | 7        | 0.1           |
| (1,721) | 1:129:B:DG:C5  | 3:81:A:HIS:CE1  | 20       | 0.1           |
| (1,706) | 1:129:B:DG:C5' | 3:60:A:ARG:CD   | 9        | 0.1           |
| (1,706) | 1:129:B:DG:C5' | 3:60:A:ARG:CD   | 10       | 0.1           |
| (1,706) | 1:129:B:DG:C5' | 3:60:A:ARG:CD   | 13       | 0.1           |
| (1,706) | 1:129:B:DG:C5' | 3:60:A:ARG:CD   | 15       | 0.1           |
| (1,696) | 1:128:B:DG:N7  | 3:81:A:HIS:CB   | 8        | 0.1           |
| (1,696) | 1:128:B:DG:N7  | 3:81:A:HIS:CB   | 15       | 0.1           |
| (1,691) | 1:128:B:DG:C6  | 3:81:A:HIS:CE1  | 14       | 0.1           |
| (1,659) | 3:80:A:ASP:HA  | 2:150:C:DC:H6   | 1        | 0.1           |
| (1,659) | 3:80:A:ASP:HA  | 2:150:C:DC:H6   | 9        | 0.1           |
| (1,659) | 3:80:A:ASP:HA  | 2:150:C:DC:H6   | 11       | 0.1           |
| (1,638) | 3:110:A:ASP:CB | 3:113:A:VAL:CG2 | 14       | 0.1           |
| (1,638) | 3:110:A:ASP:CB | 3:113:A:VAL:CG2 | 19       | 0.1           |
| (1,583) | 3:97:A:CYS:CB  | 3:116:A:HIS:CE1 | 2        | 0.1           |
| (1,577) | 3:97:A:CYS:CB  | 3:99:A:TRP:CB   | 2        | 0.1           |
| (1,577) | 3:97:A:CYS:CB  | 3:99:A:TRP:CB   | 7        | 0.1           |
| (1,509) | 3:76:A:PHE:CE2 | 3:85:A:HIS:CD2  | 7        | 0.1           |
| (1,484) | 3:69:A:CYS:CA  | 3:74:A:ARG:CA   | 1        | 0.1           |
| (1,458) | 3:65:A:LYS:CB  | 3:76:A:PHE:CA   | 17       | 0.1           |
| (1,452) | 3:59:A:ARG:CA  | 3:62:A:THR:CG2  | 14       | 0.1           |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,448) | 3:58:A:GLN:CA  | 3:62:A:THR:CG2  | 13       | 0.1           |
| (1,440) | 3:54:A:LEU:CA  | 3:57:A:HIS:CB   | 2        | 0.1           |
| (1,428) | 3:48:A:PHE:CE2 | 3:57:A:HIS:CD2  | 1        | 0.1           |
| (1,392) | 3:41:A:PHE:CA  | 3:44:A:CYS:CB   | 10       | 0.1           |
| (1,382) | 3:38:A:GLN:CA  | 3:47:A:ARG:CA   | 8        | 0.1           |
| (1,368) | 3:31:A:HIS:CB  | 3:34:A:GLU:CB   | 19       | 0.1           |
| (1,341) | 3:19:A:PHE:CB  | 3:23:A:HIS:CD2  | 12       | 0.1           |
| (1,341) | 3:19:A:PHE:CB  | 3:23:A:HIS:CD2  | 17       | 0.1           |
| (1,329) | 3:18:A:TYR:CE2 | 3:24:A:LEU:CB   | 5        | 0.1           |
| (1,308) | 3:11:A:TYR:CD2 | 3:34:A:GLU:CB   | 8        | 0.1           |
| (1,300) | 3:11:A:TYR:CE1 | 3:34:A:GLU:CB   | 8        | 0.1           |
| (1,299) | 3:11:A:TYR:CE1 | 3:34:A:GLU:CA   | 16       | 0.1           |
| (1,299) | 3:11:A:TYR:CE1 | 3:34:A:GLU:CA   | 20       | 0.1           |
| (1,288) | 3:11:A:TYR:CA  | 3:31:A:HIS:CE1  | 7        | 0.1           |
| (1,288) | 3:11:A:TYR:CA  | 3:31:A:HIS:CE1  | 19       | 0.1           |
| (1,270) | 3:7:A:PHE:CE1  | 3:21:A:LEU:CD1  | 8        | 0.1           |
| (1,268) | 3:7:A:PHE:CE1  | 3:21:A:LEU:CA   | 7        | 0.1           |
| (1,262) | 3:7:A:PHE:CB   | 3:18:A:TYR:CB   | 12       | 0.1           |
| (1,262) | 3:7:A:PHE:CB   | 3:18:A:TYR:CB   | 16       | 0.1           |
| (1,211) | 3:96:A:SER:HA  | 3:104:A:LYS:H   | 16       | 0.1           |
| (1,211) | 3:96:A:SER:HA  | 3:104:A:LYS:H   | 17       | 0.1           |
| (1,208) | 3:96:A:SER:HA  | 3:106:A:PHE:H   | 2        | 0.1           |
| (1,208) | 3:96:A:SER:HA  | 3:106:A:PHE:H   | 7        | 0.1           |
| (1,208) | 3:96:A:SER:HA  | 3:106:A:PHE:H   | 14       | 0.1           |
| (1,200) | 3:83:A:LYS:HA  | 3:86:A:THR:HG21 | 19       | 0.1           |
| (1,200) | 3:83:A:LYS:HA  | 3:86:A:THR:HG22 | 19       | 0.1           |
| (1,200) | 3:83:A:LYS:HA  | 3:86:A:THR:HG23 | 19       | 0.1           |
| (1,197) | 3:81:A:HIS:HA  | 3:84:A:THR:HG21 | 12       | 0.1           |
| (1,197) | 3:81:A:HIS:HA  | 3:84:A:THR:HG22 | 12       | 0.1           |
| (1,197) | 3:81:A:HIS:HA  | 3:84:A:THR:HG23 | 12       | 0.1           |
| (1,143) | 3:68:A:GLN:HA  | 3:74:A:ARG:H    | 1        | 0.1           |
| (1,140) | 3:68:A:GLN:HA  | 3:76:A:PHE:H    | 7        | 0.1           |
| (1,77)  | 3:38:A:GLN:HA  | 3:46:A:ARG:H    | 5        | 0.1           |
| (1,74)  | 3:38:A:GLN:HA  | 3:48:A:PHE:H    | 7        | 0.1           |
| (1,11)  | 3:8:A:MET:HA   | 3:16:A:LYS:H    | 11       | 0.1           |
| (1,11)  | 3:8:A:MET:HA   | 3:16:A:LYS:H    | 20       | 0.1           |

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

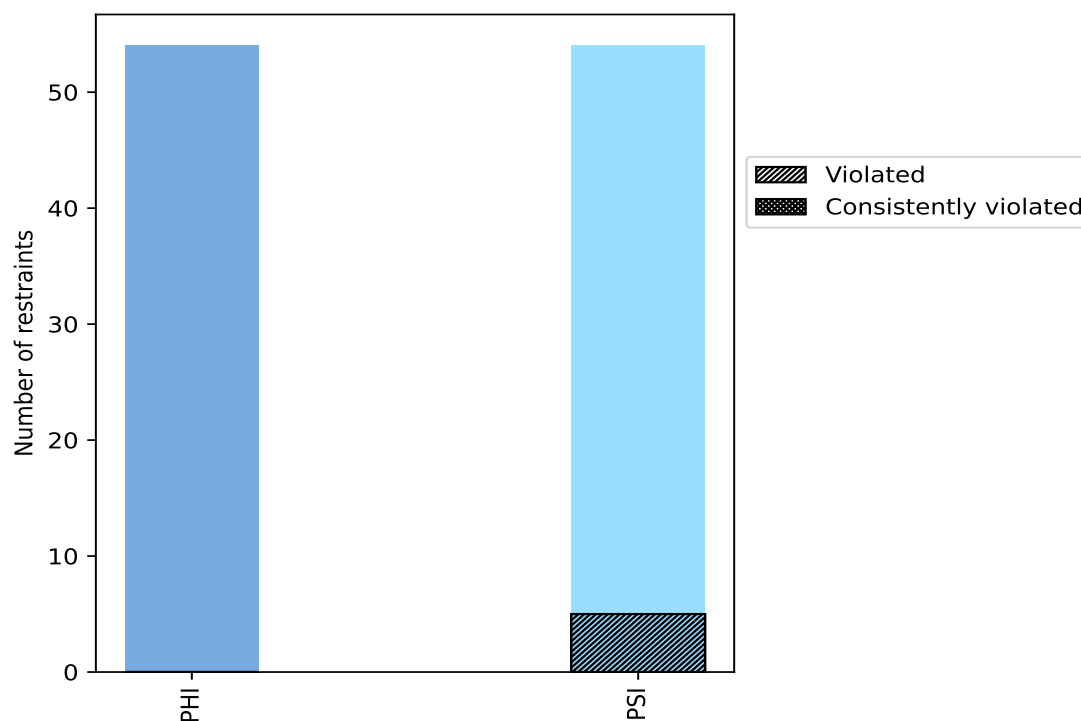
### 10.1 Summary of dihedral-angle violations [i](#)

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> |
| PHI        | 54    | 50.0           | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| PSI        | 54    | 50.0           | 5                     | 9.3            | 4.6            | 0                                  | 0.0            | 0.0            |
| Total      | 108   | 100.0          | 5                     | 4.6            | 4.6            | 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](#)



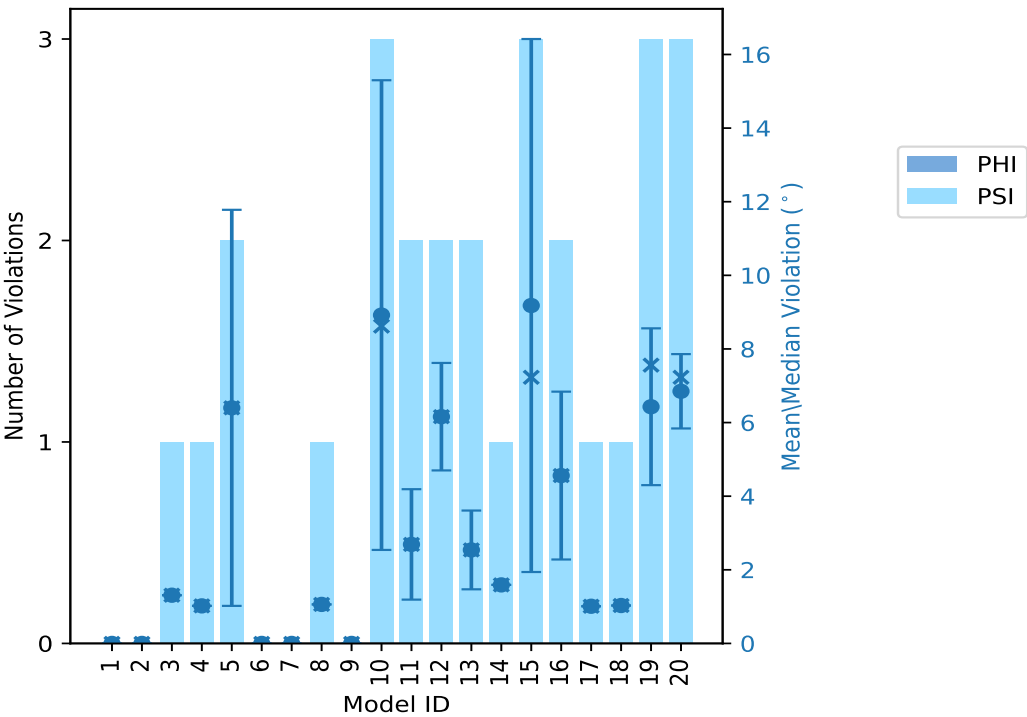
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

## 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 (°) |
|----------|----------------------|-----|-------|----------|---------|--------|------------|
|          | PHI                  | PSI | Total |          |         |        |            |
| 1        | 0                    | 0   | 0     | 0.0      | 0.0     | 0.0    | 0.0        |
| 2        | 0                    | 0   | 0     | 0.0      | 0.0     | 0.0    | 0.0        |
| 3        | 0                    | 1   | 1     | 1.31     | 1.31    | 0.0    | 1.31       |
| 4        | 0                    | 1   | 1     | 1.02     | 1.02    | 0.0    | 1.02       |
| 5        | 0                    | 2   | 2     | 6.4      | 11.78   | 5.38   | 6.4        |
| 6        | 0                    | 0   | 0     | 0.0      | 0.0     | 0.0    | 0.0        |
| 7        | 0                    | 0   | 0     | 0.0      | 0.0     | 0.0    | 0.0        |
| 8        | 0                    | 1   | 1     | 1.06     | 1.06    | 0.0    | 1.06       |
| 9        | 0                    | 0   | 0     | 0.0      | 0.0     | 0.0    | 0.0        |
| 10       | 0                    | 3   | 3     | 8.92     | 16.88   | 6.38   | 8.62       |
| 11       | 0                    | 2   | 2     | 2.69     | 4.19    | 1.5    | 2.69       |
| 12       | 0                    | 2   | 2     | 6.16     | 7.62    | 1.46   | 6.16       |
| 13       | 0                    | 2   | 2     | 2.54     | 3.61    | 1.07   | 2.54       |
| 14       | 0                    | 1   | 1     | 1.59     | 1.59    | 0.0    | 1.59       |
| 15       | 0                    | 3   | 3     | 9.18     | 18.87   | 7.24   | 7.23       |
| 16       | 0                    | 2   | 2     | 4.56     | 6.84    | 2.28   | 4.56       |
| 17       | 0                    | 1   | 1     | 1.01     | 1.01    | 0.0    | 1.01       |
| 18       | 0                    | 1   | 1     | 1.03     | 1.03    | 0.0    | 1.03       |
| 19       | 0                    | 3   | 3     | 6.43     | 8.28    | 2.13   | 7.56       |
| 20       | 0                    | 3   | 3     | 6.85     | 7.86    | 1.01   | 7.23       |

10.2.1 Bar graph : Dihedral 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

10.3 Dihedral-angle violation statistics for the ensemble [i](#)

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 |      |
|-------------------------------|-----|-------|--------------------------|------|
| PHI                           | PSI | Total | Count <sup>1</sup>       | %    |
| 0                             | 1   | 1     | 1                        | 5.0  |
| 0                             | 0   | 0     | 2                        | 10.0 |
| 0                             | 0   | 0     | 3                        | 15.0 |
| 0                             | 0   | 0     | 4                        | 20.0 |
| 0                             | 1   | 1     | 5                        | 25.0 |
| 0                             | 0   | 0     | 6                        | 30.0 |
| 0                             | 2   | 2     | 7                        | 35.0 |
| 0                             | 1   | 1     | 8                        | 40.0 |
| 0                             | 0   | 0     | 9                        | 45.0 |
| 0                             | 0   | 0     | 10                       | 50.0 |
| 0                             | 0   | 0     | 11                       | 55.0 |

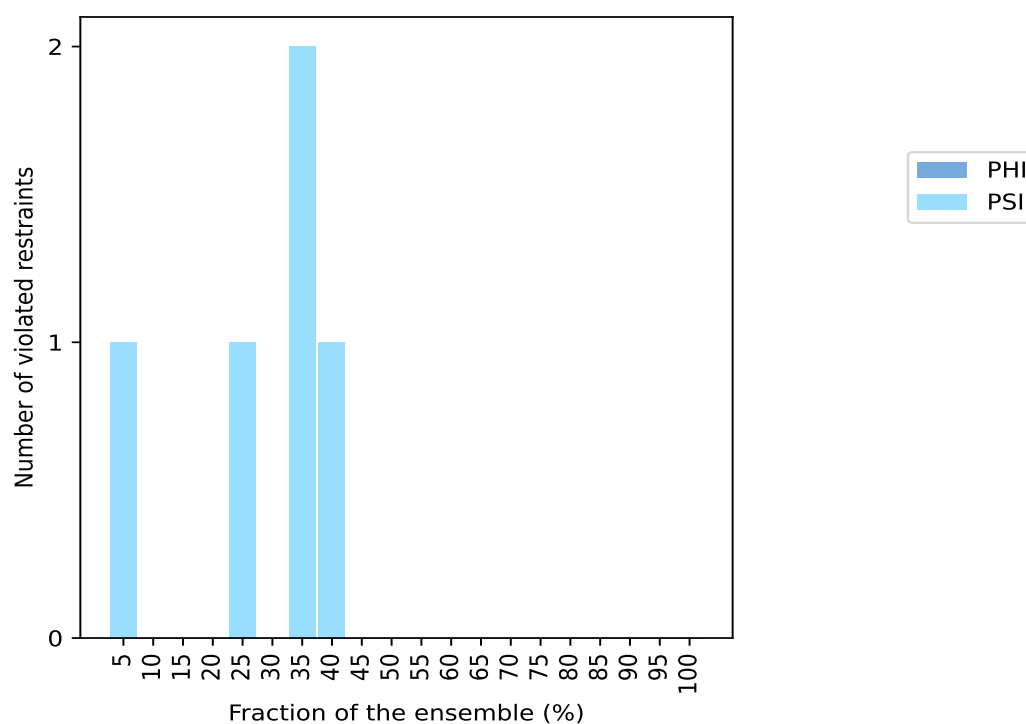
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| Number of violated restraints |     |       | Fraction of the ensemble |       |
|-------------------------------|-----|-------|--------------------------|-------|
| PHI                           | PSI | Total | Count <sup>1</sup>       | %     |
| 0                             | 0   | 0     | 12                       | 60.0  |
| 0                             | 0   | 0     | 13                       | 65.0  |
| 0                             | 0   | 0     | 14                       | 70.0  |
| 0                             | 0   | 0     | 15                       | 75.0  |
| 0                             | 0   | 0     | 16                       | 80.0  |
| 0                             | 0   | 0     | 17                       | 85.0  |
| 0                             | 0   | 0     | 18                       | 90.0  |
| 0                             | 0   | 0     | 19                       | 95.0  |
| 0                             | 0   | 0     | 20                       | 100.0 |

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

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

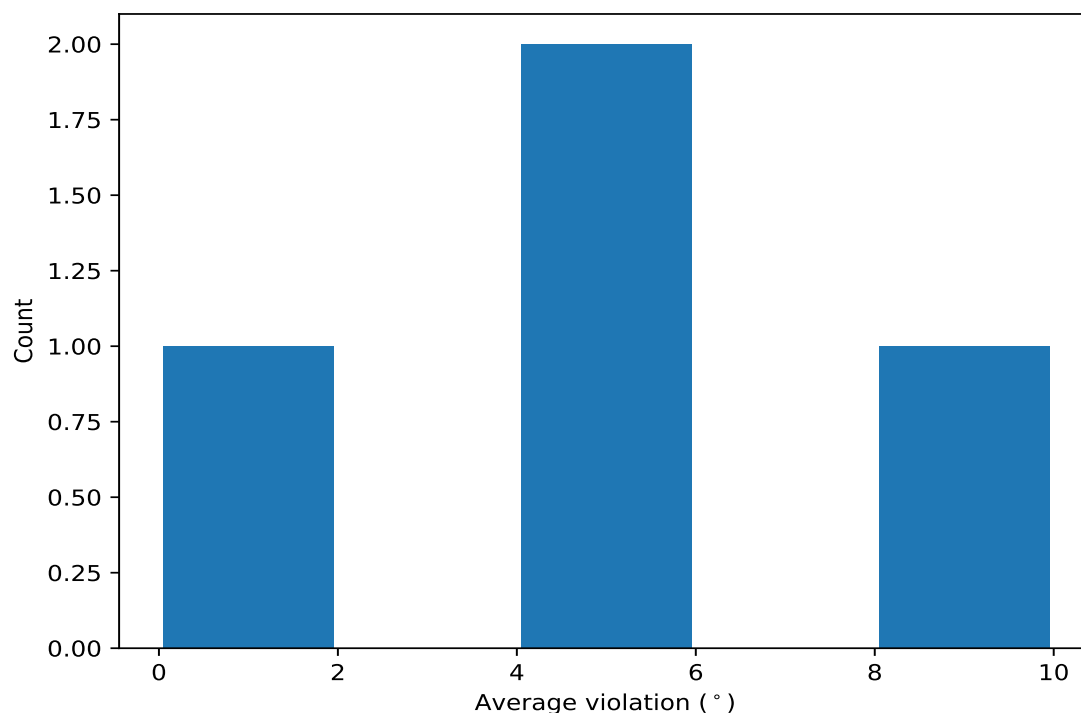


## 10.4 Most violated dihedral-angle restraints in the ensemble ⓘ

### 10.4.1 Histogram : Distribution of mean dihedral-angle violations ⓘ

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

in the ensemble



#### 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.

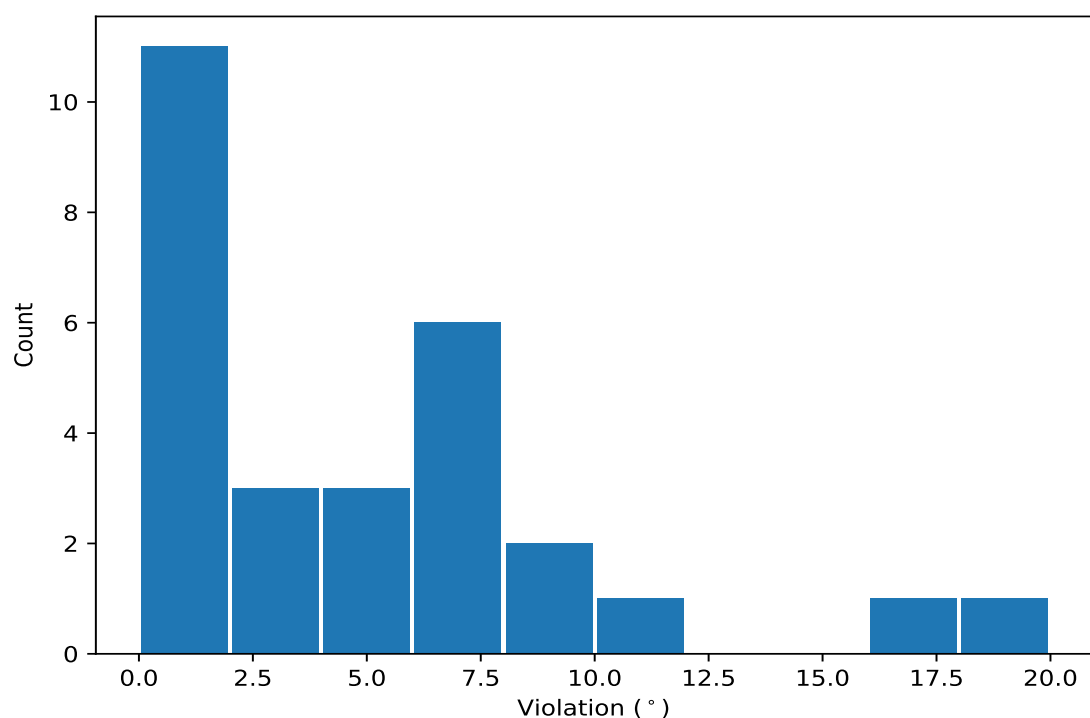
| Key    | Atom-1       | Atom-2        | Atom-3       | Atom-4       | Models <sup>1</sup> | Mean | SD <sup>2</sup> | Median |
|--------|--------------|---------------|--------------|--------------|---------------------|------|-----------------|--------|
| (1,20) | 3:28:A:SER:N | 3:28:A:SER:CA | 3:28:A:SER:C | 3:29:A:ARG:N | 8                   | 5.38 | 2.76            | 6.35   |
| (1,48) | 3:58:A:GLN:N | 3:58:A:GLN:CA | 3:58:A:GLN:C | 3:59:A:ARG:N | 7                   | 5.77 | 3.59            | 6.84   |
| (1,74) | 3:86:A:THR:N | 3:86:A:THR:CA | 3:86:A:THR:C | 3:87:A:ARG:N | 7                   | 1.71 | 0.81            | 1.45   |
| (1,26) | 3:31:A:HIS:N | 3:31:A:HIS:CA | 3:31:A:HIS:C | 3:32:A:THR:N | 5                   | 9.9  | 6.87            | 7.86   |

<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 (°) |
|--------|--------------|---------------|--------------|--------------|----------|---------------|
| (1,26) | 3:31:A:HIS:N | 3:31:A:HIS:CA | 3:31:A:HIS:C | 3:32:A:THR:N | 15       | 18.87         |
| (1,26) | 3:31:A:HIS:N | 3:31:A:HIS:CA | 3:31:A:HIS:C | 3:32:A:THR:N | 10       | 16.88         |
| (1,48) | 3:58:A:GLN:N | 3:58:A:GLN:CA | 3:58:A:GLN:C | 3:59:A:ARG:N | 5        | 11.78         |
| (1,20) | 3:28:A:SER:N | 3:28:A:SER:CA | 3:28:A:SER:C | 3:29:A:ARG:N | 10       | 8.62          |
| (1,48) | 3:58:A:GLN:N | 3:58:A:GLN:CA | 3:58:A:GLN:C | 3:59:A:ARG:N | 19       | 8.28          |
| (1,26) | 3:31:A:HIS:N | 3:31:A:HIS:CA | 3:31:A:HIS:C | 3:32:A:THR:N | 20       | 7.86          |
| (1,20) | 3:28:A:SER:N | 3:28:A:SER:CA | 3:28:A:SER:C | 3:29:A:ARG:N | 12       | 7.62          |
| (1,20) | 3:28:A:SER:N | 3:28:A:SER:CA | 3:28:A:SER:C | 3:29:A:ARG:N | 19       | 7.56          |
| (1,48) | 3:58:A:GLN:N | 3:58:A:GLN:CA | 3:58:A:GLN:C | 3:59:A:ARG:N | 20       | 7.23          |
| (1,20) | 3:28:A:SER:N | 3:28:A:SER:CA | 3:28:A:SER:C | 3:29:A:ARG:N | 15       | 7.23          |
| (1,48) | 3:58:A:GLN:N | 3:58:A:GLN:CA | 3:58:A:GLN:C | 3:59:A:ARG:N | 16       | 6.84          |
| (1,20) | 3:28:A:SER:N | 3:28:A:SER:CA | 3:28:A:SER:C | 3:29:A:ARG:N | 20       | 5.47          |
| (1,26) | 3:31:A:HIS:N | 3:31:A:HIS:CA | 3:31:A:HIS:C | 3:32:A:THR:N | 12       | 4.71          |
| (1,20) | 3:28:A:SER:N | 3:28:A:SER:CA | 3:28:A:SER:C | 3:29:A:ARG:N | 11       | 4.19          |
| (1,48) | 3:58:A:GLN:N | 3:58:A:GLN:CA | 3:58:A:GLN:C | 3:59:A:ARG:N | 13       | 3.61          |
| (1,74) | 3:86:A:THR:N | 3:86:A:THR:CA | 3:86:A:THR:C | 3:87:A:ARG:N | 19       | 3.45          |
| (1,74) | 3:86:A:THR:N | 3:86:A:THR:CA | 3:86:A:THR:C | 3:87:A:ARG:N | 16       | 2.29          |
| (1,48) | 3:58:A:GLN:N | 3:58:A:GLN:CA | 3:58:A:GLN:C | 3:59:A:ARG:N | 14       | 1.59          |
| (1,74) | 3:86:A:THR:N | 3:86:A:THR:CA | 3:86:A:THR:C | 3:87:A:ARG:N | 13       | 1.47          |
| (1,74) | 3:86:A:THR:N | 3:86:A:THR:CA | 3:86:A:THR:C | 3:87:A:ARG:N | 15       | 1.45          |
| (1,20) | 3:28:A:SER:N | 3:28:A:SER:CA | 3:28:A:SER:C | 3:29:A:ARG:N | 3        | 1.31          |

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| Key    | Atom-1       | Atom-2        | Atom-3       | Atom-4       | Model ID | Violation (°) |
|--------|--------------|---------------|--------------|--------------|----------|---------------|
| (1,74) | 3:86:A:THR:N | 3:86:A:THR:CA | 3:86:A:THR:C | 3:87:A:ARG:N | 10       | 1.27          |
| (1,26) | 3:31:A:HIS:N | 3:31:A:HIS:CA | 3:31:A:HIS:C | 3:32:A:THR:N | 11       | 1.19          |
| (1,48) | 3:58:A:GLN:N | 3:58:A:GLN:CA | 3:58:A:GLN:C | 3:59:A:ARG:N | 8        | 1.06          |
| (1,70) | 3:84:A:THR:N | 3:84:A:THR:CA | 3:84:A:THR:C | 3:85:A:HIS:N | 18       | 1.03          |
| (1,74) | 3:86:A:THR:N | 3:86:A:THR:CA | 3:86:A:THR:C | 3:87:A:ARG:N | 4        | 1.02          |
| (1,74) | 3:86:A:THR:N | 3:86:A:THR:CA | 3:86:A:THR:C | 3:87:A:ARG:N | 17       | 1.01          |
| (1,20) | 3:28:A:SER:N | 3:28:A:SER:CA | 3:28:A:SER:C | 3:29:A:ARG:N | 5        | 1.01          |