



# Full wwPDB NMR Structure Validation Report ⓘ

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PDB ID : 2LU5 / pdb\_00002lu5  
BMRB ID : 18509  
Title : Structure and chemical shifts of Cu(I),Zn(II) superoxide dismutase by solid-state NMR  
Authors : Knight, M.J.; Pell, A.J.; Bertini, I.; Felli, I.C.; Gonnelli, L.; Pierattelli, R.; Herrmann, T.; Emsley, L.; Pintacuda, G.  
Deposited on : 2012-06-08

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0  
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

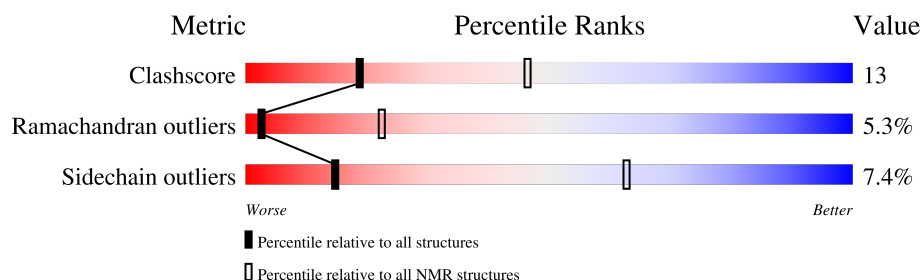
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLID-STATE NMR*

The overall completeness of chemical shifts assignment is 27%.

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



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

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 153    |                  |

## 2 Ensemble composition and analysis

This entry contains 19 models. Model 14 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest target function*.

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:1-A:80, A:84-A:153 (150) | 2.05              | 14           |

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 12 single-model clusters were found.

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

### 3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2195 atoms, of which 1085 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Superoxide dismutase [Cu-Zn].

| Mol | Chain | Residues | Atoms |     |      |     |     |   | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|-------|
| 1   | A     | 153      | Total | C   | H    | N   | O   | S | 0     |
|     |       |          | 2194  | 679 | 1085 | 203 | 225 | 2 |       |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| A     | 6       | ALA      | CYS    | engineered mutation | UNP P00441 |
| A     | 111     | SER      | CYS    | engineered mutation | UNP P00441 |

- Molecule 2 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

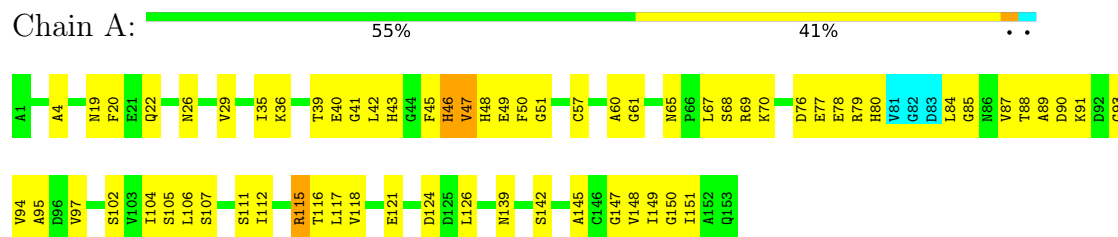
| Mol | Chain | Residues | Atoms |    |
|-----|-------|----------|-------|----|
| 2   | A     | 1        | Total | Cu |
|     |       |          | 1     | 1  |

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

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

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

- Molecule 1: Superoxide dismutase [Cu-Zn]

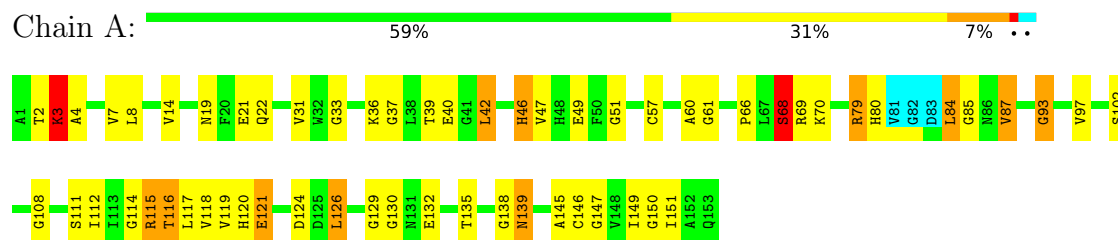


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1

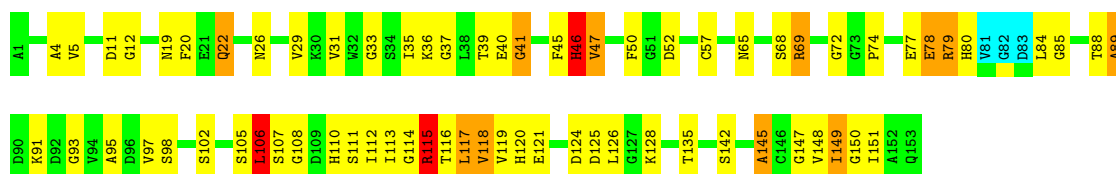
- Molecule 1: Superoxide dismutase [Cu-Zn]



#### 4.2.2 Score per residue for model 2

- Molecule 1: Superoxide dismutase [Cu-Zn]

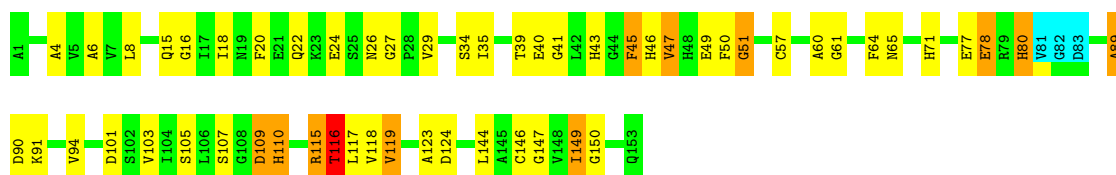




#### 4.2.3 Score per residue for model 3

- Molecule 1: Superoxide dismutase [Cu-Zn]

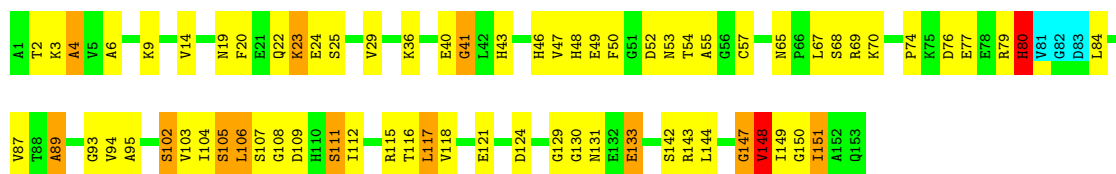
Chain A: 62% 28% 7% ..



#### 4.2.4 Score per residue for model 4

- Molecule 1: Superoxide dismutase [Cu-Zn]

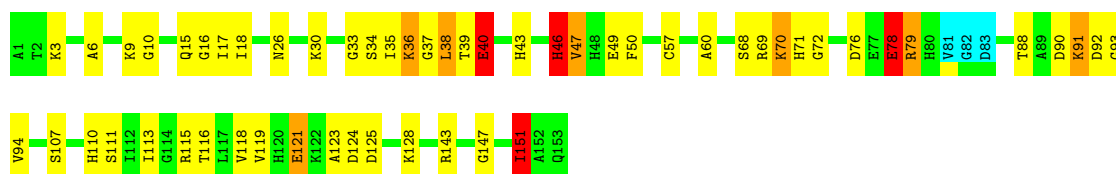
Chain A: 52% 37% 8% ..



#### 4.2.5 Score per residue for model 5

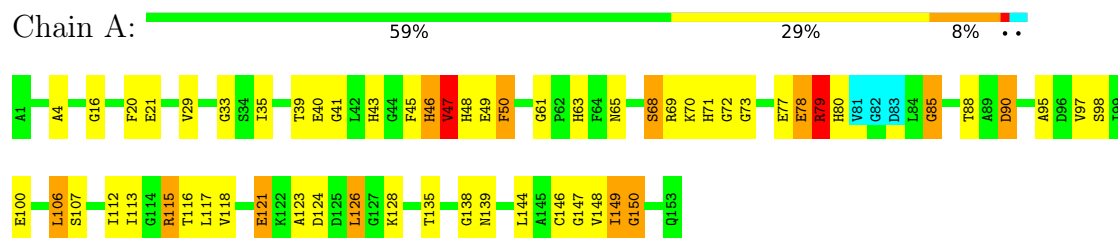
- Molecule 1: Superoxide dismutase [Cu-Zn]

Chain A: 62% 29% 5% ..



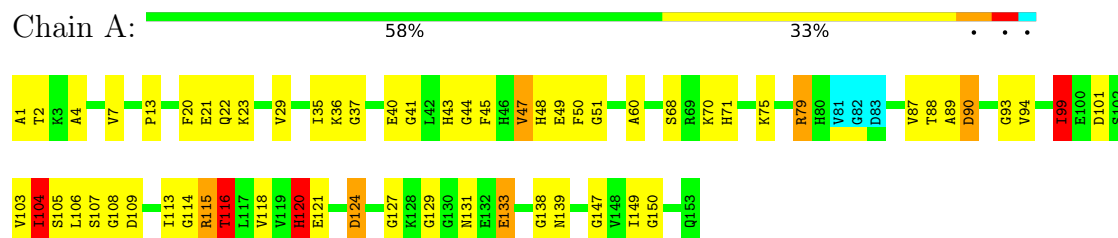
#### 4.2.6 Score per residue for model 6

- Molecule 1: Superoxide dismutase [Cu-Zn]



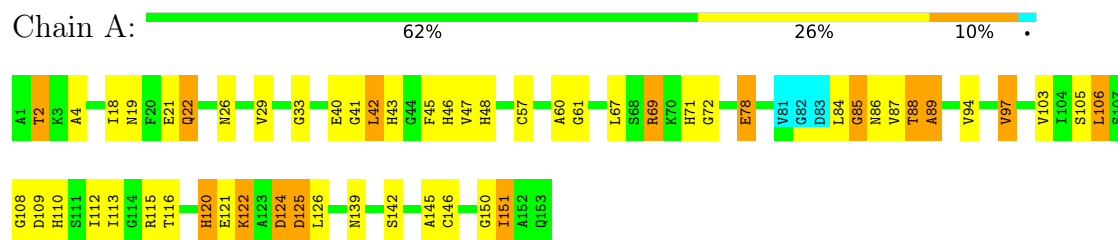
#### 4.2.7 Score per residue for model 7

- Molecule 1: Superoxide dismutase [Cu-Zn]



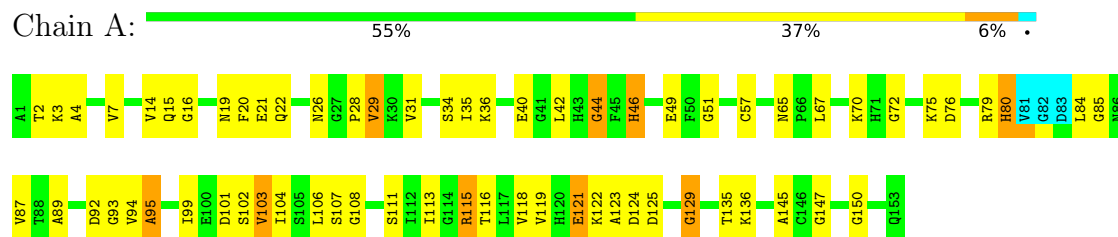
#### 4.2.8 Score per residue for model 8

- Molecule 1: Superoxide dismutase [Cu-Zn]



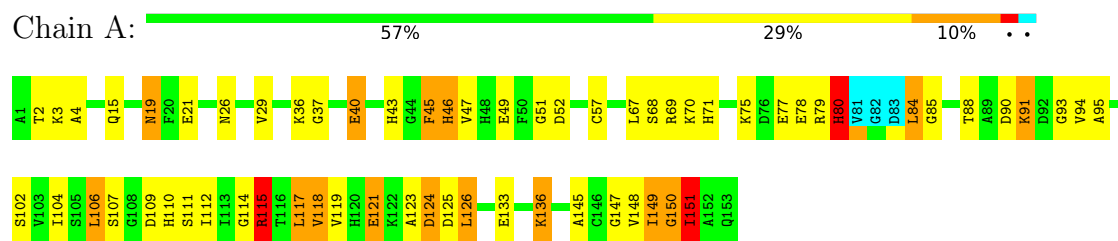
#### 4.2.9 Score per residue for model 9

- Molecule 1: Superoxide dismutase [Cu-Zn]



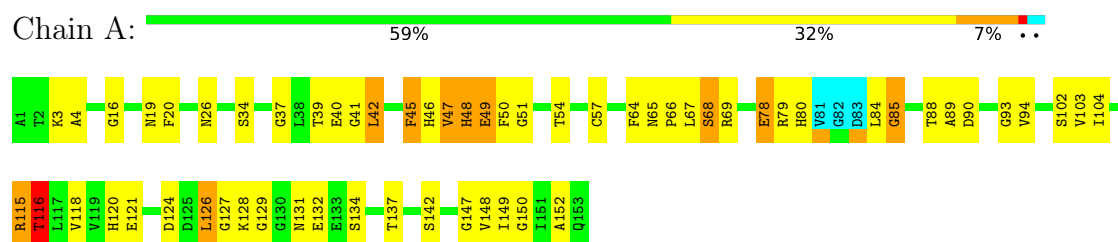
### 4.2.10 Score per residue for model 10

- Molecule 1: Superoxide dismutase [Cu-Zn]



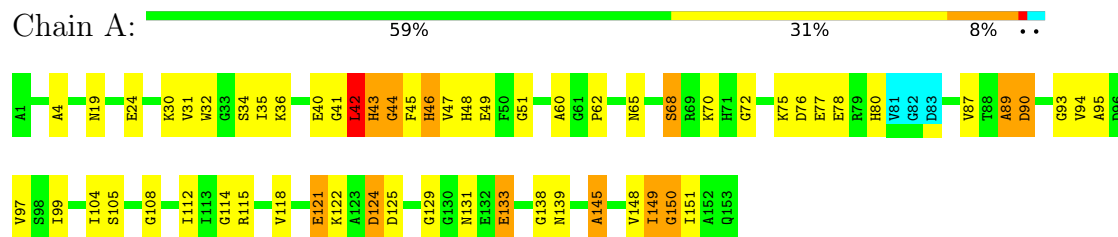
### 4.2.11 Score per residue for model 11

- Molecule 1: Superoxide dismutase [Cu-Zn]



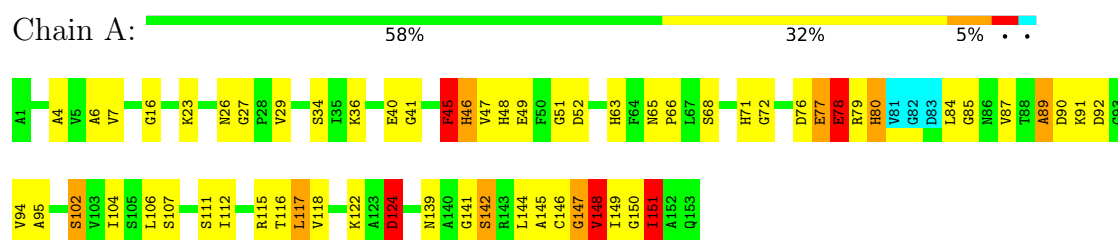
### 4.2.12 Score per residue for model 12

- Molecule 1: Superoxide dismutase [Cu-Zn]



### 4.2.13 Score per residue for model 13

- Molecule 1: Superoxide dismutase [Cu-Zn]



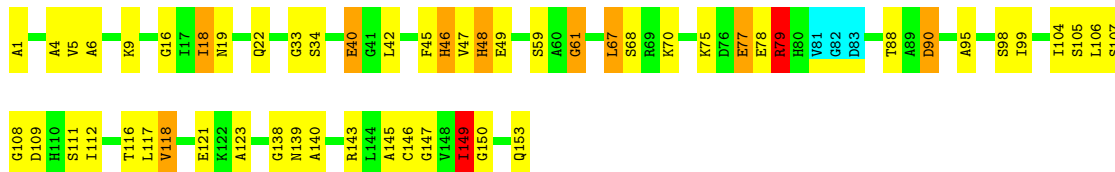




#### 4.2.18 Score per residue for model 18

- Molecule 1: Superoxide dismutase [Cu-Zn]

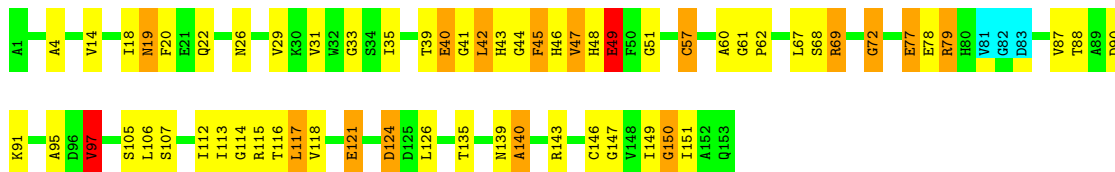
Chain A: 62% 29% 6% ..



#### 4.2.19 Score per residue for model 19

- Molecule 1: Superoxide dismutase [Cu-Zn]

Chain A: 58% 29% 10% ..



## 5 Refinement protocol and experimental data overview

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

Of the 80 calculated structures, 19 were deposited, based on the following criterion: *target function*.

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

| Software name | Classification     | Version |
|---------------|--------------------|---------|
| CYANA         | structure solution |         |
| CNS           | refinement         |         |

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

| Chemical shift file(s)                       | working_cs.cif |
|----------------------------------------------|----------------|
| Number of chemical shift lists               | 1              |
| Total number of shifts                       | 517            |
| Number of shifts mapped to atoms             | 517            |
| Number of unparsed shifts                    | 0              |
| Number of shifts with mapping errors         | 0              |
| Number of shifts with mapping warnings       | 0              |
| Assignment completeness (well-defined parts) | 27%            |

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

## 6 Model quality

### 6.1 Standard geometry

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

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   | A     | 1.67±0.06    | 16±4/1108 ( 1.4± 0.3%) | 1.25±0.06   | 6±3/1493 ( 0.4± 0.2%) |
| All | All   | 1.68         | 301/21052 ( 1.4%)      | 1.25        | 109/28367 ( 0.4%)     |

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   | A     | 0.0±0.0   | 0.3±0.6   |
| All | All   | 0         | 6         |

All unique bond 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(Å) | Ideal(Å) | Models |       |
|-----|-------|-----|------|-------|--------|-------------|----------|--------|-------|
|     |       |     |      |       |        |             |          | Worst  | Total |
| 1   | A     | 118 | VAL  | C-O   | 12.59  | 1.38        | 1.24     | 18     | 7     |
| 1   | A     | 138 | GLY  | C-O   | 11.47  | 1.39        | 1.23     | 18     | 2     |
| 1   | A     | 107 | SER  | C-N   | -10.99 | 1.26        | 1.33     | 4      | 4     |
| 1   | A     | 45  | PHE  | C-O   | 9.39   | 1.35        | 1.23     | 18     | 3     |
| 1   | A     | 105 | SER  | C-N   | -9.16  | 1.20        | 1.33     | 18     | 2     |
| 1   | A     | 89  | ALA  | C-N   | -9.07  | 1.25        | 1.33     | 2      | 9     |
| 1   | A     | 106 | LEU  | N-CA  | -8.94  | 1.35        | 1.45     | 18     | 5     |
| 1   | A     | 46  | HIS  | C-O   | 8.80   | 1.34        | 1.23     | 9      | 5     |
| 1   | A     | 105 | SER  | N-CA  | -8.69  | 1.35        | 1.46     | 4      | 1     |
| 1   | A     | 149 | ILE  | C-N   | -8.60  | 1.24        | 1.33     | 16     | 9     |
| 1   | A     | 107 | SER  | N-CA  | -8.56  | 1.35        | 1.47     | 9      | 10    |
| 1   | A     | 106 | LEU  | C-N   | -8.49  | 1.21        | 1.33     | 8      | 9     |
| 1   | A     | 150 | GLY  | CA-C  | -8.49  | 1.42        | 1.51     | 16     | 15    |
| 1   | A     | 108 | GLY  | CA-C  | -8.30  | 1.43        | 1.51     | 7      | 4     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) | Models |       |
|-----|-------|-----|------|-------|-------|-------------|----------|--------|-------|
|     |       |     |      |       |       |             |          | Worst  | Total |
| 1   | A     | 37  | GLY  | N-CA  | -8.18 | 1.37        | 1.45     | 5      | 2     |
| 1   | A     | 90  | ASP  | C-N   | -8.11 | 1.21        | 1.33     | 7      | 4     |
| 1   | A     | 145 | ALA  | N-CA  | -8.00 | 1.35        | 1.46     | 13     | 5     |
| 1   | A     | 139 | ASN  | C-O   | 7.97  | 1.34        | 1.24     | 7      | 4     |
| 1   | A     | 61  | GLY  | C-N   | 7.95  | 1.40        | 1.33     | 14     | 2     |
| 1   | A     | 68  | SER  | N-CA  | -7.86 | 1.36        | 1.46     | 11     | 4     |
| 1   | A     | 79  | ARG  | N-CA  | -7.70 | 1.36        | 1.46     | 17     | 2     |
| 1   | A     | 88  | THR  | C-N   | -7.54 | 1.22        | 1.33     | 16     | 3     |
| 1   | A     | 141 | GLY  | N-CA  | -7.44 | 1.38        | 1.45     | 15     | 1     |
| 1   | A     | 67  | LEU  | CA-C  | -7.37 | 1.42        | 1.52     | 15     | 1     |
| 1   | A     | 103 | VAL  | N-CA  | -7.26 | 1.39        | 1.46     | 8      | 2     |
| 1   | A     | 116 | THR  | N-CA  | -7.22 | 1.37        | 1.46     | 7      | 7     |
| 1   | A     | 22  | GLN  | N-CA  | -7.20 | 1.37        | 1.46     | 17     | 5     |
| 1   | A     | 68  | SER  | CA-CB | -7.16 | 1.45        | 1.54     | 12     | 1     |
| 1   | A     | 150 | GLY  | N-CA  | -7.11 | 1.38        | 1.45     | 11     | 9     |
| 1   | A     | 47  | VAL  | C-N   | -7.11 | 1.23        | 1.33     | 2      | 2     |
| 1   | A     | 111 | SER  | C-N   | -7.10 | 1.27        | 1.33     | 5      | 1     |
| 1   | A     | 140 | ALA  | C-O   | 7.02  | 1.33        | 1.23     | 15     | 1     |
| 1   | A     | 48  | HIS  | C-N   | -6.86 | 1.24        | 1.33     | 17     | 3     |
| 1   | A     | 46  | HIS  | N-CA  | -6.85 | 1.36        | 1.47     | 5      | 4     |
| 1   | A     | 43  | HIS  | CA-C  | -6.82 | 1.44        | 1.52     | 19     | 1     |
| 1   | A     | 14  | VAL  | N-CA  | -6.74 | 1.38        | 1.46     | 15     | 5     |
| 1   | A     | 106 | LEU  | CA-C  | -6.74 | 1.44        | 1.52     | 18     | 1     |
| 1   | A     | 148 | VAL  | C-N   | -6.72 | 1.23        | 1.33     | 13     | 1     |
| 1   | A     | 42  | LEU  | N-CA  | -6.68 | 1.37        | 1.45     | 19     | 3     |
| 1   | A     | 40  | GLU  | C-N   | -6.66 | 1.23        | 1.33     | 2      | 9     |
| 1   | A     | 89  | ALA  | C-O   | -6.59 | 1.15        | 1.23     | 12     | 1     |
| 1   | A     | 89  | ALA  | N-CA  | -6.58 | 1.37        | 1.45     | 16     | 1     |
| 1   | A     | 46  | HIS  | C-N   | -6.54 | 1.29        | 1.33     | 5      | 2     |
| 1   | A     | 14  | VAL  | C-N   | -6.53 | 1.25        | 1.33     | 15     | 3     |
| 1   | A     | 108 | GLY  | N-CA  | -6.52 | 1.36        | 1.45     | 4      | 2     |
| 1   | A     | 48  | HIS  | CA-C  | -6.49 | 1.45        | 1.52     | 19     | 2     |
| 1   | A     | 84  | LEU  | C-N   | -6.41 | 1.25        | 1.33     | 11     | 2     |
| 1   | A     | 47  | VAL  | N-CA  | -6.41 | 1.38        | 1.46     | 16     | 2     |
| 1   | A     | 47  | VAL  | CA-CB | 6.39  | 1.62        | 1.55     | 7      | 4     |
| 1   | A     | 148 | VAL  | CA-CB | 6.37  | 1.63        | 1.54     | 4      | 1     |
| 1   | A     | 150 | GLY  | C-N   | -6.36 | 1.27        | 1.33     | 3      | 3     |
| 1   | A     | 95  | ALA  | N-CA  | -6.33 | 1.38        | 1.46     | 9      | 2     |
| 1   | A     | 42  | LEU  | C-N   | -6.31 | 1.25        | 1.33     | 9      | 1     |
| 1   | A     | 113 | ILE  | N-CA  | -6.29 | 1.38        | 1.46     | 7      | 1     |
| 1   | A     | 69  | ARG  | C-N   | -6.25 | 1.25        | 1.33     | 15     | 1     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) | Models |       |
|-----|-------|-----|------|--------|-------|-------------|----------|--------|-------|
|     |       |     |      |        |       |             |          | Worst  | Total |
| 1   | A     | 37  | GLY  | CA-C   | -6.23 | 1.46        | 1.52     | 5      | 1     |
| 1   | A     | 107 | SER  | CA-C   | -6.20 | 1.46        | 1.53     | 13     | 4     |
| 1   | A     | 94  | VAL  | C-N    | -6.14 | 1.24        | 1.33     | 9      | 1     |
| 1   | A     | 142 | SER  | C-N    | -6.08 | 1.25        | 1.33     | 8      | 4     |
| 1   | A     | 114 | GLY  | C-N    | -6.07 | 1.25        | 1.33     | 2      | 1     |
| 1   | A     | 114 | GLY  | CA-C   | -6.06 | 1.43        | 1.51     | 7      | 1     |
| 1   | A     | 70  | LYS  | N-CA   | -6.05 | 1.38        | 1.46     | 15     | 2     |
| 1   | A     | 151 | ILE  | CA-CB  | 6.05  | 1.60        | 1.53     | 10     | 3     |
| 1   | A     | 115 | ARG  | NE-CZ  | 6.01  | 1.39        | 1.33     | 10     | 1     |
| 1   | A     | 80  | HIS  | C-N    | -5.97 | 1.25        | 1.33     | 10     | 1     |
| 1   | A     | 88  | THR  | N-CA   | -5.92 | 1.39        | 1.46     | 5      | 1     |
| 1   | A     | 77  | GLU  | C-N    | -5.92 | 1.25        | 1.33     | 3      | 1     |
| 1   | A     | 78  | GLU  | C-O    | -5.88 | 1.16        | 1.23     | 2      | 2     |
| 1   | A     | 115 | ARG  | C-O    | -5.88 | 1.16        | 1.23     | 10     | 2     |
| 1   | A     | 16  | GLY  | N-CA   | -5.86 | 1.38        | 1.45     | 13     | 1     |
| 1   | A     | 147 | GLY  | C-N    | -5.84 | 1.27        | 1.33     | 6      | 3     |
| 1   | A     | 140 | ALA  | C-N    | -5.82 | 1.27        | 1.33     | 19     | 1     |
| 1   | A     | 36  | LYS  | C-N    | -5.77 | 1.27        | 1.33     | 13     | 2     |
| 1   | A     | 91  | LYS  | CA-C   | 5.76  | 1.60        | 1.52     | 17     | 1     |
| 1   | A     | 144 | LEU  | CA-C   | -5.76 | 1.45        | 1.52     | 13     | 1     |
| 1   | A     | 85  | GLY  | N-CA   | -5.76 | 1.39        | 1.45     | 1      | 1     |
| 1   | A     | 126 | LEU  | N-CA   | -5.75 | 1.40        | 1.47     | 1      | 2     |
| 1   | A     | 149 | ILE  | CA-CB  | 5.74  | 1.59        | 1.53     | 18     | 1     |
| 1   | A     | 137 | THR  | N-CA   | -5.73 | 1.39        | 1.46     | 14     | 1     |
| 1   | A     | 45  | PHE  | C-N    | -5.72 | 1.26        | 1.33     | 13     | 1     |
| 1   | A     | 98  | SER  | N-CA   | -5.72 | 1.39        | 1.46     | 18     | 3     |
| 1   | A     | 124 | ASP  | CG-OD1 | -5.71 | 1.14        | 1.25     | 15     | 1     |
| 1   | A     | 147 | GLY  | N-CA   | -5.69 | 1.40        | 1.45     | 17     | 2     |
| 1   | A     | 94  | VAL  | N-CA   | -5.66 | 1.39        | 1.46     | 9      | 1     |
| 1   | A     | 149 | ILE  | N-CA   | -5.66 | 1.39        | 1.46     | 12     | 2     |
| 1   | A     | 78  | GLU  | C-N    | -5.66 | 1.26        | 1.33     | 13     | 1     |
| 1   | A     | 115 | ARG  | CD-NE  | 5.63  | 1.54        | 1.46     | 10     | 1     |
| 1   | A     | 124 | ASP  | C-N    | -5.62 | 1.25        | 1.33     | 9      | 1     |
| 1   | A     | 102 | SER  | C-N    | -5.60 | 1.27        | 1.33     | 9      | 1     |
| 1   | A     | 40  | GLU  | CA-C   | -5.58 | 1.46        | 1.52     | 2      | 4     |
| 1   | A     | 16  | GLY  | CA-C   | -5.56 | 1.45        | 1.51     | 13     | 1     |
| 1   | A     | 124 | ASP  | CA-C   | -5.56 | 1.46        | 1.53     | 9      | 1     |
| 1   | A     | 57  | CYS  | N-CA   | -5.55 | 1.39        | 1.46     | 8      | 3     |
| 1   | A     | 2   | THR  | C-O    | -5.48 | 1.16        | 1.23     | 8      | 1     |
| 1   | A     | 41  | GLY  | CA-C   | -5.46 | 1.44        | 1.51     | 2      | 1     |
| 1   | A     | 125 | ASP  | N-CA   | -5.46 | 1.39        | 1.46     | 9      | 1     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) | Models |       |
|-----|-------|-----|------|-------|-------|-------------|----------|--------|-------|
|     |       |     |      |       |       |             |          | Worst  | Total |
| 1   | A     | 4   | ALA  | CA-C  | -5.43 | 1.45        | 1.52     | 4      | 1     |
| 1   | A     | 68  | SER  | C-N   | -5.41 | 1.25        | 1.33     | 1      | 1     |
| 1   | A     | 69  | ARG  | N-CA  | -5.38 | 1.40        | 1.46     | 8      | 2     |
| 1   | A     | 143 | ARG  | CA-C  | -5.38 | 1.46        | 1.52     | 4      | 1     |
| 1   | A     | 143 | ARG  | N-CA  | -5.38 | 1.40        | 1.46     | 16     | 1     |
| 1   | A     | 29  | VAL  | C-N   | -5.37 | 1.24        | 1.33     | 9      | 1     |
| 1   | A     | 46  | HIS  | CA-C  | -5.35 | 1.44        | 1.53     | 5      | 1     |
| 1   | A     | 111 | SER  | N-CA  | -5.34 | 1.40        | 1.46     | 4      | 1     |
| 1   | A     | 3   | LYS  | CA-C  | -5.34 | 1.46        | 1.52     | 1      | 1     |
| 1   | A     | 85  | GLY  | CA-C  | -5.33 | 1.45        | 1.51     | 11     | 1     |
| 1   | A     | 22  | GLN  | C-N   | -5.33 | 1.26        | 1.33     | 16     | 1     |
| 1   | A     | 87  | VAL  | C-N   | -5.33 | 1.26        | 1.33     | 8      | 1     |
| 1   | A     | 34  | SER  | N-CA  | -5.33 | 1.39        | 1.45     | 12     | 2     |
| 1   | A     | 97  | VAL  | CA-CB | 5.30  | 1.59        | 1.53     | 8      | 1     |
| 1   | A     | 91  | LYS  | N-CA  | 5.28  | 1.53        | 1.46     | 16     | 1     |
| 1   | A     | 39  | THR  | CA-CB | 5.26  | 1.59        | 1.53     | 1      | 1     |
| 1   | A     | 29  | VAL  | N-CA  | -5.24 | 1.40        | 1.46     | 9      | 2     |
| 1   | A     | 122 | LYS  | C-N   | -5.24 | 1.26        | 1.33     | 13     | 1     |
| 1   | A     | 44  | GLY  | C-N   | -5.24 | 1.26        | 1.33     | 15     | 1     |
| 1   | A     | 94  | VAL  | CA-C  | -5.22 | 1.46        | 1.52     | 15     | 1     |
| 1   | A     | 40  | GLU  | N-CA  | -5.19 | 1.40        | 1.46     | 8      | 1     |
| 1   | A     | 61  | GLY  | N-CA  | 5.17  | 1.51        | 1.44     | 18     | 1     |
| 1   | A     | 115 | ARG  | C-N   | -5.14 | 1.27        | 1.34     | 7      | 2     |
| 1   | A     | 62  | PRO  | N-CA  | -5.14 | 1.40        | 1.47     | 12     | 1     |
| 1   | A     | 77  | GLU  | CA-C  | -5.13 | 1.45        | 1.52     | 13     | 1     |
| 1   | A     | 39  | THR  | C-N   | -5.13 | 1.26        | 1.33     | 11     | 1     |
| 1   | A     | 120 | HIS  | C-N   | -5.12 | 1.26        | 1.33     | 11     | 2     |
| 1   | A     | 114 | GLY  | N-CA  | -5.11 | 1.38        | 1.45     | 7      | 1     |
| 1   | A     | 31  | VAL  | N-CA  | -5.08 | 1.40        | 1.46     | 12     | 1     |
| 1   | A     | 115 | ARG  | N-CA  | -5.07 | 1.40        | 1.45     | 9      | 1     |
| 1   | A     | 118 | VAL  | CA-C  | -5.05 | 1.47        | 1.52     | 2      | 1     |
| 1   | A     | 41  | GLY  | N-CA  | -5.05 | 1.38        | 1.45     | 2      | 1     |
| 1   | A     | 67  | LEU  | C-N   | -5.05 | 1.26        | 1.33     | 11     | 1     |
| 1   | A     | 141 | GLY  | C-N   | -5.04 | 1.26        | 1.33     | 13     | 1     |
| 1   | A     | 148 | VAL  | N-CA  | -5.02 | 1.41        | 1.46     | 2      | 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 |
| 1   | A     | 103 | VAL  | N-CA-C | -10.25 | 103.12      | 113.47   | 4      | 5     |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) | Models |       |
|-----|-------|-----|------|------------|-------|-------------|----------|--------|-------|
|     |       |     |      |            |       |             |          | Worst  | Total |
| 1   | A     | 112 | ILE  | N-CA-C     | -9.44 | 103.84      | 112.90   | 6      | 4     |
| 1   | A     | 118 | VAL  | N-CA-C     | 9.01  | 120.71      | 107.37   | 10     | 1     |
| 1   | A     | 124 | ASP  | CA-CB-CG   | 8.97  | 121.58      | 112.60   | 10     | 4     |
| 1   | A     | 48  | HIS  | CA-CB-CG   | 7.54  | 121.34      | 113.80   | 14     | 1     |
| 1   | A     | 79  | ARG  | N-CA-C     | -7.38 | 104.30      | 113.38   | 19     | 2     |
| 1   | A     | 97  | VAL  | CB-CA-C    | -7.21 | 102.64      | 111.08   | 19     | 1     |
| 1   | A     | 67  | LEU  | N-CA-C     | -6.79 | 104.80      | 113.23   | 18     | 1     |
| 1   | A     | 49  | GLU  | N-CA-C     | 6.70  | 118.32      | 108.14   | 19     | 1     |
| 1   | A     | 106 | LEU  | N-CA-C     | -6.67 | 99.27       | 109.41   | 8      | 1     |
| 1   | A     | 11  | ASP  | N-CA-C     | -6.43 | 104.92      | 112.89   | 2      | 1     |
| 1   | A     | 117 | LEU  | CA-C-N     | -6.30 | 114.54      | 123.11   | 10     | 5     |
| 1   | A     | 117 | LEU  | C-N-CA     | -6.30 | 114.54      | 123.11   | 10     | 5     |
| 1   | A     | 46  | HIS  | CA-CB-CG   | 6.28  | 120.08      | 113.80   | 2      | 3     |
| 1   | A     | 69  | ARG  | N-CA-C     | -6.20 | 103.01      | 111.56   | 1      | 3     |
| 1   | A     | 76  | ASP  | CA-CB-CG   | 6.20  | 118.80      | 112.60   | 14     | 1     |
| 1   | A     | 124 | ASP  | OD1-CG-OD2 | -6.19 | 108.04      | 122.90   | 13     | 16    |
| 1   | A     | 120 | HIS  | CA-C-O     | -6.11 | 114.91      | 121.38   | 2      | 2     |
| 1   | A     | 77  | GLU  | N-CA-C     | 5.95  | 117.98      | 110.24   | 17     | 1     |
| 1   | A     | 78  | GLU  | N-CA-C     | -5.90 | 107.31      | 114.75   | 17     | 1     |
| 1   | A     | 71  | HIS  | N-CA-C     | 5.90  | 117.22      | 107.20   | 6      | 1     |
| 1   | A     | 60  | ALA  | N-CA-C     | -5.79 | 106.05      | 113.23   | 12     | 1     |
| 1   | A     | 141 | GLY  | CA-C-N     | 5.77  | 132.55      | 121.54   | 15     | 1     |
| 1   | A     | 141 | GLY  | C-N-CA     | 5.77  | 132.55      | 121.54   | 15     | 1     |
| 1   | A     | 40  | GLU  | N-CA-C     | 5.76  | 117.98      | 110.43   | 5      | 2     |
| 1   | A     | 102 | SER  | CA-C-N     | -5.75 | 117.06      | 123.16   | 2      | 2     |
| 1   | A     | 102 | SER  | C-N-CA     | -5.75 | 117.06      | 123.16   | 2      | 2     |
| 1   | A     | 124 | ASP  | N-CA-C     | -5.75 | 104.65      | 111.03   | 10     | 1     |
| 1   | A     | 43  | HIS  | CA-CB-CG   | 5.75  | 119.55      | 113.80   | 19     | 1     |
| 1   | A     | 38  | LEU  | N-CA-C     | -5.70 | 103.12      | 110.19   | 5      | 1     |
| 1   | A     | 86  | ASN  | CA-CB-CG   | 5.69  | 118.29      | 112.60   | 14     | 1     |
| 1   | A     | 63  | HIS  | CA-CB-CG   | 5.64  | 119.44      | 113.80   | 15     | 1     |
| 1   | A     | 80  | HIS  | N-CA-C     | -5.56 | 108.28      | 114.62   | 2      | 2     |
| 1   | A     | 65  | ASN  | CA-C-N     | 5.52  | 126.73      | 119.84   | 13     | 1     |
| 1   | A     | 65  | ASN  | C-N-CA     | 5.52  | 126.73      | 119.84   | 13     | 1     |
| 1   | A     | 12  | GLY  | N-CA-C     | -5.45 | 101.22      | 112.34   | 2      | 1     |
| 1   | A     | 120 | HIS  | CA-CB-CG   | 5.43  | 119.23      | 113.80   | 2      | 2     |
| 1   | A     | 45  | PHE  | CA-CB-CG   | 5.38  | 119.18      | 113.80   | 14     | 3     |
| 1   | A     | 68  | SER  | N-CA-C     | -5.38 | 105.42      | 112.41   | 16     | 1     |
| 1   | A     | 9   | LYS  | CA-C-N     | -5.37 | 117.48      | 121.61   | 18     | 1     |
| 1   | A     | 9   | LYS  | C-N-CA     | -5.37 | 117.48      | 121.61   | 18     | 1     |
| 1   | A     | 92  | ASP  | N-CA-C     | -5.36 | 104.36      | 112.99   | 5      | 2     |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) | Models |       |
|-----|-------|-----|------|----------|-------|-------------|----------|--------|-------|
|     |       |     |      |          |       |             |          | Worst  | Total |
| 1   | A     | 110 | HIS  | CA-CB-CG | 5.32  | 119.12      | 113.80   | 3      | 1     |
| 1   | A     | 105 | SER  | N-CA-C   | 5.29  | 117.73      | 108.52   | 2      | 1     |
| 1   | A     | 99  | ILE  | N-CA-C   | 5.26  | 115.43      | 107.80   | 7      | 1     |
| 1   | A     | 47  | VAL  | N-CA-CB  | -5.25 | 107.40      | 112.65   | 17     | 1     |
| 1   | A     | 62  | PRO  | N-CA-C   | -5.25 | 107.32      | 114.98   | 14     | 1     |
| 1   | A     | 40  | GLU  | CA-C-N   | 5.21  | 129.49      | 121.37   | 10     | 1     |
| 1   | A     | 40  | GLU  | C-N-CA   | 5.21  | 129.49      | 121.37   | 10     | 1     |
| 1   | A     | 142 | SER  | N-CA-C   | 5.13  | 118.32      | 111.75   | 17     | 1     |
| 1   | A     | 68  | SER  | CA-C-N   | -5.12 | 114.59      | 123.25   | 12     | 1     |
| 1   | A     | 68  | SER  | C-N-CA   | -5.12 | 114.59      | 123.25   | 12     | 1     |
| 1   | A     | 126 | LEU  | N-CA-C   | 5.12  | 121.70      | 110.80   | 11     | 1     |
| 1   | A     | 77  | GLU  | N-CA-CB  | 5.10  | 119.11      | 110.49   | 13     | 1     |
| 1   | A     | 138 | GLY  | CA-C-N   | 5.09  | 131.27      | 121.54   | 6      | 1     |
| 1   | A     | 138 | GLY  | C-N-CA   | 5.09  | 131.27      | 121.54   | 6      | 1     |
| 1   | A     | 119 | VAL  | CB-CA-C  | -5.07 | 103.32      | 110.82   | 3      | 1     |
| 1   | A     | 108 | GLY  | N-CA-C   | -5.07 | 105.34      | 112.13   | 7      | 1     |
| 1   | A     | 73  | GLY  | CA-C-N   | 5.04  | 125.72      | 120.12   | 14     | 1     |
| 1   | A     | 73  | GLY  | C-N-CA   | 5.04  | 125.72      | 120.12   | 14     | 1     |
| 1   | A     | 80  | HIS  | N-CA-CB  | 5.04  | 119.00      | 110.49   | 9      | 2     |

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) |
|-----|-------|-----|------|-----------|----------------|
| 1   | A     | 115 | ARG  | Sidechain | 2              |
| 1   | A     | 69  | ARG  | Sidechain | 1              |
| 1   | A     | 80  | HIS  | Peptide   | 1              |
| 1   | A     | 45  | PHE  | Mainchain | 1              |
| 1   | A     | 79  | 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   | A     | 1090  | 1069     | 1061     | 28±5    |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes |
|-----|-------|-------|----------|----------|---------|
| All | All   | 20729 | 20311    | 20159    | 529     |

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 13.

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

| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:116:THR:HB   | 1:A:146:CYS:SG   | 0.77     | 2.19        | 6      | 3     |
| 1:A:60:ALA:HB2   | 1:A:116:THR:HB   | 0.76     | 1.57        | 7      | 1     |
| 1:A:87:VAL:HB    | 1:A:95:ALA:HB1   | 0.75     | 1.58        | 9      | 4     |
| 1:A:57:CYS:SG    | 1:A:143:ARG:HA   | 0.73     | 2.22        | 19     | 3     |
| 1:A:67:LEU:O     | 1:A:78:GLU:HA    | 0.71     | 1.86        | 10     | 1     |
| 1:A:41:GLY:HA3   | 1:A:89:ALA:O     | 0.70     | 1.86        | 13     | 5     |
| 1:A:57:CYS:SG    | 1:A:118:VAL:HG21 | 0.70     | 2.26        | 10     | 1     |
| 1:A:4:ALA:HB3    | 1:A:20:PHE:H     | 0.70     | 1.45        | 3      | 10    |
| 1:A:115:ARG:HD3  | 1:A:149:ILE:O    | 0.69     | 1.86        | 6      | 2     |
| 1:A:116:THR:HA   | 1:A:147:GLY:O    | 0.68     | 1.89        | 5      | 8     |
| 1:A:51:GLY:HA2   | 1:A:114:GLY:O    | 0.66     | 1.91        | 17     | 4     |
| 1:A:35:ILE:O     | 1:A:94:VAL:HA    | 0.65     | 1.92        | 5      | 4     |
| 1:A:36:LYS:HA    | 1:A:93:GLY:O     | 0.64     | 1.92        | 10     | 8     |
| 1:A:40:GLU:HB3   | 1:A:90:ASP:C     | 0.64     | 2.18        | 10     | 2     |
| 1:A:37:GLY:O     | 1:A:93:GLY:HA3   | 0.64     | 1.92        | 11     | 5     |
| 1:A:75:LYS:O     | 1:A:102:SER:HA   | 0.63     | 1.94        | 15     | 1     |
| 1:A:4:ALA:O      | 1:A:19:ASN:HA    | 0.63     | 1.94        | 8      | 9     |
| 1:A:110:HIS:HA   | 1:A:115:ARG:NE   | 0.63     | 2.08        | 10     | 1     |
| 1:A:72:GLY:HA3   | 1:A:80:HIS:C     | 0.62     | 2.19        | 6      | 1     |
| 1:A:143:ARG:HA   | 1:A:146:CYS:SG   | 0.62     | 2.35        | 18     | 1     |
| 1:A:43:HIS:O     | 1:A:123:ALA:HA   | 0.62     | 1.94        | 3      | 5     |
| 1:A:115:ARG:NH1  | 1:A:148:VAL:HB   | 0.62     | 2.10        | 6      | 1     |
| 1:A:67:LEU:O     | 1:A:79:ARG:HA    | 0.61     | 1.95        | 18     | 2     |
| 1:A:46:HIS:HB2   | 1:A:124:ASP:OD1  | 0.61     | 1.95        | 14     | 1     |
| 1:A:78:GLU:O     | 1:A:79:ARG:HG2   | 0.60     | 1.95        | 2      | 1     |
| 1:A:51:GLY:HA3   | 1:A:114:GLY:O    | 0.60     | 1.95        | 10     | 1     |
| 1:A:33:GLY:O     | 1:A:97:VAL:HB    | 0.60     | 1.97        | 1      | 2     |
| 1:A:48:HIS:CE1   | 1:A:60:ALA:HB3   | 0.60     | 2.31        | 8      | 1     |
| 1:A:117:LEU:HB3  | 1:A:149:ILE:HG21 | 0.60     | 1.74        | 17     | 2     |
| 1:A:68:SER:OG    | 1:A:76:ASP:HA    | 0.60     | 1.97        | 12     | 1     |
| 1:A:87:VAL:HG22  | 1:A:95:ALA:HB1   | 0.59     | 1.73        | 15     | 1     |
| 1:A:117:LEU:HD22 | 1:A:149:ILE:HB   | 0.59     | 1.72        | 16     | 1     |
| 1:A:57:CYS:HB2   | 1:A:60:ALA:HB3   | 0.59     | 1.73        | 16     | 3     |
| 1:A:39:THR:OG1   | 1:A:91:LYS:HA    | 0.59     | 1.97        | 17     | 2     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:68:SER:HA    | 1:A:79:ARG:O     | 0.59     | 1.98        | 1      | 4     |
| 1:A:79:ARG:NE    | 1:A:79:ARG:HA    | 0.59     | 2.13        | 13     | 1     |
| 1:A:46:HIS:CE1   | 1:A:85:GLY:HA3   | 0.58     | 2.34        | 6      | 1     |
| 1:A:118:VAL:HA   | 1:A:146:CYS:HB3  | 0.58     | 1.74        | 13     | 1     |
| 1:A:22:GLN:HG2   | 1:A:105:SER:O    | 0.57     | 1.99        | 16     | 1     |
| 1:A:46:HIS:HA    | 1:A:118:VAL:O    | 0.57     | 2.00        | 5      | 1     |
| 1:A:119:VAL:O    | 1:A:145:ALA:HB3  | 0.57     | 1.99        | 1      | 5     |
| 1:A:115:ARG:HD3  | 1:A:116:THR:N    | 0.57     | 2.15        | 11     | 1     |
| 1:A:115:ARG:O    | 1:A:115:ARG:HD2  | 0.57     | 2.00        | 6      | 1     |
| 1:A:115:ARG:O    | 1:A:148:VAL:HA   | 0.57     | 1.99        | 16     | 3     |
| 1:A:88:THR:O     | 1:A:95:ALA:HA    | 0.57     | 2.00        | 15     | 5     |
| 1:A:129:GLY:HA2  | 1:A:134:SER:O    | 0.57     | 2.00        | 15     | 1     |
| 1:A:47:VAL:HB    | 1:A:49:GLU:OE2   | 0.57     | 2.00        | 12     | 1     |
| 1:A:53:ASN:HB3   | 1:A:56:GLY:O     | 0.56     | 2.01        | 17     | 3     |
| 1:A:112:ILE:HG13 | 1:A:151:ILE:O    | 0.56     | 2.00        | 2      | 1     |
| 1:A:48:HIS:ND1   | 1:A:60:ALA:HB3   | 0.56     | 2.14        | 8      | 1     |
| 1:A:51:GLY:H     | 1:A:115:ARG:HD3  | 0.56     | 1.60        | 10     | 1     |
| 1:A:112:ILE:O    | 1:A:150:GLY:HA2  | 0.56     | 2.00        | 8      | 3     |
| 1:A:29:VAL:HG12  | 1:A:31:VAL:HG13  | 0.55     | 1.76        | 19     | 1     |
| 1:A:9:LYS:O      | 1:A:55:ALA:HA    | 0.55     | 2.01        | 4      | 1     |
| 1:A:7:VAL:O      | 1:A:147:GLY:HA3  | 0.55     | 2.01        | 7      | 4     |
| 1:A:48:HIS:CG    | 1:A:60:ALA:HB3   | 0.55     | 2.36        | 8      | 1     |
| 1:A:111:SER:HB3  | 1:A:115:ARG:CZ   | 0.55     | 2.31        | 1      | 1     |
| 1:A:2:THR:O      | 1:A:3:LYS:HD2    | 0.55     | 2.02        | 4      | 1     |
| 1:A:124:ASP:HA   | 1:A:139:ASN:O    | 0.55     | 2.02        | 8      | 1     |
| 1:A:131:ASN:HB3  | 1:A:133:GLU:OE1  | 0.55     | 2.02        | 7      | 3     |
| 1:A:18:ILE:HG22  | 1:A:33:GLY:HA3   | 0.55     | 1.78        | 14     | 2     |
| 1:A:2:THR:O      | 1:A:21:GLU:HB3   | 0.54     | 2.02        | 1      | 2     |
| 1:A:115:ARG:O    | 1:A:149:ILE:HG12 | 0.54     | 2.01        | 1      | 1     |
| 1:A:49:GLU:CD    | 1:A:65:ASN:HB3   | 0.54     | 2.27        | 4      | 1     |
| 1:A:48:HIS:HB2   | 1:A:116:THR:O    | 0.54     | 2.02        | 13     | 1     |
| 1:A:43:HIS:HA    | 1:A:87:VAL:O     | 0.54     | 2.01        | 14     | 1     |
| 1:A:68:SER:HA    | 1:A:79:ARG:HB2   | 0.54     | 1.76        | 18     | 1     |
| 1:A:60:ALA:HB2   | 1:A:116:THR:CB   | 0.54     | 2.30        | 7      | 1     |
| 1:A:3:LYS:HG3    | 1:A:152:ALA:O    | 0.54     | 2.02        | 11     | 1     |
| 1:A:131:ASN:N    | 1:A:134:SER:HB2  | 0.54     | 2.17        | 11     | 1     |
| 1:A:115:ARG:O    | 1:A:149:ILE:HB   | 0.54     | 2.02        | 4      | 1     |
| 1:A:29:VAL:HG11  | 1:A:103:VAL:HG12 | 0.54     | 1.79        | 14     | 1     |
| 1:A:22:GLN:HG3   | 1:A:106:LEU:HB3  | 0.54     | 1.78        | 2      | 1     |
| 1:A:68:SER:HA    | 1:A:78:GLU:OE1   | 0.54     | 2.03        | 13     | 1     |
| 1:A:65:ASN:OD1   | 1:A:66:PRO:HD2   | 0.54     | 2.03        | 11     | 1     |

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| Atom-1          | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|-----------------|------------------|----------|-------------|--------|-------|
|                 |                  |          |             | Worst  | Total |
| 1:A:27:GLY:O    | 1:A:102:SER:HB3  | 0.54     | 2.02        | 13     | 1     |
| 1:A:111:SER:O   | 1:A:115:ARG:HD3  | 0.54     | 2.03        | 16     | 1     |
| 1:A:68:SER:O    | 1:A:80:HIS:HA    | 0.53     | 2.03        | 10     | 1     |
| 1:A:64:PHE:O    | 1:A:66:PRO:HD3   | 0.53     | 2.03        | 16     | 1     |
| 1:A:68:SER:HB2  | 1:A:79:ARG:O     | 0.53     | 2.02        | 5      | 1     |
| 1:A:115:ARG:HD2 | 1:A:115:ARG:N    | 0.53     | 2.19        | 1      | 1     |
| 1:A:128:LYS:O   | 1:A:128:LYS:HD3  | 0.53     | 2.04        | 5      | 1     |
| 1:A:45:PHE:CG   | 1:A:124:ASP:HB3  | 0.53     | 2.39        | 13     | 1     |
| 1:A:115:ARG:NH2 | 1:A:148:VAL:HG13 | 0.53     | 2.18        | 17     | 1     |
| 1:A:45:PHE:CE1  | 1:A:47:VAL:HB    | 0.53     | 2.39        | 2      | 1     |
| 1:A:57:CYS:SG   | 1:A:118:VAL:HG22 | 0.53     | 2.43        | 9      | 3     |
| 1:A:125:ASP:HB3 | 1:A:128:LYS:HB3  | 0.53     | 1.79        | 5      | 1     |
| 1:A:2:THR:C     | 1:A:21:GLU:HG3   | 0.53     | 2.28        | 9      | 1     |
| 1:A:2:THR:O     | 1:A:21:GLU:HA    | 0.53     | 2.03        | 8      | 1     |
| 1:A:44:GLY:HA2  | 1:A:87:VAL:N     | 0.53     | 2.19        | 12     | 1     |
| 1:A:46:HIS:CB   | 1:A:119:VAL:HA   | 0.53     | 2.33        | 15     | 1     |
| 1:A:33:GLY:H    | 1:A:97:VAL:HG11  | 0.53     | 1.63        | 6      | 2     |
| 1:A:22:GLN:HG3  | 1:A:105:SER:C    | 0.53     | 2.29        | 19     | 1     |
| 1:A:15:GLN:O    | 1:A:35:ILE:HA    | 0.52     | 2.03        | 5      | 2     |
| 1:A:16:GLY:HA2  | 1:A:34:SER:O     | 0.52     | 2.04        | 5      | 3     |
| 1:A:19:ASN:O    | 1:A:31:VAL:HB    | 0.52     | 2.03        | 16     | 2     |
| 1:A:24:GLU:H    | 1:A:24:GLU:CD    | 0.52     | 2.13        | 14     | 3     |
| 1:A:76:ASP:HA   | 1:A:80:HIS:CG    | 0.52     | 2.39        | 16     | 1     |
| 1:A:1:ALA:HA    | 1:A:22:GLN:O     | 0.52     | 2.05        | 18     | 1     |
| 1:A:45:PHE:HB3  | 1:A:85:GLY:C     | 0.52     | 2.28        | 2      | 1     |
| 1:A:77:GLU:O    | 1:A:78:GLU:HB3   | 0.52     | 2.04        | 12     | 1     |
| 1:A:7:VAL:N     | 1:A:148:VAL:HG11 | 0.52     | 2.20        | 13     | 1     |
| 1:A:61:GLY:HA2  | 1:A:142:SER:HB3  | 0.52     | 1.82        | 16     | 1     |
| 1:A:35:ILE:HB   | 1:A:95:ALA:HB3   | 0.52     | 1.81        | 17     | 1     |
| 1:A:57:CYS:SG   | 1:A:142:SER:HA   | 0.52     | 2.45        | 15     | 2     |
| 1:A:5:VAL:HA    | 1:A:18:ILE:O     | 0.52     | 2.05        | 18     | 1     |
| 1:A:47:VAL:CB   | 1:A:117:LEU:HD23 | 0.52     | 2.35        | 16     | 1     |
| 1:A:6:ALA:HB2   | 1:A:149:ILE:HA   | 0.51     | 1.82        | 18     | 1     |
| 1:A:57:CYS:SG   | 1:A:116:THR:HB   | 0.51     | 2.45        | 2      | 1     |
| 1:A:67:LEU:C    | 1:A:79:ARG:HB2   | 0.51     | 2.31        | 19     | 1     |
| 1:A:6:ALA:HB3   | 1:A:18:ILE:H     | 0.51     | 1.64        | 5      | 2     |
| 1:A:45:PHE:O    | 1:A:124:ASP:HB3  | 0.51     | 2.05        | 7      | 1     |
| 1:A:75:LYS:C    | 1:A:105:SER:HB3  | 0.51     | 2.31        | 12     | 1     |
| 1:A:22:GLN:HE21 | 1:A:106:LEU:HG   | 0.51     | 1.65        | 19     | 1     |
| 1:A:42:LEU:HD23 | 1:A:43:HIS:N     | 0.51     | 2.21        | 16     | 1     |
| 1:A:20:PHE:CE1  | 1:A:106:LEU:HG   | 0.51     | 2.40        | 4      | 1     |

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| Atom-1          | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|-----------------|------------------|----------|-------------|--------|-------|
|                 |                  |          |             | Worst  | Total |
| 1:A:42:LEU:HG   | 1:A:120:HIS:O    | 0.51     | 2.06        | 1      | 1     |
| 1:A:112:ILE:H   | 1:A:112:ILE:HD13 | 0.51     | 1.66        | 14     | 1     |
| 1:A:6:ALA:HA    | 1:A:148:VAL:O    | 0.51     | 2.06        | 4      | 1     |
| 1:A:80:HIS:NE2  | 1:A:105:SER:HB2  | 0.51     | 2.20        | 14     | 1     |
| 1:A:42:LEU:HD22 | 1:A:87:VAL:HB    | 0.51     | 1.82        | 16     | 1     |
| 1:A:69:ARG:N    | 1:A:79:ARG:HB2   | 0.51     | 2.21        | 17     | 1     |
| 1:A:51:GLY:HA2  | 1:A:115:ARG:N    | 0.51     | 2.21        | 7      | 1     |
| 1:A:87:VAL:CB   | 1:A:95:ALA:HB1   | 0.51     | 2.35        | 9      | 1     |
| 1:A:6:ALA:HA    | 1:A:148:VAL:HG21 | 0.51     | 1.83        | 13     | 1     |
| 1:A:68:SER:HA   | 1:A:77:GLU:OE1   | 0.51     | 2.06        | 19     | 1     |
| 1:A:42:LEU:HB2  | 1:A:123:ALA:HB2  | 0.50     | 1.84        | 18     | 1     |
| 1:A:115:ARG:HD3 | 1:A:149:ILE:C    | 0.50     | 2.31        | 6      | 2     |
| 1:A:69:ARG:C    | 1:A:78:GLU:HA    | 0.50     | 2.32        | 2      | 1     |
| 1:A:118:VAL:HA  | 1:A:146:CYS:CB   | 0.50     | 2.36        | 13     | 1     |
| 1:A:73:GLY:O    | 1:A:77:GLU:HG3   | 0.50     | 2.07        | 14     | 1     |
| 1:A:49:GLU:OE1  | 1:A:49:GLU:HA    | 0.50     | 2.04        | 19     | 1     |
| 1:A:67:LEU:C    | 1:A:69:ARG:H     | 0.50     | 2.14        | 15     | 3     |
| 1:A:121:GLU:H   | 1:A:121:GLU:CD   | 0.50     | 2.13        | 12     | 7     |
| 1:A:68:SER:HB2  | 1:A:79:ARG:C     | 0.50     | 2.32        | 5      | 1     |
| 1:A:69:ARG:O    | 1:A:70:LYS:HB2   | 0.50     | 2.06        | 5      | 1     |
| 1:A:113:ILE:HA  | 1:A:150:GLY:HA3  | 0.50     | 1.83        | 19     | 1     |
| 1:A:51:GLY:N    | 1:A:115:ARG:HD3  | 0.50     | 2.22        | 19     | 2     |
| 1:A:84:LEU:HD23 | 1:A:85:GLY:N     | 0.50     | 2.21        | 13     | 2     |
| 1:A:72:GLY:HA3  | 1:A:80:HIS:O     | 0.50     | 2.07        | 12     | 1     |
| 1:A:46:HIS:CD2  | 1:A:117:LEU:HD12 | 0.50     | 2.41        | 3      | 1     |
| 1:A:89:ALA:HA   | 1:A:94:VAL:O     | 0.49     | 2.07        | 3      | 2     |
| 1:A:49:GLU:N    | 1:A:115:ARG:HD2  | 0.49     | 2.22        | 11     | 1     |
| 1:A:67:LEU:O    | 1:A:78:GLU:HB3   | 0.49     | 2.07        | 19     | 1     |
| 1:A:68:SER:HA   | 1:A:77:GLU:C     | 0.49     | 2.31        | 6      | 1     |
| 1:A:45:PHE:CG   | 1:A:84:LEU:HB3   | 0.49     | 2.42        | 8      | 1     |
| 1:A:113:ILE:HA  | 1:A:115:ARG:NH1  | 0.49     | 2.22        | 17     | 1     |
| 1:A:69:ARG:HB2  | 1:A:78:GLU:HA    | 0.49     | 1.83        | 11     | 1     |
| 1:A:9:LYS:HD3   | 1:A:10:GLY:N     | 0.49     | 2.21        | 5      | 1     |
| 1:A:80:HIS:CD2  | 1:A:126:LEU:HG   | 0.49     | 2.42        | 10     | 1     |
| 1:A:129:GLY:CA  | 1:A:135:THR:HA   | 0.49     | 2.36        | 15     | 1     |
| 1:A:46:HIS:CD2  | 1:A:126:LEU:HB2  | 0.49     | 2.43        | 19     | 1     |
| 1:A:29:VAL:HG12 | 1:A:104:ILE:HG23 | 0.49     | 1.83        | 7      | 1     |
| 1:A:84:LEU:HD23 | 1:A:85:GLY:H     | 0.49     | 1.68        | 13     | 1     |
| 1:A:16:GLY:HA3  | 1:A:34:SER:O     | 0.49     | 2.07        | 9      | 2     |
| 1:A:99:ILE:H    | 1:A:99:ILE:HD13  | 0.49     | 1.67        | 7      | 1     |
| 1:A:121:GLU:O   | 1:A:122:LYS:HG2  | 0.49     | 2.08        | 8      | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:70:LYS:CB    | 1:A:79:ARG:HB2   | 0.49     | 2.38        | 15     | 1     |
| 1:A:66:PRO:O     | 1:A:70:LYS:HA    | 0.48     | 2.08        | 1      | 1     |
| 1:A:38:LEU:HA    | 1:A:92:ASP:OD1   | 0.48     | 2.08        | 15     | 1     |
| 1:A:3:LYS:O      | 1:A:151:ILE:HG12 | 0.48     | 2.08        | 10     | 2     |
| 1:A:40:GLU:HG3   | 1:A:121:GLU:O    | 0.48     | 2.08        | 11     | 1     |
| 1:A:68:SER:HA    | 1:A:79:ARG:C     | 0.48     | 2.33        | 17     | 1     |
| 1:A:48:HIS:O     | 1:A:115:ARG:HG3  | 0.48     | 2.09        | 8      | 1     |
| 1:A:49:GLU:HG3   | 1:A:109:ASP:OD1  | 0.48     | 2.09        | 10     | 1     |
| 1:A:49:GLU:HB3   | 1:A:109:ASP:OD2  | 0.48     | 2.08        | 3      | 1     |
| 1:A:51:GLY:HA2   | 1:A:115:ARG:HA   | 0.48     | 1.86        | 11     | 4     |
| 1:A:124:ASP:OD2  | 1:A:140:ALA:HB2  | 0.48     | 2.09        | 19     | 1     |
| 1:A:117:LEU:HD22 | 1:A:148:VAL:O    | 0.48     | 2.09        | 13     | 1     |
| 1:A:22:GLN:CG    | 1:A:106:LEU:HB3  | 0.48     | 2.38        | 2      | 1     |
| 1:A:45:PHE:O     | 1:A:47:VAL:HG12  | 0.48     | 2.09        | 3      | 1     |
| 1:A:39:THR:HB    | 1:A:90:ASP:O     | 0.48     | 2.09        | 6      | 1     |
| 1:A:57:CYS:SG    | 1:A:118:VAL:HB   | 0.48     | 2.49        | 11     | 1     |
| 1:A:19:ASN:O     | 1:A:31:VAL:HA    | 0.47     | 2.09        | 1      | 3     |
| 1:A:40:GLU:O     | 1:A:90:ASP:HA    | 0.47     | 2.09        | 11     | 1     |
| 1:A:51:GLY:HA3   | 1:A:115:ARG:HA   | 0.47     | 1.86        | 13     | 1     |
| 1:A:75:LYS:O     | 1:A:104:ILE:HG13 | 0.47     | 2.09        | 12     | 1     |
| 1:A:21:GLU:O     | 1:A:29:VAL:HG23  | 0.47     | 2.09        | 6      | 1     |
| 1:A:90:ASP:CG    | 1:A:91:LYS:H     | 0.47     | 2.17        | 19     | 1     |
| 1:A:110:HIS:HB3  | 1:A:113:ILE:O    | 0.47     | 2.10        | 2      | 2     |
| 1:A:65:ASN:O     | 1:A:70:LYS:HA    | 0.47     | 2.09        | 6      | 2     |
| 1:A:69:ARG:HA    | 1:A:78:GLU:HA    | 0.47     | 1.86        | 8      | 1     |
| 1:A:33:GLY:O     | 1:A:97:VAL:HG22  | 0.47     | 2.09        | 19     | 1     |
| 1:A:35:ILE:HG22  | 1:A:95:ALA:HB2   | 0.47     | 1.87        | 2      | 1     |
| 1:A:68:SER:HA    | 1:A:80:HIS:HB3   | 0.47     | 1.87        | 4      | 1     |
| 1:A:111:SER:O    | 1:A:115:ARG:HG3  | 0.47     | 2.09        | 9      | 1     |
| 1:A:86:ASN:O     | 1:A:97:VAL:HA    | 0.47     | 2.10        | 15     | 1     |
| 1:A:28:PRO:HB3   | 1:A:101:ASP:N    | 0.47     | 2.24        | 9      | 1     |
| 1:A:117:LEU:HB3  | 1:A:149:ILE:CD1  | 0.47     | 2.40        | 13     | 1     |
| 1:A:46:HIS:CB    | 1:A:119:VAL:HB   | 0.47     | 2.39        | 5      | 1     |
| 1:A:42:LEU:HA    | 1:A:122:LYS:C    | 0.47     | 2.35        | 16     | 1     |
| 1:A:22:GLN:HA    | 1:A:104:ILE:O    | 0.46     | 2.10        | 14     | 1     |
| 1:A:44:GLY:HA2   | 1:A:85:GLY:O     | 0.46     | 2.10        | 9      | 1     |
| 1:A:57:CYS:O     | 1:A:142:SER:HB2  | 0.46     | 2.10        | 14     | 1     |
| 1:A:40:GLU:O     | 1:A:121:GLU:HB3  | 0.46     | 2.09        | 4      | 4     |
| 1:A:45:PHE:HA    | 1:A:85:GLY:O     | 0.46     | 2.09        | 11     | 1     |
| 1:A:117:LEU:HD13 | 1:A:149:ILE:HB   | 0.46     | 1.87        | 16     | 1     |
| 1:A:127:GLY:C    | 1:A:128:LYS:HD2  | 0.46     | 2.35        | 11     | 1     |

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| Atom-1           | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|------------------|-----------------|----------|-------------|--------|-------|
|                  |                 |          |             | Worst  | Total |
| 1:A:112:ILE:HG22 | 1:A:150:GLY:HA2 | 0.46     | 1.88        | 15     | 1     |
| 1:A:112:ILE:O    | 1:A:115:ARG:HG2 | 0.46     | 2.10        | 19     | 1     |
| 1:A:103:VAL:C    | 1:A:105:SER:H   | 0.46     | 2.19        | 7      | 1     |
| 1:A:89:ALA:HB3   | 1:A:121:GLU:HG2 | 0.46     | 1.88        | 11     | 2     |
| 1:A:50:PHE:CD2   | 1:A:59:SER:HB3  | 0.46     | 2.45        | 14     | 1     |
| 1:A:21:GLU:O     | 1:A:29:VAL:HB   | 0.46     | 2.10        | 9      | 1     |
| 1:A:74:PRO:C     | 1:A:76:ASP:H    | 0.46     | 2.19        | 14     | 1     |
| 1:A:77:GLU:HB2   | 1:A:79:ARG:HD2  | 0.46     | 1.86        | 18     | 1     |
| 1:A:72:GLY:C     | 1:A:126:LEU:HB3 | 0.46     | 2.36        | 6      | 1     |
| 1:A:84:LEU:HD13  | 1:A:85:GLY:N    | 0.46     | 2.26        | 10     | 1     |
| 1:A:40:GLU:OE2   | 1:A:122:LYS:HG2 | 0.46     | 2.09        | 14     | 1     |
| 1:A:69:ARG:CB    | 1:A:78:GLU:HA   | 0.46     | 2.41        | 11     | 1     |
| 1:A:14:VAL:HA    | 1:A:36:LYS:O    | 0.46     | 2.11        | 9      | 2     |
| 1:A:35:ILE:H     | 1:A:95:ALA:HB3  | 0.46     | 1.70        | 16     | 1     |
| 1:A:68:SER:HA    | 1:A:77:GLU:CD   | 0.46     | 2.35        | 19     | 1     |
| 1:A:116:THR:HB   | 1:A:147:GLY:HA2 | 0.45     | 1.88        | 13     | 1     |
| 1:A:22:GLN:NE2   | 1:A:106:LEU:HG  | 0.45     | 2.26        | 19     | 1     |
| 1:A:42:LEU:HA    | 1:A:87:VAL:O    | 0.45     | 2.11        | 19     | 1     |
| 1:A:111:SER:O    | 1:A:115:ARG:HD2 | 0.45     | 2.11        | 14     | 1     |
| 1:A:117:LEU:O    | 1:A:146:CYS:HA  | 0.45     | 2.11        | 3      | 1     |
| 1:A:42:LEU:CB    | 1:A:88:THR:HA   | 0.45     | 2.41        | 8      | 1     |
| 1:A:2:THR:O      | 1:A:21:GLU:HB2  | 0.45     | 2.12        | 10     | 1     |
| 1:A:45:PHE:CD1   | 1:A:45:PHE:O    | 0.45     | 2.70        | 13     | 1     |
| 1:A:72:GLY:HA2   | 1:A:77:GLU:CG   | 0.45     | 2.41        | 19     | 1     |
| 1:A:76:ASP:HB3   | 1:A:78:GLU:OE1  | 0.45     | 2.11        | 5      | 1     |
| 1:A:40:GLU:N     | 1:A:90:ASP:HA   | 0.45     | 2.27        | 18     | 2     |
| 1:A:49:GLU:OE2   | 1:A:64:PHE:HA   | 0.45     | 2.12        | 3      | 1     |
| 1:A:46:HIS:O     | 1:A:47:VAL:HG23 | 0.45     | 2.12        | 13     | 1     |
| 1:A:90:ASP:C     | 1:A:92:ASP:H    | 0.45     | 2.19        | 13     | 3     |
| 1:A:46:HIS:O     | 1:A:47:VAL:HG13 | 0.45     | 2.12        | 6      | 1     |
| 1:A:3:LYS:NZ     | 1:A:3:LYS:HB3   | 0.45     | 2.27        | 1      | 1     |
| 1:A:13:PRO:HB3   | 1:A:120:HIS:HA  | 0.45     | 1.88        | 7      | 1     |
| 1:A:4:ALA:HA     | 1:A:151:ILE:HA  | 0.45     | 1.88        | 19     | 4     |
| 1:A:23:LYS:HG3   | 1:A:24:GLU:H    | 0.45     | 1.72        | 4      | 1     |
| 1:A:113:ILE:HA   | 1:A:115:ARG:NE  | 0.45     | 2.26        | 6      | 1     |
| 1:A:107:SER:O    | 1:A:112:ILE:HA  | 0.45     | 2.11        | 19     | 1     |
| 1:A:46:HIS:HB2   | 1:A:125:ASP:HA  | 0.44     | 1.89        | 2      | 1     |
| 1:A:54:THR:O     | 1:A:147:GLY:HA2 | 0.44     | 2.12        | 17     | 1     |
| 1:A:60:ALA:C     | 1:A:62:PRO:HD3  | 0.44     | 2.36        | 19     | 1     |
| 1:A:49:GLU:HB3   | 1:A:110:HIS:HB2 | 0.44     | 1.88        | 5      | 1     |
| 1:A:57:CYS:HB2   | 1:A:60:ALA:CB   | 0.44     | 2.42        | 5      | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:116:THR:HG22 | 1:A:146:CYS:HB3  | 0.44     | 1.89        | 8      | 1     |
| 1:A:47:VAL:HG13  | 1:A:117:LEU:HA   | 0.44     | 1.90        | 1      | 1     |
| 1:A:110:HIS:CG   | 1:A:115:ARG:HG2  | 0.44     | 2.47        | 3      | 1     |
| 1:A:125:ASP:HB3  | 1:A:128:LYS:CB   | 0.44     | 2.43        | 5      | 1     |
| 1:A:120:HIS:CD2  | 1:A:124:ASP:HB2  | 0.44     | 2.48        | 8      | 1     |
| 1:A:22:GLN:HG3   | 1:A:105:SER:O    | 0.44     | 2.12        | 19     | 1     |
| 1:A:22:GLN:HG3   | 1:A:29:VAL:HG12  | 0.44     | 1.89        | 4      | 1     |
| 1:A:60:ALA:HB1   | 1:A:118:VAL:HG13 | 0.44     | 1.89        | 7      | 1     |
| 1:A:42:LEU:HB3   | 1:A:88:THR:HG22  | 0.44     | 1.89        | 19     | 1     |
| 1:A:88:THR:HA    | 1:A:121:GLU:OE1  | 0.44     | 2.12        | 7      | 1     |
| 1:A:40:GLU:HB3   | 1:A:91:LYS:N     | 0.44     | 2.28        | 10     | 1     |
| 1:A:21:GLU:O     | 1:A:104:ILE:HA   | 0.44     | 2.13        | 14     | 1     |
| 1:A:47:VAL:HA    | 1:A:117:LEU:HA   | 0.44     | 1.89        | 14     | 1     |
| 1:A:75:LYS:O     | 1:A:101:ASP:HA   | 0.44     | 2.13        | 7      | 1     |
| 1:A:133:GLU:O    | 1:A:136:LYS:HG3  | 0.44     | 2.13        | 10     | 1     |
| 1:A:115:ARG:HH21 | 1:A:148:VAL:HG13 | 0.44     | 1.72        | 17     | 1     |
| 1:A:45:PHE:CD1   | 1:A:85:GLY:HA3   | 0.44     | 2.48        | 2      | 1     |
| 1:A:116:THR:CB   | 1:A:147:GLY:HA2  | 0.44     | 2.43        | 13     | 1     |
| 1:A:124:ASP:OD2  | 1:A:140:ALA:HA   | 0.44     | 2.13        | 16     | 1     |
| 1:A:74:PRO:HA    | 1:A:84:LEU:HG    | 0.44     | 1.90        | 2      | 1     |
| 1:A:4:ALA:HB3    | 1:A:20:PHE:N     | 0.44     | 2.28        | 16     | 1     |
| 1:A:49:GLU:CG    | 1:A:60:ALA:HB2   | 0.43     | 2.43        | 1      | 1     |
| 1:A:40:GLU:O     | 1:A:121:GLU:HB2  | 0.43     | 2.13        | 6      | 1     |
| 1:A:22:GLN:HB2   | 1:A:106:LEU:HA   | 0.43     | 1.89        | 8      | 1     |
| 1:A:50:PHE:C     | 1:A:115:ARG:HG2  | 0.43     | 2.38        | 11     | 1     |
| 1:A:57:CYS:O     | 1:A:142:SER:HB3  | 0.43     | 2.13        | 11     | 1     |
| 1:A:39:THR:HB    | 1:A:91:LYS:HB3   | 0.43     | 1.90        | 16     | 1     |
| 1:A:48:HIS:NE2   | 1:A:65:ASN:HB2   | 0.43     | 2.28        | 4      | 1     |
| 1:A:1:ALA:O      | 1:A:21:GLU:HA    | 0.43     | 2.12        | 7      | 2     |
| 1:A:113:ILE:HD12 | 1:A:113:ILE:H    | 0.43     | 1.72        | 19     | 1     |
| 1:A:45:PHE:CE1   | 1:A:126:LEU:HA   | 0.43     | 2.48        | 6      | 1     |
| 1:A:112:ILE:O    | 1:A:149:ILE:HG22 | 0.43     | 2.13        | 13     | 1     |
| 1:A:46:HIS:CE1   | 1:A:138:GLY:HA3  | 0.43     | 2.47        | 1      | 1     |
| 1:A:49:GLU:CB    | 1:A:110:HIS:HB2  | 0.43     | 2.44        | 5      | 1     |
| 1:A:89:ALA:CB    | 1:A:121:GLU:HB3  | 0.43     | 2.43        | 8      | 1     |
| 1:A:48:HIS:NE2   | 1:A:118:VAL:HG23 | 0.43     | 2.29        | 12     | 1     |
| 1:A:126:LEU:HA   | 1:A:135:THR:O    | 0.43     | 2.14        | 2      | 1     |
| 1:A:38:LEU:HD23  | 1:A:39:THR:N     | 0.43     | 2.29        | 5      | 1     |
| 1:A:44:GLY:HA3   | 1:A:87:VAL:H     | 0.43     | 1.73        | 7      | 1     |
| 1:A:42:LEU:HA    | 1:A:88:THR:HA    | 0.43     | 1.89        | 11     | 1     |
| 1:A:42:LEU:O     | 1:A:43:HIS:HB2   | 0.43     | 2.13        | 12     | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:48:HIS:CD2   | 1:A:118:VAL:HB   | 0.43     | 2.48        | 18     | 1     |
| 1:A:5:VAL:O      | 1:A:149:ILE:HA   | 0.43     | 2.14        | 2      | 1     |
| 1:A:50:PHE:HA    | 1:A:111:SER:OG   | 0.43     | 2.13        | 4      | 1     |
| 1:A:40:GLU:OE2   | 1:A:122:LYS:HD3  | 0.43     | 2.14        | 9      | 1     |
| 1:A:47:VAL:HG23  | 1:A:116:THR:C    | 0.43     | 2.39        | 14     | 1     |
| 1:A:52:ASP:OD1   | 1:A:57:CYS:HA    | 0.43     | 2.13        | 14     | 1     |
| 1:A:129:GLY:HA2  | 1:A:135:THR:HA   | 0.43     | 1.91        | 15     | 1     |
| 1:A:39:THR:HA    | 1:A:91:LYS:N     | 0.43     | 2.29        | 19     | 1     |
| 1:A:57:CYS:N     | 1:A:146:CYS:SG   | 0.43     | 2.87        | 15     | 3     |
| 1:A:31:VAL:HG13  | 1:A:99:ILE:HG21  | 0.43     | 1.91        | 15     | 1     |
| 1:A:46:HIS:O     | 1:A:47:VAL:HB    | 0.43     | 2.13        | 5      | 1     |
| 1:A:79:ARG:NH1   | 1:A:80:HIS:HB2   | 0.43     | 2.29        | 6      | 1     |
| 1:A:65:ASN:HB3   | 1:A:68:SER:OG    | 0.43     | 2.14        | 2      | 1     |
| 1:A:110:HIS:HA   | 1:A:115:ARG:HE   | 0.43     | 1.72        | 10     | 1     |
| 1:A:115:ARG:HH11 | 1:A:115:ARG:CA   | 0.43     | 2.26        | 10     | 1     |
| 1:A:50:PHE:CZ    | 1:A:60:ALA:HA    | 0.43     | 2.49        | 15     | 1     |
| 1:A:89:ALA:CB    | 1:A:121:GLU:HB2  | 0.43     | 2.44        | 16     | 1     |
| 1:A:49:GLU:CB    | 1:A:108:GLY:HA2  | 0.42     | 2.43        | 12     | 1     |
| 1:A:7:VAL:H      | 1:A:148:VAL:HG11 | 0.42     | 1.74        | 13     | 1     |
| 1:A:117:LEU:HB3  | 1:A:149:ILE:CG2  | 0.42     | 2.44        | 6      | 2     |
| 1:A:4:ALA:CB     | 1:A:151:ILE:HA   | 0.42     | 2.44        | 13     | 1     |
| 1:A:117:LEU:HD12 | 1:A:117:LEU:N    | 0.42     | 2.28        | 16     | 1     |
| 1:A:74:PRO:O     | 1:A:84:LEU:HD13  | 0.42     | 2.14        | 4      | 1     |
| 1:A:17:ILE:O     | 1:A:33:GLY:HA2   | 0.42     | 2.15        | 5      | 1     |
| 1:A:41:GLY:N     | 1:A:90:ASP:HA    | 0.42     | 2.29        | 7      | 1     |
| 1:A:42:LEU:HB3   | 1:A:87:VAL:O     | 0.42     | 2.14        | 16     | 1     |
| 1:A:104:ILE:HD12 | 1:A:105:SER:N    | 0.42     | 2.30        | 4      | 1     |
| 1:A:147:GLY:O    | 1:A:148:VAL:HG23 | 0.42     | 2.14        | 4      | 1     |
| 1:A:71:HIS:O     | 1:A:127:GLY:HA2  | 0.42     | 2.14        | 7      | 1     |
| 1:A:46:HIS:HB2   | 1:A:117:LEU:HD12 | 0.42     | 1.90        | 13     | 1     |
| 1:A:68:SER:C     | 1:A:70:LYS:H     | 0.42     | 2.23        | 15     | 1     |
| 1:A:54:THR:HA    | 1:A:147:GLY:O    | 0.42     | 2.14        | 4      | 1     |
| 1:A:70:LYS:HE2   | 1:A:76:ASP:OD2   | 0.42     | 2.14        | 4      | 1     |
| 1:A:18:ILE:HG12  | 1:A:46:HIS:HE2   | 0.42     | 1.74        | 8      | 1     |
| 1:A:116:THR:CG2  | 1:A:146:CYS:HB3  | 0.42     | 2.44        | 8      | 1     |
| 1:A:68:SER:OG    | 1:A:80:HIS:HB2   | 0.42     | 2.15        | 13     | 1     |
| 1:A:68:SER:N     | 1:A:79:ARG:HB2   | 0.42     | 2.28        | 19     | 1     |
| 1:A:29:VAL:HG22  | 1:A:101:ASP:H    | 0.42     | 1.74        | 3      | 1     |
| 1:A:39:THR:HA    | 1:A:91:LYS:HA    | 0.42     | 1.89        | 5      | 1     |
| 1:A:29:VAL:HG23  | 1:A:102:SER:HA   | 0.42     | 1.91        | 13     | 1     |
| 1:A:50:PHE:N     | 1:A:115:ARG:HG3  | 0.42     | 2.29        | 5      | 1     |

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| Atom-1          | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|-----------------|------------------|----------|-------------|--------|-------|
|                 |                  |          |             | Worst  | Total |
| 1:A:90:ASP:OD2  | 1:A:91:LYS:HG2   | 0.42     | 2.14        | 3      | 1     |
| 1:A:129:GLY:HA3 | 1:A:135:THR:HA   | 0.42     | 1.90        | 9      | 1     |
| 1:A:134:SER:HA  | 1:A:137:THR:HG22 | 0.42     | 1.91        | 11     | 1     |
| 1:A:117:LEU:O   | 1:A:146:CYS:HB2  | 0.42     | 2.13        | 13     | 1     |
| 1:A:115:ARG:NE  | 1:A:150:GLY:HA3  | 0.42     | 2.30        | 6      | 1     |
| 1:A:59:SER:O    | 1:A:62:PRO:HD3   | 0.42     | 2.15        | 14     | 1     |
| 1:A:46:HIS:HB3  | 1:A:119:VAL:HB   | 0.42     | 1.90        | 5      | 1     |
| 1:A:49:GLU:O    | 1:A:50:PHE:HB2   | 0.42     | 2.15        | 6      | 1     |
| 1:A:84:LEU:H    | 1:A:103:VAL:HG11 | 0.42     | 1.74        | 9      | 1     |
| 1:A:47:VAL:HB   | 1:A:63:HIS:CD2   | 0.41     | 2.50        | 6      | 1     |
| 1:A:79:ARG:O    | 1:A:80:HIS:HB2   | 0.41     | 2.15        | 4      | 1     |
| 1:A:57:CYS:HB2  | 1:A:60:ALA:HB2   | 0.41     | 1.92        | 5      | 1     |
| 1:A:2:THR:HA    | 1:A:21:GLU:HG3   | 0.41     | 1.92        | 10     | 1     |
| 1:A:41:GLY:HA2  | 1:A:121:GLU:C    | 0.41     | 2.40        | 12     | 1     |
| 1:A:44:GLY:HA2  | 1:A:87:VAL:H     | 0.41     | 1.73        | 12     | 1     |
| 1:A:69:ARG:HA   | 1:A:79:ARG:H     | 0.41     | 1.75        | 2      | 1     |
| 1:A:41:GLY:N    | 1:A:90:ASP:HB3   | 0.41     | 2.31        | 6      | 1     |
| 1:A:128:LYS:C   | 1:A:135:THR:HB   | 0.41     | 2.41        | 6      | 1     |
| 1:A:21:GLU:HB2  | 1:A:29:VAL:HG23  | 0.41     | 1.91        | 8      | 1     |
| 1:A:106:LEU:HG  | 1:A:112:ILE:HG22 | 0.41     | 1.92        | 17     | 1     |
| 1:A:39:THR:HA   | 1:A:90:ASP:C     | 0.41     | 2.40        | 19     | 1     |
| 1:A:16:GLY:HA3  | 1:A:35:ILE:HD13  | 0.41     | 1.93        | 6      | 1     |
| 1:A:27:GLY:H    | 1:A:103:VAL:HG22 | 0.41     | 1.75        | 3      | 1     |
| 1:A:45:PHE:HB3  | 1:A:124:ASP:CB   | 0.41     | 2.45        | 10     | 1     |
| 1:A:68:SER:HB3  | 1:A:78:GLU:H     | 0.41     | 1.75        | 12     | 1     |
| 1:A:67:LEU:O    | 1:A:79:ARG:HB2   | 0.41     | 2.15        | 17     | 1     |
| 1:A:72:GLY:HA2  | 1:A:79:ARG:HB2   | 0.41     | 1.92        | 2      | 1     |
| 1:A:8:LEU:HB3   | 1:A:117:LEU:HD21 | 0.41     | 1.92        | 3      | 1     |
| 1:A:22:GLN:O    | 1:A:22:GLN:HG3   | 0.41     | 2.14        | 8      | 1     |
| 1:A:3:LYS:N     | 1:A:21:GLU:HG3   | 0.41     | 2.30        | 9      | 1     |
| 1:A:48:HIS:HB2  | 1:A:115:ARG:HB3  | 0.41     | 1.92        | 11     | 1     |
| 1:A:54:THR:HA   | 1:A:148:VAL:HG23 | 0.41     | 1.92        | 11     | 1     |
| 1:A:90:ASP:HB3  | 1:A:93:GLY:HA3   | 0.41     | 1.93        | 5      | 1     |
| 1:A:110:HIS:O   | 1:A:115:ARG:HB2  | 0.41     | 2.15        | 10     | 1     |
| 1:A:108:GLY:HA3 | 1:A:111:SER:O    | 0.41     | 2.16        | 1      | 1     |
| 1:A:132:GLU:O   | 1:A:135:THR:HB   | 0.41     | 2.16        | 1      | 1     |
| 1:A:22:GLN:HA   | 1:A:29:VAL:HG12  | 0.41     | 1.92        | 2      | 1     |
| 1:A:65:ASN:HB2  | 1:A:109:ASP:OD2  | 0.41     | 2.15        | 3      | 1     |
| 1:A:69:ARG:HB3  | 1:A:79:ARG:HA    | 0.41     | 1.93        | 6      | 1     |
| 1:A:67:LEU:CB   | 1:A:109:ASP:HB2  | 0.41     | 2.46        | 8      | 1     |
| 1:A:16:GLY:HA3  | 1:A:35:ILE:HG22  | 0.41     | 1.93        | 9      | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:34:SER:HA    | 1:A:95:ALA:O     | 0.41     | 2.16        | 9      | 1     |
| 1:A:65:ASN:ND2   | 1:A:108:GLY:HA2  | 0.41     | 2.31        | 9      | 1     |
| 1:A:69:ARG:O     | 1:A:69:ARG:HD2   | 0.41     | 2.16        | 10     | 1     |
| 1:A:79:ARG:O     | 1:A:80:HIS:HB3   | 0.41     | 2.15        | 10     | 1     |
| 1:A:68:SER:CB    | 1:A:78:GLU:H     | 0.41     | 2.28        | 12     | 1     |
| 1:A:87:VAL:HB    | 1:A:95:ALA:CB    | 0.41     | 2.45        | 12     | 1     |
| 1:A:125:ASP:O    | 1:A:138:GLY:HA2  | 0.41     | 2.16        | 12     | 1     |
| 1:A:69:ARG:HB3   | 1:A:78:GLU:OE1   | 0.41     | 2.16        | 14     | 1     |
| 1:A:76:ASP:HB2   | 1:A:102:SER:O    | 0.41     | 2.16        | 14     | 1     |
| 1:A:39:THR:HB    | 1:A:91:LYS:CA    | 0.41     | 2.45        | 16     | 1     |
| 1:A:115:ARG:O    | 1:A:149:ILE:HG22 | 0.41     | 2.16        | 19     | 1     |
| 1:A:42:LEU:HD22  | 1:A:87:VAL:HG23  | 0.41     | 1.92        | 1      | 1     |
| 1:A:149:ILE:O    | 1:A:149:ILE:HG23 | 0.41     | 2.16        | 6      | 1     |
| 1:A:69:ARG:O     | 1:A:71:HIS:N     | 0.41     | 2.52        | 10     | 1     |
| 1:A:129:GLY:C    | 1:A:135:THR:HA   | 0.41     | 2.40        | 15     | 1     |
| 1:A:68:SER:HA    | 1:A:79:ARG:CB    | 0.41     | 2.45        | 18     | 1     |
| 1:A:118:VAL:HA   | 1:A:145:ALA:O    | 0.40     | 2.16        | 12     | 1     |
| 1:A:66:PRO:HB3   | 1:A:69:ARG:NH2   | 0.40     | 2.31        | 16     | 1     |
| 1:A:33:GLY:C     | 1:A:97:VAL:HG12  | 0.40     | 2.41        | 8      | 1     |
| 1:A:45:PHE:HB3   | 1:A:124:ASP:HB2  | 0.40     | 1.93        | 10     | 1     |
| 1:A:46:HIS:NE2   | 1:A:117:LEU:HG   | 0.40     | 2.30        | 10     | 1     |
| 1:A:67:LEU:HG    | 1:A:109:ASP:CG   | 0.40     | 2.41        | 4      | 1     |
| 1:A:32:TRP:HA    | 1:A:97:VAL:O     | 0.40     | 2.17        | 12     | 1     |
| 1:A:89:ALA:HB1   | 1:A:93:GLY:HA2   | 0.40     | 1.94        | 7      | 1     |
| 1:A:22:GLN:HB2   | 1:A:104:ILE:HB   | 0.40     | 1.93        | 9      | 1     |
| 1:A:45:PHE:CD2   | 1:A:124:ASP:HB3  | 0.40     | 2.51        | 13     | 1     |
| 1:A:118:VAL:HG22 | 1:A:140:ALA:HB3  | 0.40     | 1.92        | 18     | 1     |
| 1:A:47:VAL:HG22  | 1:A:117:LEU:CD1  | 0.40     | 2.45        | 4      | 1     |
| 1:A:53:ASN:O     | 1:A:147:GLY:HA3  | 0.40     | 2.16        | 4      | 1     |
| 1:A:69:ARG:C     | 1:A:71:HIS:H     | 0.40     | 2.24        | 8      | 1     |
| 1:A:115:ARG:NH1  | 1:A:150:GLY:HA3  | 0.40     | 2.32        | 17     | 1     |
| 1:A:126:LEU:HD12 | 1:A:135:THR:O    | 0.40     | 2.17        | 19     | 1     |

## 6.3 Torsion angles ⓘ

### 6.3.1 Protein backbone ⓘ

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

| Mol | Chain | Analysed        | Favoured      | Allowed      | Outliers   | Percentiles |    |
|-----|-------|-----------------|---------------|--------------|------------|-------------|----|
| 1   | A     | 148/153 (97%)   | 113±4 (76±3%) | 27±5 (19±3%) | 8±3 (5±2%) | 2           | 22 |
| All | All   | 2812/2907 (97%) | 2141 (76%)    | 522 (19%)    | 149 (5%)   | 2           | 22 |

All 42 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 26  | ASN  | 10             |
| 1   | A     | 61  | GLY  | 6              |
| 1   | A     | 79  | ARG  | 6              |
| 1   | A     | 80  | HIS  | 6              |
| 1   | A     | 129 | GLY  | 6              |
| 1   | A     | 139 | ASN  | 6              |
| 1   | A     | 52  | ASP  | 6              |
| 1   | A     | 94  | VAL  | 6              |
| 1   | A     | 78  | GLU  | 6              |
| 1   | A     | 50  | PHE  | 5              |
| 1   | A     | 77  | GLU  | 5              |
| 1   | A     | 70  | LYS  | 5              |
| 1   | A     | 91  | LYS  | 5              |
| 1   | A     | 111 | SER  | 4              |
| 1   | A     | 109 | ASP  | 4              |
| 1   | A     | 41  | GLY  | 4              |
| 1   | A     | 102 | SER  | 4              |
| 1   | A     | 47  | VAL  | 4              |
| 1   | A     | 104 | ILE  | 4              |
| 1   | A     | 76  | ASP  | 4              |
| 1   | A     | 42  | LEU  | 3              |
| 1   | A     | 23  | LYS  | 3              |
| 1   | A     | 71  | HIS  | 3              |
| 1   | A     | 72  | GLY  | 3              |
| 1   | A     | 44  | GLY  | 3              |
| 1   | A     | 68  | SER  | 2              |
| 1   | A     | 93  | GLY  | 2              |
| 1   | A     | 130 | GLY  | 2              |
| 1   | A     | 43  | HIS  | 2              |
| 1   | A     | 147 | GLY  | 2              |
| 1   | A     | 148 | VAL  | 2              |
| 1   | A     | 151 | ILE  | 2              |
| 1   | A     | 85  | GLY  | 2              |
| 1   | A     | 138 | GLY  | 2              |
| 1   | A     | 125 | ASP  | 2              |
| 1   | A     | 142 | SER  | 2              |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 51  | GLY  | 1              |
| 1   | A     | 123 | ALA  | 1              |
| 1   | A     | 126 | LEU  | 1              |
| 1   | A     | 90  | ASP  | 1              |
| 1   | A     | 63  | HIS  | 1              |
| 1   | A     | 73  | GLY  | 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 |    |
|-----|-------|-----------------|---------------|------------|-------------|----|
| 1   | A     | 115/117 (98%)   | 107±2 (93±2%) | 8±2 (7±2%) | 15          | 63 |
| All | All   | 2185/2223 (98%) | 2024 (93%)    | 161 (7%)   | 15          | 63 |

All 70 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 121 | GLU  | 8              |
| 1   | A     | 115 | ARG  | 7              |
| 1   | A     | 49  | GLU  | 7              |
| 1   | A     | 126 | LEU  | 5              |
| 1   | A     | 149 | ILE  | 5              |
| 1   | A     | 22  | GLN  | 4              |
| 1   | A     | 116 | THR  | 4              |
| 1   | A     | 78  | GLU  | 4              |
| 1   | A     | 151 | ILE  | 4              |
| 1   | A     | 79  | ARG  | 4              |
| 1   | A     | 99  | ILE  | 4              |
| 1   | A     | 104 | ILE  | 4              |
| 1   | A     | 75  | LYS  | 4              |
| 1   | A     | 18  | ILE  | 4              |
| 1   | A     | 84  | LEU  | 3              |
| 1   | A     | 46  | HIS  | 3              |
| 1   | A     | 80  | HIS  | 3              |
| 1   | A     | 144 | LEU  | 3              |
| 1   | A     | 133 | GLU  | 3              |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 48  | HIS  | 3              |
| 1   | A     | 19  | ASN  | 3              |
| 1   | A     | 3   | LYS  | 2              |
| 1   | A     | 8   | LEU  | 2              |
| 1   | A     | 57  | CYS  | 2              |
| 1   | A     | 112 | ILE  | 2              |
| 1   | A     | 106 | LEU  | 2              |
| 1   | A     | 39  | THR  | 2              |
| 1   | A     | 71  | HIS  | 2              |
| 1   | A     | 25  | SER  | 2              |
| 1   | A     | 36  | LYS  | 2              |
| 1   | A     | 30  | LYS  | 2              |
| 1   | A     | 40  | GLU  | 2              |
| 1   | A     | 113 | ILE  | 2              |
| 1   | A     | 43  | HIS  | 2              |
| 1   | A     | 86  | ASN  | 2              |
| 1   | A     | 122 | LYS  | 2              |
| 1   | A     | 15  | GLN  | 2              |
| 1   | A     | 136 | LYS  | 2              |
| 1   | A     | 77  | GLU  | 2              |
| 1   | A     | 132 | GLU  | 2              |
| 1   | A     | 42  | LEU  | 2              |
| 1   | A     | 124 | ASP  | 2              |
| 1   | A     | 117 | LEU  | 2              |
| 1   | A     | 69  | ARG  | 2              |
| 1   | A     | 87  | VAL  | 1              |
| 1   | A     | 102 | SER  | 1              |
| 1   | A     | 118 | VAL  | 1              |
| 1   | A     | 128 | LYS  | 1              |
| 1   | A     | 119 | VAL  | 1              |
| 1   | A     | 47  | VAL  | 1              |
| 1   | A     | 100 | GLU  | 1              |
| 1   | A     | 23  | LYS  | 1              |
| 1   | A     | 120 | HIS  | 1              |
| 1   | A     | 125 | ASP  | 1              |
| 1   | A     | 67  | LEU  | 1              |
| 1   | A     | 66  | PRO  | 1              |
| 1   | A     | 142 | SER  | 1              |
| 1   | A     | 24  | GLU  | 1              |
| 1   | A     | 26  | ASN  | 1              |
| 1   | A     | 50  | PHE  | 1              |
| 1   | A     | 65  | ASN  | 1              |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 68  | SER  | 1              |
| 1   | A     | 91  | LYS  | 1              |
| 1   | A     | 45  | PHE  | 1              |
| 1   | A     | 70  | LYS  | 1              |
| 1   | A     | 137 | THR  | 1              |
| 1   | A     | 59  | SER  | 1              |
| 1   | A     | 153 | GLN  | 1              |
| 1   | A     | 35  | ILE  | 1              |
| 1   | A     | 97  | VAL  | 1              |

### 6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 6.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is 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 27% for the well-defined parts and 27% 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                  | 517 |
| Number of shifts mapped to atoms        | 517 |
| 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         |
|------------------------|----------|---------------------------------|--------------------------|
| $^{13}\text{C}_\alpha$ | 125      | $3.23 \pm 0.20$                 | Should be checked        |
| $^{13}\text{C}_\beta$  | 0        | —                               | None (insufficient data) |
| $^{13}\text{C}'$       | 120      | $3.49 \pm 0.23$                 | Should be applied        |
| $^{15}\text{N}$        | 136      | $1.07 \pm 0.58$                 | None needed (imprecise)  |

#### 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 27%, i.e. 508 atoms were assigned a chemical shift out of a possible 1863. 0 out of 22 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total         | $^1\text{H}$  | $^{13}\text{C}$ | $^{15}\text{N}$ |
|-----------|---------------|---------------|-----------------|-----------------|
| Backbone  | 508/764 (66%) | 134/319 (42%) | 240/300 (80%)   | 134/145 (92%)   |
| Sidechain | 0/983 (0%)    | 0/638 (0%)    | 0/312 (0%)      | 0/33 (0%)       |

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|          | <b>Total</b>   | <b><sup>1</sup>H</b> | <b><sup>13</sup>C</b> | <b><sup>15</sup>N</b> |
|----------|----------------|----------------------|-----------------------|-----------------------|
| Aromatic | 0/116 (0%)     | 0/58 (0%)            | 0/41 (0%)             | 0/17 (0%)             |
| Overall  | 508/1863 (27%) | 134/1015 (13%)       | 240/653 (37%)         | 134/195 (69%)         |

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 27%, i.e. 517 atoms were assigned a chemical shift out of a possible 1893. 0 out of 23 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | <b>Total</b>   | <b><sup>1</sup>H</b> | <b><sup>13</sup>C</b> | <b><sup>15</sup>N</b> |
|-----------|----------------|----------------------|-----------------------|-----------------------|
| Backbone  | 517/780 (66%)  | 136/326 (42%)        | 245/306 (80%)         | 136/148 (92%)         |
| Sidechain | 0/997 (0%)     | 0/647 (0%)           | 0/317 (0%)            | 0/33 (0%)             |
| Aromatic  | 0/116 (0%)     | 0/58 (0%)            | 0/41 (0%)             | 0/17 (0%)             |
| Overall   | 517/1893 (27%) | 136/1031 (13%)       | 245/664 (37%)         | 136/198 (69%)         |

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

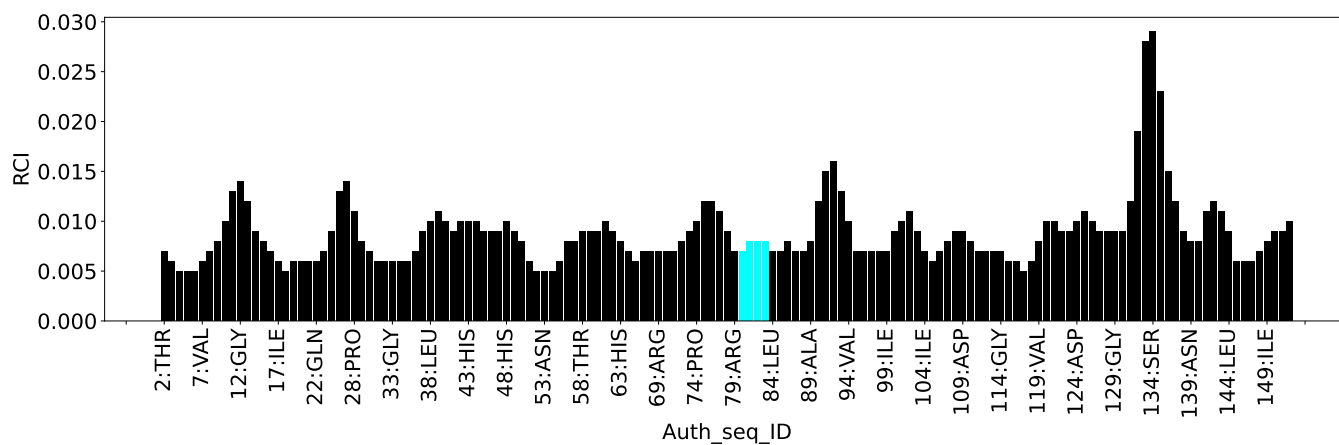
#### 7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

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

Random coil index (RCI) for chain A:



## 8 NMR restraints analysis

### 8.1 Conformationally restricting restraints

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

| Description                                              | Value |
|----------------------------------------------------------|-------|
| Total distance restraints                                | 20826 |
| Intra-residue ( $ i-j =0$ )                              | 0     |
| Sequential ( $ i-j =1$ )                                 | 1     |
| Medium range ( $ i-j >1$ and $ i-j <5$ )                 | 10922 |
| Long range ( $ i-j \geq 5$ )                             | 9524  |
| Inter-chain                                              | 0     |
| Hydrogen bond restraints                                 | 0     |
| Disulfide bond restraints                                | 1     |
| Total dihedral-angle restraints                          | 363   |
| Number of unmapped restraints                            | 0     |
| Number of restraints per residue                         | 137.6 |
| Number of long range restraints per residue <sup>1</sup> | 61.9  |

<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)  | 40.2                                   | 0.2     |
| 0.2-0.5 (Medium) | 39.5                                   | 0.5     |
| >0.5 (Large)     | 42.1                                   | 2.81    |

### 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)   | 3.6                                    | 8.78    |
| 10.0-20.0 (Medium) | 0.1                                    | 11.34   |
| >20.0 (Large)      | None                                   | None    |

## 9 Distance violation analysis

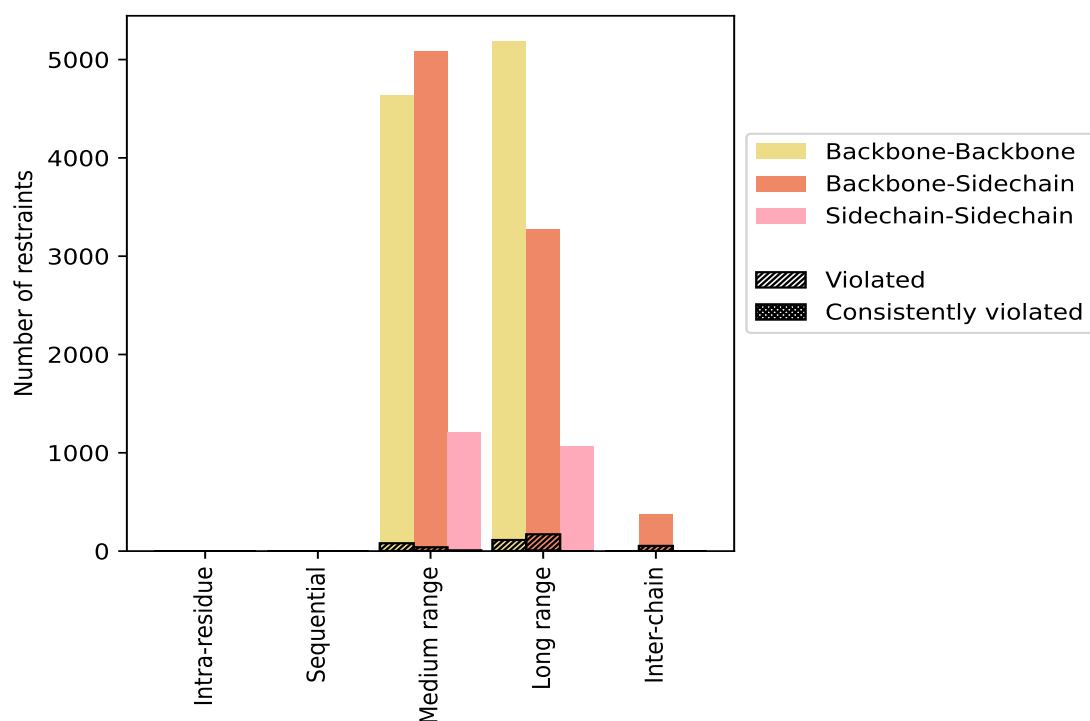
### 9.1 Summary of distance violations

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> |
| Intra-residue ( $ i-j =0$ )            | 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            |
| Sequential ( $ i-j =1$ )               | 1     | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Backbone                      | 1     | 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            |
| Medium range ( $ i-j >1$ & $ i-j <5$ ) | 10922 | 52.4           | 127                   | 1.2            | 0.6            | 2                                  | 0.0            | 0.0            |
| Backbone-Backbone                      | 4635  | 22.3           | 80                    | 1.7            | 0.4            | 1                                  | 0.0            | 0.0            |
| Backbone-Sidechain                     | 5083  | 24.4           | 39                    | 0.8            | 0.2            | 1                                  | 0.0            | 0.0            |
| Sidechain-Sidechain                    | 1204  | 5.8            | 8                     | 0.7            | 0.0            | 0                                  | 0.0            | 0.0            |
| Long range ( $ i-j \geq 5$ )           | 9524  | 45.7           | 284                   | 3.0            | 1.4            | 8                                  | 0.1            | 0.0            |
| Backbone-Backbone                      | 5186  | 24.9           | 113                   | 2.2            | 0.5            | 1                                  | 0.0            | 0.0            |
| Backbone-Sidechain                     | 3273  | 15.7           | 171                   | 5.2            | 0.8            | 7                                  | 0.2            | 0.0            |
| Sidechain-Sidechain                    | 1065  | 5.1            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Inter-chain                            | 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            |
| Hydrogen bond                          | 0     | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Disulfide bond                         | 1     | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Total                                  | 20826 | 100.0          | 464                   | 2.2            | 2.2            | 10                                 | 0.0            | 0.0            |
| Backbone-Backbone                      | 9822  | 47.2           | 193                   | 2.0            | 0.9            | 2                                  | 0.0            | 0.0            |
| Backbone-Sidechain                     | 8734  | 41.9           | 263                   | 3.0            | 1.3            | 8                                  | 0.1            | 0.0            |
| Sidechain-Sidechain                    | 2270  | 10.9           | 8                     | 0.4            | 0.0            | 0                                  | 0.0            | 0.0            |

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

### 9.1.1 Bar chart : Distribution of distance restraints and violations [i](#)



Violated and consistently violated restraints are shown using different hatch patterns in their respective categories. The hydrogen bonds and disulfied bonds are counted in their appropriate category on the x-axis

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

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

| Model ID | Number of violations |                 |                 |                 |                 |       | Mean (Å) | Max (Å) | SD <sup>6</sup> (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
|          | IR <sup>1</sup>      | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total |          |         |                     |            |
| 1        | 0                    | 0               | 18              | 88              | 11              | 117   | 0.43     | 2.02    | 0.4                 | 0.27       |
| 2        | 0                    | 0               | 20              | 96              | 11              | 127   | 0.45     | 2.81    | 0.42                | 0.31       |
| 3        | 0                    | 0               | 23              | 91              | 8               | 122   | 0.48     | 2.09    | 0.4                 | 0.32       |
| 4        | 0                    | 0               | 24              | 78              | 13              | 115   | 0.44     | 2.77    | 0.38                | 0.34       |
| 5        | 0                    | 0               | 23              | 87              | 11              | 121   | 0.48     | 2.01    | 0.38                | 0.33       |
| 6        | 0                    | 0               | 22              | 86              | 13              | 121   | 0.44     | 2.15    | 0.39                | 0.28       |
| 7        | 0                    | 0               | 17              | 92              | 11              | 120   | 0.46     | 1.99    | 0.36                | 0.32       |
| 8        | 0                    | 0               | 23              | 108             | 19              | 150   | 0.44     | 1.69    | 0.36                | 0.28       |
| 9        | 0                    | 0               | 18              | 94              | 13              | 125   | 0.46     | 1.57    | 0.37                | 0.35       |
| 10       | 0                    | 0               | 20              | 87              | 13              | 120   | 0.42     | 1.8     | 0.35                | 0.29       |

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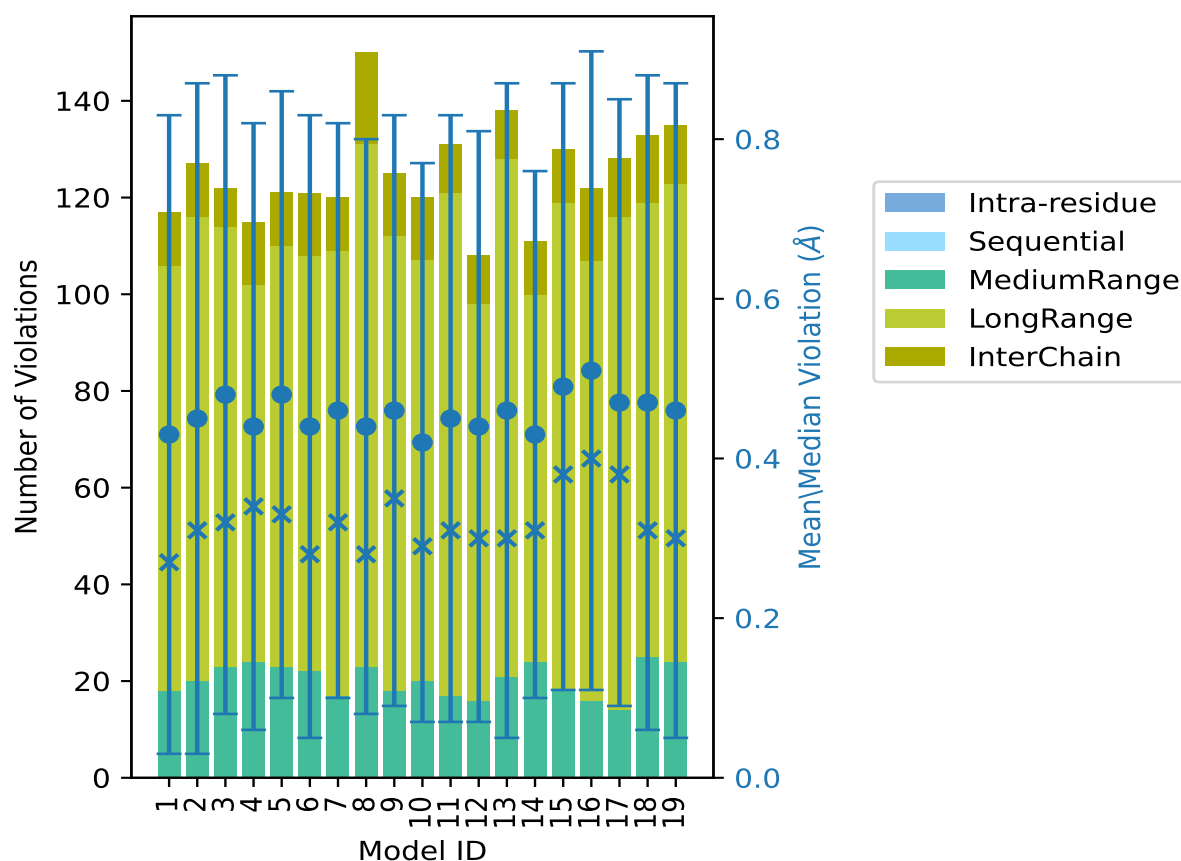
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| Model ID | Number of violations |                 |                 |                 |                 |       | Mean (Å) | Max (Å) | SD <sup>6</sup> (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
|          | IR <sup>1</sup>      | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total |          |         |                     |            |
| 11       | 0                    | 0               | 17              | 104             | 10              | 131   | 0.45     | 2.2     | 0.38                | 0.31       |
| 12       | 0                    | 0               | 16              | 82              | 10              | 108   | 0.44     | 1.9     | 0.37                | 0.3        |
| 13       | 0                    | 0               | 21              | 107             | 10              | 138   | 0.46     | 2.16    | 0.41                | 0.3        |
| 14       | 0                    | 0               | 24              | 76              | 11              | 111   | 0.43     | 1.78    | 0.33                | 0.31       |
| 15       | 0                    | 0               | 18              | 101             | 11              | 130   | 0.49     | 1.8     | 0.38                | 0.38       |
| 16       | 0                    | 0               | 16              | 91              | 15              | 122   | 0.51     | 2.13    | 0.4                 | 0.4        |
| 17       | 0                    | 0               | 14              | 102             | 12              | 128   | 0.47     | 1.81    | 0.38                | 0.38       |
| 18       | 0                    | 0               | 25              | 94              | 14              | 133   | 0.47     | 2.6     | 0.41                | 0.31       |
| 19       | 0                    | 0               | 24              | 99              | 12              | 135   | 0.46     | 2.3     | 0.41                | 0.3        |

<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

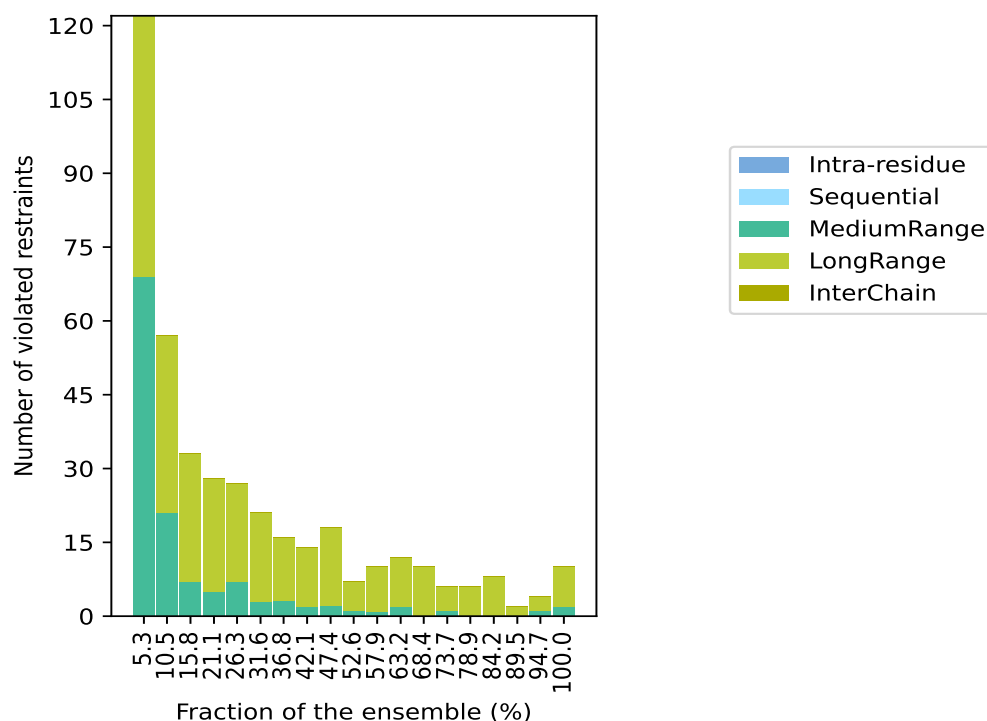
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 20036(IR:0, SQ:1, MR:10795, LR:9240, IC:0) restraints are not violated in the ensemble.

| Number of violated restraints |                 |                 |                 |                 |       | Fraction of the ensemble |       |
|-------------------------------|-----------------|-----------------|-----------------|-----------------|-------|--------------------------|-------|
| IR <sup>1</sup>               | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total | Count <sup>6</sup>       | %     |
| 0                             | 0               | 69              | 53              | 0               | 122   | 1                        | 5.3   |
| 0                             | 0               | 21              | 36              | 0               | 57    | 2                        | 10.5  |
| 0                             | 0               | 7               | 26              | 0               | 33    | 3                        | 15.8  |
| 0                             | 0               | 5               | 23              | 0               | 28    | 4                        | 21.1  |
| 0                             | 0               | 7               | 20              | 0               | 27    | 5                        | 26.3  |
| 0                             | 0               | 3               | 18              | 0               | 21    | 6                        | 31.6  |
| 0                             | 0               | 3               | 13              | 0               | 16    | 7                        | 36.8  |
| 0                             | 0               | 2               | 12              | 0               | 14    | 8                        | 42.1  |
| 0                             | 0               | 2               | 16              | 0               | 18    | 9                        | 47.4  |
| 0                             | 0               | 1               | 6               | 0               | 7     | 10                       | 52.6  |
| 0                             | 0               | 1               | 9               | 0               | 10    | 11                       | 57.9  |
| 0                             | 0               | 2               | 10              | 0               | 12    | 12                       | 63.2  |
| 0                             | 0               | 0               | 10              | 0               | 10    | 13                       | 68.4  |
| 0                             | 0               | 1               | 5               | 0               | 6     | 14                       | 73.7  |
| 0                             | 0               | 0               | 6               | 0               | 6     | 15                       | 78.9  |
| 0                             | 0               | 0               | 8               | 0               | 8     | 16                       | 84.2  |
| 0                             | 0               | 0               | 2               | 0               | 2     | 17                       | 89.5  |
| 0                             | 0               | 1               | 3               | 0               | 4     | 18                       | 94.7  |
| 0                             | 0               | 2               | 8               | 0               | 10    | 19                       | 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

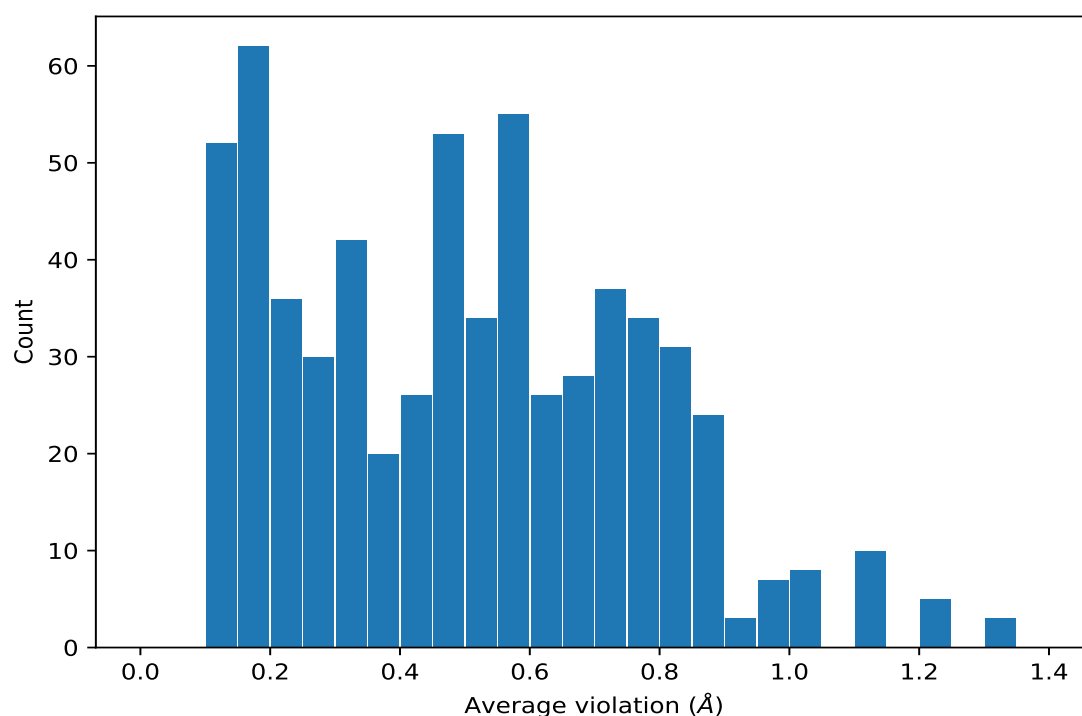
### 9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



## 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) |
|----------|---------------|---------------|---------------------|----------|---------------------|------------|
| (1,4480) | 1:56:A:GLY:O  | 1:147:A:GLY:H | 19                  | 1.31     | 0.45                | 1.32       |
| (1,4480) | 1:56:A:GLY:O  | 1:146:A:CYS:H | 19                  | 1.31     | 0.45                | 1.32       |
| (1,4480) | 1:56:A:GLY:O  | 1:116:A:THR:H | 19                  | 1.31     | 0.45                | 1.32       |
| (1,4589) | 1:112:A:ILE:H | 1:149:A:ILE:O | 19                  | 1.11     | 0.33                | 1.21       |
| (1,4589) | 1:112:A:ILE:H | 1:151:A:ILE:O | 19                  | 1.11     | 0.33                | 1.21       |
| (1,4589) | 1:105:A:SER:O | 1:112:A:ILE:H | 19                  | 1.11     | 0.33                | 1.21       |
| (1,4589) | 1:50:A:PHE:O  | 1:112:A:ILE:H | 19                  | 1.11     | 0.33                | 1.21       |
| (1,4589) | 1:104:A:ILE:O | 1:112:A:ILE:H | 19                  | 1.11     | 0.33                | 1.21       |
| (1,4589) | 1:48:A:HIS:O  | 1:112:A:ILE:H | 19                  | 1.11     | 0.33                | 1.21       |
| (1,4589) | 1:49:A:GLU:O  | 1:112:A:ILE:H | 19                  | 1.11     | 0.33                | 1.21       |
| (1,4436) | 1:41:A:GLY:O  | 1:121:A:GLU:H | 19                  | 1.03     | 0.57                | 0.84       |
| (1,4436) | 1:41:A:GLY:O  | 1:91:A:LYS:H  | 19                  | 1.03     | 0.57                | 0.84       |
| (1,4436) | 1:41:A:GLY:O  | 1:44:A:GLY:H  | 19                  | 1.03     | 0.57                | 0.84       |
| (1,4436) | 1:41:A:GLY:O  | 1:94:A:VAL:H  | 19                  | 1.03     | 0.57                | 0.84       |
| (1,4484) | 1:57:A:CYS:O  | 1:143:A:ARG:H | 19                  | 0.85     | 0.34                | 0.75       |
| (1,4629) | 1:57:A:CYS:O  | 1:143:A:ARG:H | 19                  | 0.81     | 0.31                | 0.75       |

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| Key      | Atom-1        | Atom-2        | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|---------------|---------------|---------------------|----------|---------------------|------------|
| (1,4629) | 1:119:A:VAL:O | 1:143:A:ARG:H | 19                  | 0.81     | 0.31                | 0.75       |
| (1,4428) | 1:39:A:THR:O  | 1:93:A:GLY:H  | 19                  | 0.76     | 0.29                | 0.77       |
| (1,4428) | 1:39:A:THR:O  | 1:91:A:LYS:H  | 19                  | 0.76     | 0.29                | 0.77       |
| (1,4428) | 1:39:A:THR:O  | 1:121:A:GLU:H | 19                  | 0.76     | 0.29                | 0.77       |
| (1,4428) | 1:39:A:THR:O  | 1:92:A:ASP:H  | 19                  | 0.76     | 0.29                | 0.77       |
| (1,4501) | 1:75:A:LYS:H  | 1:85:A:GLY:O  | 19                  | 0.75     | 0.36                | 0.71       |
| (1,4501) | 1:75:A:LYS:H  | 1:101:A:ASP:O | 19                  | 0.75     | 0.36                | 0.71       |
| (1,4501) | 1:75:A:LYS:H  | 1:102:A:SER:O | 19                  | 0.75     | 0.36                | 0.71       |
| (1,4501) | 1:75:A:LYS:H  | 1:84:A:LEU:O  | 19                  | 0.75     | 0.36                | 0.71       |
| (1,4501) | 1:44:A:GLY:O  | 1:75:A:LYS:H  | 19                  | 0.75     | 0.36                | 0.71       |
| (1,4501) | 1:75:A:LYS:H  | 1:100:A:GLU:O | 19                  | 0.75     | 0.36                | 0.71       |
| (1,4501) | 1:69:A:ARG:O  | 1:75:A:LYS:H  | 19                  | 0.75     | 0.36                | 0.71       |
| (1,91)   | 1:119:A:VAL:H | 1:121:A:GLU:H | 19                  | 0.73     | 0.1                 | 0.73       |
| (1,91)   | 1:15:A:GLN:H  | 1:121:A:GLU:H | 19                  | 0.73     | 0.1                 | 0.73       |
| (1,91)   | 1:12:A:GLY:H  | 1:121:A:GLU:H | 19                  | 0.73     | 0.1                 | 0.73       |
| (1,4356) | 1:10:A:GLY:O  | 1:14:A:VAL:H  | 19                  | 0.57     | 0.34                | 0.5        |
| (1,4356) | 1:10:A:GLY:O  | 1:146:A:CYS:H | 19                  | 0.57     | 0.34                | 0.5        |
| (1,28)   | 1:149:A:ILE:H | 1:151:A:ILE:H | 19                  | 0.46     | 0.13                | 0.48       |
| (1,28)   | 1:118:A:VAL:H | 1:149:A:ILE:H | 19                  | 0.46     | 0.13                | 0.48       |
| (1,4473) | 1:54:A:THR:H  | 1:114:A:GLY:O | 18                  | 1.23     | 0.36                | 1.27       |
| (1,4473) | 1:7:A:VAL:O   | 1:54:A:THR:H  | 18                  | 1.23     | 0.36                | 1.27       |
| (1,4473) | 1:54:A:THR:H  | 1:147:A:GLY:O | 18                  | 1.23     | 0.36                | 1.27       |
| (1,4473) | 1:54:A:THR:H  | 1:146:A:CYS:O | 18                  | 1.23     | 0.36                | 1.27       |
| (1,4473) | 1:54:A:THR:H  | 1:115:A:ARG:O | 18                  | 1.23     | 0.36                | 1.27       |
| (1,4388) | 1:2:A:THR:H   | 1:22:A:GLN:O  | 18                  | 0.81     | 0.34                | 0.76       |
| (1,4388) | 1:22:A:GLN:O  | 1:29:A:VAL:H  | 18                  | 0.81     | 0.34                | 0.76       |
| (1,4388) | 1:22:A:GLN:O  | 1:112:A:ILE:H | 18                  | 0.81     | 0.34                | 0.76       |
| (1,4388) | 1:22:A:GLN:O  | 1:105:A:SER:H | 18                  | 0.81     | 0.34                | 0.76       |
| (3,371)  | 1:132:A:GLU:N | 2:201:A:CU:CU | 18                  | 0.8      | 0.88                | 0.32       |
| (1,4548) | 1:86:A:ASN:H  | 1:96:A:ASP:O  | 18                  | 0.76     | 0.37                | 0.74       |
| (1,4548) | 1:33:A:GLY:H  | 1:96:A:ASP:O  | 18                  | 0.76     | 0.37                | 0.74       |
| (1,4548) | 1:35:A:ILE:H  | 1:96:A:ASP:O  | 18                  | 0.76     | 0.37                | 0.74       |
| (3,198)  | 1:143:A:ARG:C | 2:201:A:CU:CU | 18                  | 0.57     | 0.5                 | 0.37       |
| (1,176)  | 1:86:A:ASN:H  | 1:88:A:THR:H  | 18                  | 0.55     | 0.17                | 0.54       |
| (1,4620) | 1:42:A:LEU:H  | 1:120:A:HIS:O | 17                  | 0.89     | 0.51                | 0.73       |
| (1,4620) | 1:14:A:VAL:H  | 1:120:A:HIS:O | 17                  | 0.89     | 0.51                | 0.73       |
| (1,4620) | 1:45:A:PHE:H  | 1:120:A:HIS:O | 17                  | 0.89     | 0.51                | 0.73       |
| (1,4620) | 1:46:A:HIS:H  | 1:120:A:HIS:O | 17                  | 0.89     | 0.51                | 0.73       |
| (1,4620) | 1:44:A:GLY:H  | 1:120:A:HIS:O | 17                  | 0.89     | 0.51                | 0.73       |
| (1,4536) | 1:39:A:THR:H  | 1:92:A:ASP:O  | 17                  | 0.81     | 0.35                | 0.92       |
| (1,4536) | 1:36:A:LYS:H  | 1:92:A:ASP:O  | 17                  | 0.81     | 0.35                | 0.92       |
| (1,4536) | 1:40:A:GLU:H  | 1:92:A:ASP:O  | 17                  | 0.81     | 0.35                | 0.92       |

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| Key      | Atom-1        | Atom-2        | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|---------------|---------------|---------------------|----------|---------------------|------------|
| (1,4537) | 1:40:A:GLU:O  | 1:92:A:ASP:H  | 16                  | 0.75     | 0.32                | 0.7        |
| (1,4537) | 1:38:A:LEU:O  | 1:92:A:ASP:H  | 16                  | 0.75     | 0.32                | 0.7        |
| (1,4537) | 1:39:A:THR:O  | 1:92:A:ASP:H  | 16                  | 0.75     | 0.32                | 0.7        |
| (1,4576) | 1:29:A:VAL:H  | 1:103:A:VAL:O | 16                  | 0.71     | 0.35                | 0.72       |
| (1,4576) | 1:22:A:GLN:H  | 1:103:A:VAL:O | 16                  | 0.71     | 0.35                | 0.72       |
| (1,4576) | 1:84:A:LEU:H  | 1:103:A:VAL:O | 16                  | 0.71     | 0.35                | 0.72       |
| (1,4576) | 1:21:A:GLU:H  | 1:103:A:VAL:O | 16                  | 0.71     | 0.35                | 0.72       |
| (1,4576) | 1:78:A:GLU:H  | 1:103:A:VAL:O | 16                  | 0.71     | 0.35                | 0.72       |
| (1,4621) | 1:44:A:GLY:O  | 1:120:A:HIS:H | 16                  | 0.7      | 0.34                | 0.66       |
| (1,4621) | 1:120:A:HIS:H | 1:145:A:ALA:O | 16                  | 0.7      | 0.34                | 0.66       |
| (1,4621) | 1:45:A:PHE:O  | 1:120:A:HIS:H | 16                  | 0.7      | 0.34                | 0.66       |
| (1,4621) | 1:42:A:LEU:O  | 1:120:A:HIS:H | 16                  | 0.7      | 0.34                | 0.66       |
| (1,4621) | 1:46:A:HIS:O  | 1:120:A:HIS:H | 16                  | 0.7      | 0.34                | 0.66       |
| (1,4584) | 1:22:A:GLN:H  | 1:105:A:SER:O | 16                  | 0.67     | 0.36                | 0.72       |
| (1,4584) | 1:78:A:GLU:H  | 1:105:A:SER:O | 16                  | 0.67     | 0.36                | 0.72       |
| (1,4584) | 1:105:A:SER:O | 1:112:A:ILE:H | 16                  | 0.67     | 0.36                | 0.72       |
| (1,4584) | 1:77:A:GLU:H  | 1:105:A:SER:O | 16                  | 0.67     | 0.36                | 0.72       |
| (1,4584) | 1:79:A:ARG:H  | 1:105:A:SER:O | 16                  | 0.67     | 0.36                | 0.72       |
| (1,4584) | 1:84:A:LEU:H  | 1:105:A:SER:O | 16                  | 0.67     | 0.36                | 0.72       |
| (1,4625) | 1:41:A:GLY:O  | 1:121:A:GLU:H | 16                  | 0.58     | 0.32                | 0.56       |
| (1,4625) | 1:38:A:LEU:O  | 1:121:A:GLU:H | 16                  | 0.58     | 0.32                | 0.56       |
| (1,4625) | 1:40:A:GLU:O  | 1:121:A:GLU:H | 16                  | 0.58     | 0.32                | 0.56       |
| (1,4625) | 1:121:A:GLU:H | 1:144:A:LEU:O | 16                  | 0.58     | 0.32                | 0.56       |
| (1,88)   | 1:15:A:GLN:H  | 1:35:A:ILE:H  | 16                  | 0.39     | 0.15                | 0.32       |
| (1,181)  | 1:18:A:ILE:H  | 1:150:A:GLY:H | 16                  | 0.27     | 0.07                | 0.26       |
| (3,213)  | 1:10:A:GLY:C  | 2:201:A:CU:CU | 16                  | 0.18     | 0.05                | 0.18       |
| (1,201)  | 1:16:A:GLY:H  | 1:34:A:SER:H  | 16                  | 0.16     | 0.04                | 0.16       |
| (1,4592) | 1:113:A:ILE:O | 1:149:A:ILE:H | 15                  | 1.01     | 0.24                | 1.12       |
| (1,4592) | 1:50:A:PHE:H  | 1:113:A:ILE:O | 15                  | 1.01     | 0.24                | 1.12       |
| (1,4592) | 1:113:A:ILE:O | 1:151:A:ILE:H | 15                  | 1.01     | 0.24                | 1.12       |
| (1,4592) | 1:49:A:GLU:H  | 1:113:A:ILE:O | 15                  | 1.01     | 0.24                | 1.12       |
| (1,4489) | 1:67:A:LEU:H  | 1:79:A:ARG:O  | 15                  | 0.82     | 0.55                | 0.62       |
| (1,4489) | 1:67:A:LEU:H  | 1:105:A:SER:O | 15                  | 0.82     | 0.55                | 0.62       |
| (1,4489) | 1:67:A:LEU:H  | 1:78:A:GLU:O  | 15                  | 0.82     | 0.55                | 0.62       |
| (1,4489) | 1:49:A:GLU:O  | 1:67:A:LEU:H  | 15                  | 0.82     | 0.55                | 0.62       |
| (1,4580) | 1:79:A:ARG:H  | 1:104:A:ILE:O | 15                  | 0.76     | 0.64                | 0.69       |
| (1,4580) | 1:22:A:GLN:H  | 1:104:A:ILE:O | 15                  | 0.76     | 0.64                | 0.69       |
| (1,4580) | 1:69:A:ARG:H  | 1:104:A:ILE:O | 15                  | 0.76     | 0.64                | 0.69       |
| (1,4580) | 1:76:A:ASP:H  | 1:104:A:ILE:O | 15                  | 0.76     | 0.64                | 0.69       |
| (1,4580) | 1:78:A:GLU:H  | 1:104:A:ILE:O | 15                  | 0.76     | 0.64                | 0.69       |
| (1,4580) | 1:77:A:GLU:H  | 1:104:A:ILE:O | 15                  | 0.76     | 0.64                | 0.69       |
| (1,4508) | 1:77:A:GLU:O  | 1:103:A:VAL:H | 15                  | 0.68     | 0.51                | 0.46       |

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| Key      | Atom-1        | Atom-2        | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|---------------|---------------|---------------------|----------|---------------------|------------|
| (1,4508) | 1:77:A:GLU:O  | 1:104:A:ILE:H | 15                  | 0.68     | 0.51                | 0.46       |
| (1,4508) | 1:69:A:ARG:H  | 1:77:A:GLU:O  | 15                  | 0.68     | 0.51                | 0.46       |
| (1,4508) | 1:77:A:GLU:O  | 1:102:A:SER:H | 15                  | 0.68     | 0.51                | 0.46       |
| (1,4508) | 1:77:A:GLU:O  | 1:84:A:LEU:H  | 15                  | 0.68     | 0.51                | 0.46       |
| (1,4479) | 1:56:A:GLY:O  | 1:143:A:ARG:N | 15                  | 0.49     | 0.15                | 0.45       |
| (1,4479) | 1:56:A:GLY:O  | 1:147:A:GLY:N | 15                  | 0.49     | 0.15                | 0.45       |
| (1,4479) | 1:56:A:GLY:O  | 1:116:A:THR:N | 15                  | 0.49     | 0.15                | 0.45       |
| (1,4479) | 1:56:A:GLY:O  | 1:146:A:CYS:N | 15                  | 0.49     | 0.15                | 0.45       |
| (1,26)   | 1:51:A:GLY:H  | 1:149:A:ILE:H | 15                  | 0.47     | 0.28                | 0.47       |
| (1,26)   | 1:48:A:HIS:H  | 1:149:A:ILE:H | 15                  | 0.47     | 0.28                | 0.47       |
| (1,4509) | 1:68:A:SER:O  | 1:77:A:GLU:H  | 14                  | 0.8      | 0.38                | 0.84       |
| (1,4509) | 1:77:A:GLU:H  | 1:102:A:SER:O | 14                  | 0.8      | 0.38                | 0.84       |
| (1,4509) | 1:77:A:GLU:H  | 1:101:A:ASP:O | 14                  | 0.8      | 0.38                | 0.84       |
| (1,4509) | 1:67:A:LEU:O  | 1:77:A:GLU:H  | 14                  | 0.8      | 0.38                | 0.84       |
| (1,4509) | 1:77:A:GLU:H  | 1:104:A:ILE:O | 14                  | 0.8      | 0.38                | 0.84       |
| (1,4509) | 1:69:A:ARG:O  | 1:77:A:GLU:H  | 14                  | 0.8      | 0.38                | 0.84       |
| (1,4496) | 1:69:A:ARG:O  | 1:77:A:GLU:H  | 14                  | 0.71     | 0.42                | 0.64       |
| (1,4496) | 1:69:A:ARG:O  | 1:79:A:ARG:H  | 14                  | 0.71     | 0.42                | 0.64       |
| (1,4496) | 1:69:A:ARG:O  | 1:78:A:GLU:H  | 14                  | 0.71     | 0.42                | 0.64       |
| (1,4496) | 1:69:A:ARG:O  | 1:75:A:LYS:H  | 14                  | 0.71     | 0.42                | 0.64       |
| (1,12)   | 1:53:A:ASN:H  | 1:117:A:LEU:H | 14                  | 0.58     | 0.23                | 0.63       |
| (1,12)   | 1:117:A:LEU:H | 1:150:A:GLY:H | 14                  | 0.58     | 0.23                | 0.63       |
| (1,12)   | 1:47:A:VAL:H  | 1:117:A:LEU:H | 14                  | 0.58     | 0.23                | 0.63       |
| (1,4591) | 1:113:A:ILE:O | 1:150:A:GLY:N | 14                  | 0.47     | 0.18                | 0.4        |
| (1,4591) | 1:50:A:PHE:N  | 1:113:A:ILE:O | 14                  | 0.47     | 0.18                | 0.4        |
| (1,4591) | 1:113:A:ILE:O | 1:151:A:ILE:N | 14                  | 0.47     | 0.18                | 0.4        |
| (1,120)  | 1:3:A:LYS:H   | 1:151:A:ILE:H | 14                  | 0.45     | 0.2                 | 0.48       |
| (1,120)  | 1:149:A:ILE:H | 1:151:A:ILE:H | 14                  | 0.45     | 0.2                 | 0.48       |
| (1,4404) | 1:18:A:ILE:H  | 1:32:A:TRP:O  | 14                  | 0.27     | 0.13                | 0.22       |
| (1,4633) | 1:119:A:VAL:O | 1:144:A:LEU:H | 13                  | 0.97     | 0.62                | 0.71       |
| (1,4633) | 1:55:A:ALA:O  | 1:144:A:LEU:H | 13                  | 0.97     | 0.62                | 0.71       |
| (1,4633) | 1:9:A:LYS:O   | 1:144:A:LEU:H | 13                  | 0.97     | 0.62                | 0.71       |
| (1,4464) | 1:49:A:GLU:O  | 1:116:A:THR:H | 13                  | 0.77     | 0.5                 | 0.59       |
| (1,4464) | 1:49:A:GLU:O  | 1:67:A:LEU:H  | 13                  | 0.77     | 0.5                 | 0.59       |
| (1,4504) | 1:76:A:ASP:O  | 1:103:A:VAL:H | 13                  | 0.67     | 0.34                | 0.64       |
| (1,4504) | 1:76:A:ASP:O  | 1:105:A:SER:H | 13                  | 0.67     | 0.34                | 0.64       |
| (1,4504) | 1:69:A:ARG:H  | 1:76:A:ASP:O  | 13                  | 0.67     | 0.34                | 0.64       |
| (1,4504) | 1:76:A:ASP:O  | 1:104:A:ILE:H | 13                  | 0.67     | 0.34                | 0.64       |
| (1,4504) | 1:76:A:ASP:O  | 1:101:A:ASP:H | 13                  | 0.67     | 0.34                | 0.64       |
| (1,4504) | 1:76:A:ASP:O  | 1:102:A:SER:H | 13                  | 0.67     | 0.34                | 0.64       |
| (1,4325) | 1:2:A:THR:H   | 1:22:A:GLN:O  | 13                  | 0.62     | 0.27                | 0.59       |
| (1,4325) | 1:2:A:THR:H   | 1:20:A:PHE:O  | 13                  | 0.62     | 0.27                | 0.59       |

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| Key      | Atom-1        | Atom-2        | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|---------------|---------------|---------------------|----------|---------------------|------------|
| (1,4325) | 1:2:A:THR:H   | 1:152:A:ALA:O | 13                  | 0.62     | 0.27                | 0.59       |
| (1,169)  | 1:49:A:GLU:H  | 1:111:A:SER:H | 13                  | 0.6      | 0.32                | 0.55       |
| (1,169)  | 1:49:A:GLU:H  | 1:83:A:ASP:H  | 13                  | 0.6      | 0.32                | 0.55       |
| (1,4547) | 1:86:A:ASN:N  | 1:96:A:ASP:O  | 13                  | 0.57     | 0.36                | 0.49       |
| (1,4547) | 1:33:A:GLY:N  | 1:96:A:ASP:O  | 13                  | 0.57     | 0.36                | 0.49       |
| (3,274)  | 1:120:A:HIS:C | 2:201:A:CU:CU | 13                  | 0.32     | 0.2                 | 0.25       |
| (1,131)  | 1:50:A:PHE:H  | 1:60:A:ALA:H  | 13                  | 0.24     | 0.1                 | 0.23       |
| (1,217)  | 1:87:A:VAL:H  | 1:122:A:LYS:H | 13                  | 0.24     | 0.1                 | 0.19       |
| (1,123)  | 1:22:A:GLN:H  | 1:106:A:LEU:H | 13                  | 0.2      | 0.07                | 0.17       |
| (3,295)  | 1:9:A:LYS:N   | 2:201:A:CU:CU | 13                  | 0.18     | 0.06                | 0.16       |
| (3,310)  | 1:31:A:VAL:N  | 2:201:A:CU:CU | 13                  | 0.17     | 0.05                | 0.17       |
| (1,42)   | 1:19:A:ASN:H  | 1:31:A:VAL:H  | 13                  | 0.15     | 0.03                | 0.15       |
| (1,4505) | 1:76:A:ASP:H  | 1:101:A:ASP:O | 12                  | 0.83     | 0.36                | 0.81       |
| (1,4505) | 1:76:A:ASP:H  | 1:102:A:SER:O | 12                  | 0.83     | 0.36                | 0.81       |
| (1,4505) | 1:76:A:ASP:H  | 1:84:A:LEU:O  | 12                  | 0.83     | 0.36                | 0.81       |
| (1,4505) | 1:76:A:ASP:H  | 1:104:A:ILE:O | 12                  | 0.83     | 0.36                | 0.81       |
| (1,4505) | 1:76:A:ASP:H  | 1:100:A:GLU:O | 12                  | 0.83     | 0.36                | 0.81       |
| (1,4529) | 1:44:A:GLY:O  | 1:86:A:ASN:H  | 12                  | 0.78     | 0.38                | 0.82       |
| (1,4529) | 1:86:A:ASN:H  | 1:96:A:ASP:O  | 12                  | 0.78     | 0.38                | 0.82       |
| (1,4529) | 1:86:A:ASN:H  | 1:98:A:SER:O  | 12                  | 0.78     | 0.38                | 0.82       |
| (1,4529) | 1:86:A:ASN:H  | 1:99:A:ILE:O  | 12                  | 0.78     | 0.38                | 0.82       |
| (1,4529) | 1:86:A:ASN:H  | 1:97:A:VAL:O  | 12                  | 0.78     | 0.38                | 0.82       |
| (1,4577) | 1:21:A:GLU:O  | 1:103:A:VAL:H | 12                  | 0.74     | 0.44                | 0.66       |
| (1,4577) | 1:76:A:ASP:O  | 1:103:A:VAL:H | 12                  | 0.74     | 0.44                | 0.66       |
| (1,4577) | 1:75:A:LYS:O  | 1:103:A:VAL:H | 12                  | 0.74     | 0.44                | 0.66       |
| (1,4577) | 1:77:A:GLU:O  | 1:103:A:VAL:H | 12                  | 0.74     | 0.44                | 0.66       |
| (1,4577) | 1:84:A:LEU:O  | 1:103:A:VAL:H | 12                  | 0.74     | 0.44                | 0.66       |
| (1,4533) | 1:40:A:GLU:O  | 1:91:A:LYS:H  | 12                  | 0.62     | 0.37                | 0.73       |
| (1,4533) | 1:38:A:LEU:O  | 1:91:A:LYS:H  | 12                  | 0.62     | 0.37                | 0.73       |
| (1,4533) | 1:41:A:GLY:O  | 1:91:A:LYS:H  | 12                  | 0.62     | 0.37                | 0.73       |
| (1,4405) | 1:17:A:ILE:O  | 1:32:A:TRP:H  | 12                  | 0.57     | 0.21                | 0.55       |
| (1,4405) | 1:18:A:ILE:O  | 1:32:A:TRP:H  | 12                  | 0.57     | 0.21                | 0.55       |
| (1,4405) | 1:32:A:TRP:H  | 1:97:A:VAL:O  | 12                  | 0.57     | 0.21                | 0.55       |
| (1,4405) | 1:32:A:TRP:H  | 1:98:A:SER:O  | 12                  | 0.57     | 0.21                | 0.55       |
| (1,4465) | 1:49:A:GLU:H  | 1:116:A:THR:O | 12                  | 0.55     | 0.3                 | 0.44       |
| (1,4465) | 1:49:A:GLU:H  | 1:67:A:LEU:O  | 12                  | 0.55     | 0.3                 | 0.44       |
| (1,4512) | 1:69:A:ARG:H  | 1:78:A:GLU:O  | 12                  | 0.54     | 0.28                | 0.5        |
| (1,4512) | 1:78:A:GLU:O  | 1:105:A:SER:H | 12                  | 0.54     | 0.28                | 0.5        |
| (1,4512) | 1:68:A:SER:H  | 1:78:A:GLU:O  | 12                  | 0.54     | 0.28                | 0.5        |
| (1,4512) | 1:67:A:LEU:H  | 1:78:A:GLU:O  | 12                  | 0.54     | 0.28                | 0.5        |
| (1,35)   | 1:43:A:HIS:H  | 1:45:A:PHE:H  | 12                  | 0.34     | 0.15                | 0.31       |
| (1,276)  | 1:47:A:VAL:H  | 1:85:A:GLY:H  | 12                  | 0.34     | 0.15                | 0.33       |

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| Key      | Atom-1        | Atom-2        | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|---------------|---------------|---------------------|----------|---------------------|------------|
| (1,276)  | 1:85:A:GLY:H  | 1:99:A:ILE:H  | 12                  | 0.34     | 0.15                | 0.33       |
| (1,4389) | 1:2:A:THR:O   | 1:22:A:GLN:H  | 12                  | 0.31     | 0.23                | 0.22       |
| (1,4389) | 1:22:A:GLN:H  | 1:103:A:VAL:O | 12                  | 0.31     | 0.23                | 0.22       |
| (1,4389) | 1:22:A:GLN:H  | 1:104:A:ILE:O | 12                  | 0.31     | 0.23                | 0.22       |
| (1,4389) | 1:22:A:GLN:H  | 1:105:A:SER:O | 12                  | 0.31     | 0.23                | 0.22       |
| (3,84)   | 1:150:A:GLY:C | 2:201:A:CU:CU | 12                  | 0.3      | 0.37                | 0.21       |
| (3,319)  | 1:41:A:GLY:N  | 2:201:A:CU:CU | 12                  | 0.21     | 0.06                | 0.18       |
| (2,156)  | 1:106:A:LEU:N | 1:108:A:GLY:N | 12                  | 0.19     | 0.07                | 0.17       |
| (1,43)   | 1:8:A:LEU:H   | 1:18:A:ILE:H  | 12                  | 0.18     | 0.04                | 0.16       |
| (1,4556) | 1:86:A:ASN:H  | 1:98:A:SER:O  | 11                  | 0.85     | 0.28                | 0.94       |
| (1,4556) | 1:31:A:VAL:H  | 1:98:A:SER:O  | 11                  | 0.85     | 0.28                | 0.94       |
| (1,4585) | 1:76:A:ASP:O  | 1:105:A:SER:H | 11                  | 0.85     | 0.49                | 0.83       |
| (1,4585) | 1:77:A:GLU:O  | 1:105:A:SER:H | 11                  | 0.85     | 0.49                | 0.83       |
| (1,4585) | 1:21:A:GLU:O  | 1:105:A:SER:H | 11                  | 0.85     | 0.49                | 0.83       |
| (1,4585) | 1:79:A:ARG:O  | 1:105:A:SER:H | 11                  | 0.85     | 0.49                | 0.83       |
| (1,4477) | 1:55:A:ALA:H  | 1:146:A:CYS:O | 11                  | 0.72     | 0.27                | 0.62       |
| (1,4477) | 1:9:A:LYS:O   | 1:55:A:ALA:H  | 11                  | 0.72     | 0.27                | 0.62       |
| (1,4593) | 1:113:A:ILE:H | 1:151:A:ILE:O | 11                  | 0.58     | 0.3                 | 0.51       |
| (1,4593) | 1:113:A:ILE:H | 1:149:A:ILE:O | 11                  | 0.58     | 0.3                 | 0.51       |
| (1,4593) | 1:50:A:PHE:O  | 1:113:A:ILE:H | 11                  | 0.58     | 0.3                 | 0.51       |
| (1,4593) | 1:49:A:GLU:O  | 1:113:A:ILE:H | 11                  | 0.58     | 0.3                 | 0.51       |
| (1,98)   | 1:120:A:HIS:H | 1:123:A:ALA:H | 11                  | 0.55     | 0.19                | 0.61       |
| (1,98)   | 1:44:A:GLY:H  | 1:123:A:ALA:H | 11                  | 0.55     | 0.19                | 0.61       |
| (1,4432) | 1:40:A:GLU:O  | 1:121:A:GLU:H | 11                  | 0.51     | 0.38                | 0.31       |
| (1,4432) | 1:40:A:GLU:O  | 1:91:A:LYS:H  | 11                  | 0.51     | 0.38                | 0.31       |
| (1,50)   | 1:120:A:HIS:H | 1:145:A:ALA:H | 11                  | 0.51     | 0.15                | 0.53       |
| (1,50)   | 1:118:A:VAL:H | 1:145:A:ALA:H | 11                  | 0.51     | 0.15                | 0.53       |
| (1,4632) | 1:121:A:GLU:H | 1:144:A:LEU:O | 11                  | 0.47     | 0.24                | 0.37       |
| (1,4632) | 1:9:A:LYS:H   | 1:144:A:LEU:O | 11                  | 0.47     | 0.24                | 0.37       |
| (1,4632) | 1:119:A:VAL:H | 1:144:A:LEU:O | 11                  | 0.47     | 0.24                | 0.37       |
| (1,4632) | 1:10:A:GLY:H  | 1:144:A:LEU:O | 11                  | 0.47     | 0.24                | 0.37       |
| (1,4632) | 1:14:A:VAL:H  | 1:144:A:LEU:O | 11                  | 0.47     | 0.24                | 0.37       |
| (1,85)   | 1:8:A:LEU:H   | 1:15:A:GLN:H  | 11                  | 0.42     | 0.14                | 0.45       |
| (1,4355) | 1:10:A:GLY:O  | 1:14:A:VAL:N  | 11                  | 0.32     | 0.2                 | 0.29       |
| (1,4355) | 1:10:A:GLY:O  | 1:145:A:ALA:N | 11                  | 0.32     | 0.2                 | 0.29       |
| (1,4355) | 1:10:A:GLY:O  | 1:146:A:CYS:N | 11                  | 0.32     | 0.2                 | 0.29       |
| (1,4628) | 1:57:A:CYS:H  | 1:143:A:ARG:O | 10                  | 0.85     | 0.38                | 0.8        |
| (1,4628) | 1:10:A:GLY:H  | 1:143:A:ARG:O | 10                  | 0.85     | 0.38                | 0.8        |
| (1,4513) | 1:78:A:GLU:H  | 1:105:A:SER:O | 10                  | 0.65     | 0.31                | 0.7        |
| (1,4513) | 1:68:A:SER:O  | 1:78:A:GLU:H  | 10                  | 0.65     | 0.31                | 0.7        |
| (1,4513) | 1:78:A:GLU:H  | 1:102:A:SER:O | 10                  | 0.65     | 0.31                | 0.7        |
| (1,4513) | 1:78:A:GLU:H  | 1:103:A:VAL:O | 10                  | 0.65     | 0.31                | 0.7        |

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| Key      | Atom-1       | Atom-2        | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|--------------|---------------|---------------------|----------|---------------------|------------|
| (1,4513) | 1:67:A:LEU:O | 1:78:A:GLU:H  | 10                  | 0.65     | 0.31                | 0.7        |
| (1,4435) | 1:41:A:GLY:O | 1:91:A:LYS:N  | 10                  | 0.57     | 0.44                | 0.46       |
| (1,4435) | 1:41:A:GLY:O | 1:44:A:GLY:N  | 10                  | 0.57     | 0.44                | 0.46       |
| (1,4435) | 1:41:A:GLY:O | 1:121:A:GLU:N | 10                  | 0.57     | 0.44                | 0.46       |
| (1,4481) | 1:56:A:GLY:H | 1:146:A:CYS:O | 10                  | 0.53     | 0.3                 | 0.52       |
| (1,4463) | 1:49:A:GLU:O | 1:116:A:THR:N | 10                  | 0.48     | 0.2                 | 0.42       |
| (1,4463) | 1:49:A:GLU:O | 1:114:A:GLY:N | 10                  | 0.48     | 0.2                 | 0.42       |
| (1,4463) | 1:49:A:GLU:O | 1:68:A:SER:N  | 10                  | 0.48     | 0.2                 | 0.42       |
| (1,4463) | 1:49:A:GLU:O | 1:67:A:LEU:N  | 10                  | 0.48     | 0.2                 | 0.42       |
| (1,63)   | 1:88:A:THR:H | 1:90:A:ASP:H  | 10                  | 0.45     | 0.25                | 0.4        |
| (1,63)   | 1:41:A:GLY:H | 1:90:A:ASP:H  | 10                  | 0.45     | 0.25                | 0.4        |
| (1,4660) | 1:5:A:VAL:H  | 1:151:A:ILE:O | 10                  | 0.26     | 0.15                | 0.24       |
| (1,4469) | 1:50:A:PHE:H | 1:116:A:THR:O | 9                   | 0.97     | 0.32                | 1.0        |
| (1,4469) | 1:50:A:PHE:H | 1:114:A:GLY:O | 9                   | 0.97     | 0.32                | 1.0        |
| (1,4469) | 1:50:A:PHE:H | 1:113:A:ILE:O | 9                   | 0.97     | 0.32                | 1.0        |
| (1,4469) | 1:50:A:PHE:H | 1:112:A:ILE:O | 9                   | 0.97     | 0.32                | 1.0        |
| (1,4521) | 1:84:A:LEU:H | 1:105:A:SER:O | 9                   | 0.87     | 0.45                | 0.9        |
| (1,4521) | 1:46:A:HIS:O | 1:84:A:LEU:H  | 9                   | 0.87     | 0.45                | 0.9        |
| (1,4521) | 1:84:A:LEU:H | 1:103:A:VAL:O | 9                   | 0.87     | 0.45                | 0.9        |
| (1,4521) | 1:45:A:PHE:O | 1:84:A:LEU:H  | 9                   | 0.87     | 0.45                | 0.9        |
| (1,4521) | 1:84:A:LEU:H | 1:101:A:ASP:O | 9                   | 0.87     | 0.45                | 0.9        |
| (1,4521) | 1:84:A:LEU:H | 1:149:A:ILE:O | 9                   | 0.87     | 0.45                | 0.9        |
| (1,4521) | 1:84:A:LEU:H | 1:98:A:SER:O  | 9                   | 0.87     | 0.45                | 0.9        |
| (1,4555) | 1:31:A:VAL:N | 1:98:A:SER:O  | 9                   | 0.75     | 0.23                | 0.74       |
| (1,4555) | 1:86:A:ASN:N | 1:98:A:SER:O  | 9                   | 0.75     | 0.23                | 0.74       |
| (1,4560) | 1:31:A:VAL:H | 1:99:A:ILE:O  | 9                   | 0.72     | 0.28                | 0.7        |
| (1,4560) | 1:85:A:GLY:H | 1:99:A:ILE:O  | 9                   | 0.72     | 0.28                | 0.7        |
| (1,4560) | 1:86:A:ASN:H | 1:99:A:ILE:O  | 9                   | 0.72     | 0.28                | 0.7        |
| (1,4492) | 1:68:A:SER:O | 1:78:A:GLU:H  | 9                   | 0.63     | 0.22                | 0.55       |
| (1,4492) | 1:68:A:SER:O | 1:79:A:ARG:H  | 9                   | 0.63     | 0.22                | 0.55       |
| (1,4401) | 1:31:A:VAL:H | 1:100:A:GLU:O | 9                   | 0.63     | 0.29                | 0.47       |
| (1,4401) | 1:31:A:VAL:H | 1:97:A:VAL:O  | 9                   | 0.63     | 0.29                | 0.47       |
| (1,4401) | 1:31:A:VAL:H | 1:99:A:ILE:O  | 9                   | 0.63     | 0.29                | 0.47       |
| (1,4401) | 1:31:A:VAL:H | 1:98:A:SER:O  | 9                   | 0.63     | 0.29                | 0.47       |
| (1,4401) | 1:21:A:GLU:O | 1:31:A:VAL:H  | 9                   | 0.63     | 0.29                | 0.47       |
| (1,4581) | 1:76:A:ASP:O | 1:104:A:ILE:H | 9                   | 0.61     | 0.29                | 0.67       |
| (1,4581) | 1:75:A:LYS:O | 1:104:A:ILE:H | 9                   | 0.61     | 0.29                | 0.67       |
| (1,4581) | 1:77:A:GLU:O | 1:104:A:ILE:H | 9                   | 0.61     | 0.29                | 0.67       |
| (1,4581) | 1:21:A:GLU:O | 1:104:A:ILE:H | 9                   | 0.61     | 0.29                | 0.67       |
| (1,4532) | 1:39:A:THR:H | 1:91:A:LYS:O  | 9                   | 0.57     | 0.17                | 0.57       |
| (1,4532) | 1:40:A:GLU:H | 1:91:A:LYS:O  | 9                   | 0.57     | 0.17                | 0.57       |
| (1,4485) | 1:57:A:CYS:H | 1:117:A:LEU:O | 9                   | 0.56     | 0.19                | 0.57       |

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| Key      | Atom-1       | Atom-2        | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|--------------|---------------|---------------------|----------|---------------------|------------|
| (1,4485) | 1:57:A:CYS:H | 1:145:A:ALA:O | 9                   | 0.56     | 0.19                | 0.57       |
| (1,4485) | 1:57:A:CYS:H | 1:143:A:ARG:O | 9                   | 0.56     | 0.19                | 0.57       |
| (1,4485) | 1:57:A:CYS:H | 1:146:A:CYS:O | 9                   | 0.56     | 0.19                | 0.57       |
| (1,4441) | 1:42:A:LEU:H | 1:121:A:GLU:O | 9                   | 0.56     | 0.47                | 0.42       |
| (1,4441) | 1:42:A:LEU:H | 1:120:A:HIS:O | 9                   | 0.56     | 0.47                | 0.42       |
| (1,107)  | 1:46:A:HIS:H | 1:119:A:VAL:H | 9                   | 0.47     | 0.37                | 0.3        |
| (1,107)  | 1:45:A:PHE:H | 1:119:A:VAL:H | 9                   | 0.47     | 0.37                | 0.3        |
| (1,16)   | 1:48:A:HIS:H | 1:50:A:PHE:H  | 9                   | 0.4      | 0.16                | 0.47       |
| (1,16)   | 1:48:A:HIS:H | 1:149:A:ILE:H | 9                   | 0.4      | 0.16                | 0.47       |
| (1,4417) | 1:15:A:GLN:O | 1:35:A:ILE:H  | 9                   | 0.24     | 0.08                | 0.25       |
| (1,292)  | 1:37:A:GLY:H | 1:39:A:THR:H  | 9                   | 0.23     | 0.1                 | 0.18       |
| (3,236)  | 1:49:A:GLU:C | 2:201:A:CU:CU | 9                   | 0.21     | 0.04                | 0.21       |
| (1,143)  | 1:36:A:LYS:H | 1:94:A:VAL:H  | 9                   | 0.17     | 0.04                | 0.17       |
| (3,1)    | 1:2:A:THR:C  | 2:201:A:CU:CU | 9                   | 0.17     | 0.03                | 0.17       |
| (1,159)  | 1:49:A:GLU:H | 1:118:A:VAL:H | 9                   | 0.15     | 0.04                | 0.17       |
| (1,95)   | 1:9:A:LYS:H  | 1:145:A:ALA:H | 9                   | 0.14     | 0.03                | 0.14       |
| (1,115)  | 1:20:A:PHE:H | 1:151:A:ILE:H | 9                   | 0.14     | 0.02                | 0.13       |
| (1,4559) | 1:31:A:VAL:N | 1:99:A:ILE:O  | 8                   | 0.64     | 0.28                | 0.63       |
| (1,4559) | 1:85:A:GLY:N | 1:99:A:ILE:O  | 8                   | 0.64     | 0.28                | 0.63       |
| (1,4559) | 1:86:A:ASN:N | 1:99:A:ILE:O  | 8                   | 0.64     | 0.28                | 0.63       |
| (1,4619) | 1:42:A:LEU:N | 1:120:A:HIS:O | 8                   | 0.55     | 0.25                | 0.6        |
| (1,4619) | 1:46:A:HIS:N | 1:120:A:HIS:O | 8                   | 0.55     | 0.25                | 0.6        |
| (1,4619) | 1:44:A:GLY:N | 1:120:A:HIS:O | 8                   | 0.55     | 0.25                | 0.6        |
| (1,4433) | 1:40:A:GLU:H | 1:121:A:GLU:O | 8                   | 0.52     | 0.24                | 0.5        |
| (1,4433) | 1:40:A:GLU:H | 1:91:A:LYS:O  | 8                   | 0.52     | 0.24                | 0.5        |
| (1,4444) | 1:44:A:GLY:O | 1:120:A:HIS:H | 8                   | 0.45     | 0.21                | 0.42       |
| (1,4444) | 1:44:A:GLY:O | 1:86:A:ASN:H  | 8                   | 0.45     | 0.21                | 0.42       |
| (1,4444) | 1:44:A:GLY:O | 1:85:A:GLY:H  | 8                   | 0.45     | 0.21                | 0.42       |
| (1,4565) | 1:29:A:VAL:O | 1:100:A:GLU:H | 8                   | 0.45     | 0.39                | 0.3        |
| (1,4565) | 1:84:A:LEU:O | 1:100:A:GLU:H | 8                   | 0.45     | 0.39                | 0.3        |
| (1,4324) | 1:2:A:THR:O  | 1:21:A:GLU:H  | 8                   | 0.43     | 0.25                | 0.33       |
| (1,4495) | 1:69:A:ARG:O | 1:78:A:GLU:N  | 8                   | 0.41     | 0.28                | 0.29       |
| (1,4495) | 1:69:A:ARG:O | 1:79:A:ARG:N  | 8                   | 0.41     | 0.28                | 0.29       |
| (1,4495) | 1:69:A:ARG:O | 1:75:A:LYS:N  | 8                   | 0.41     | 0.28                | 0.29       |
| (1,4429) | 1:39:A:THR:H | 1:91:A:LYS:O  | 8                   | 0.39     | 0.16                | 0.43       |
| (1,4429) | 1:39:A:THR:H | 1:92:A:ASP:O  | 8                   | 0.39     | 0.16                | 0.43       |
| (1,4552) | 1:33:A:GLY:H | 1:97:A:VAL:O  | 8                   | 0.32     | 0.18                | 0.28       |
| (1,48)   | 1:6:A:ALA:H  | 1:8:A:LEU:H   | 8                   | 0.23     | 0.07                | 0.23       |
| (1,271)  | 1:33:A:GLY:H | 1:99:A:ILE:H  | 8                   | 0.17     | 0.03                | 0.17       |
| (1,211)  | 1:41:A:GLY:H | 1:89:A:ALA:H  | 8                   | 0.16     | 0.05                | 0.15       |
| (1,198)  | 1:52:A:ASP:H | 1:56:A:GLY:H  | 8                   | 0.15     | 0.01                | 0.15       |
| (1,38)   | 1:6:A:ALA:H  | 1:152:A:ALA:H | 8                   | 0.14     | 0.02                | 0.14       |

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| Key      | Atom-1        | Atom-2        | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|---------------|---------------|---------------------|----------|---------------------|------------|
| (1,4448) | 1:45:A:PHE:O  | 1:118:A:VAL:H | 7                   | 0.84     | 0.38                | 0.81       |
| (1,4448) | 1:45:A:PHE:O  | 1:84:A:LEU:H  | 7                   | 0.84     | 0.38                | 0.81       |
| (1,4448) | 1:45:A:PHE:O  | 1:120:A:HIS:H | 7                   | 0.84     | 0.38                | 0.81       |
| (1,4448) | 1:45:A:PHE:O  | 1:85:A:GLY:H  | 7                   | 0.84     | 0.38                | 0.81       |
| (1,4468) | 1:50:A:PHE:O  | 1:116:A:THR:H | 7                   | 0.59     | 0.24                | 0.66       |
| (1,4493) | 1:68:A:SER:H  | 1:77:A:GLU:O  | 7                   | 0.54     | 0.44                | 0.34       |
| (1,4493) | 1:68:A:SER:H  | 1:78:A:GLU:O  | 7                   | 0.54     | 0.44                | 0.34       |
| (1,4493) | 1:68:A:SER:H  | 1:76:A:ASP:O  | 7                   | 0.54     | 0.44                | 0.34       |
| (1,4493) | 1:68:A:SER:H  | 1:79:A:ARG:O  | 7                   | 0.54     | 0.44                | 0.34       |
| (1,4520) | 1:84:A:LEU:O  | 1:99:A:ILE:H  | 7                   | 0.5      | 0.31                | 0.35       |
| (1,4520) | 1:75:A:LYS:H  | 1:84:A:LEU:O  | 7                   | 0.5      | 0.31                | 0.35       |
| (1,4520) | 1:46:A:HIS:H  | 1:84:A:LEU:O  | 7                   | 0.5      | 0.31                | 0.35       |
| (1,4520) | 1:45:A:PHE:H  | 1:84:A:LEU:O  | 7                   | 0.5      | 0.31                | 0.35       |
| (1,4520) | 1:20:A:PHE:H  | 1:84:A:LEU:O  | 7                   | 0.5      | 0.31                | 0.35       |
| (1,119)  | 1:45:A:PHE:H  | 1:84:A:LEU:H  | 7                   | 0.41     | 0.22                | 0.39       |
| (1,119)  | 1:46:A:HIS:H  | 1:84:A:LEU:H  | 7                   | 0.41     | 0.22                | 0.39       |
| (1,303)  | 1:69:A:ARG:H  | 1:82:A:GLY:H  | 7                   | 0.38     | 0.22                | 0.43       |
| (1,303)  | 1:49:A:GLU:H  | 1:82:A:GLY:H  | 7                   | 0.38     | 0.22                | 0.43       |
| (1,239)  | 1:131:A:ASN:H | 1:138:A:GLY:H | 7                   | 0.28     | 0.14                | 0.22       |
| (1,239)  | 1:68:A:SER:H  | 1:71:A:HIS:H  | 7                   | 0.28     | 0.14                | 0.22       |
| (1,234)  | 1:131:A:ASN:H | 1:139:A:ASN:H | 7                   | 0.24     | 0.07                | 0.2        |
| (1,157)  | 1:42:A:LEU:H  | 1:88:A:THR:H  | 7                   | 0.2      | 0.03                | 0.18       |
| (3,282)  | 1:142:A:SER:C | 2:201:A:CU:CU | 7                   | 0.18     | 0.04                | 0.18       |
| (3,253)  | 1:83:A:ASP:C  | 2:201:A:CU:CU | 7                   | 0.18     | 0.07                | 0.15       |
| (1,141)  | 1:88:A:THR:H  | 1:94:A:VAL:H  | 7                   | 0.15     | 0.05                | 0.14       |
| (1,168)  | 1:88:A:THR:H  | 1:94:A:VAL:H  | 7                   | 0.15     | 0.05                | 0.14       |
| (1,232)  | 1:116:A:THR:H | 1:148:A:VAL:H | 7                   | 0.14     | 0.04                | 0.13       |
| (1,261)  | 1:129:A:GLY:H | 1:136:A:LYS:H | 7                   | 0.14     | 0.04                | 0.12       |
| (1,14)   | 1:46:A:HIS:H  | 1:48:A:HIS:H  | 7                   | 0.13     | 0.03                | 0.13       |
| (1,187)  | 1:46:A:HIS:H  | 1:48:A:HIS:H  | 7                   | 0.13     | 0.03                | 0.13       |
| (1,273)  | 1:27:A:GLY:H  | 1:105:A:SER:H | 7                   | 0.12     | 0.01                | 0.12       |
| (1,4500) | 1:75:A:LYS:O  | 1:101:A:ASP:H | 6                   | 0.66     | 0.35                | 0.52       |
| (1,4500) | 1:75:A:LYS:O  | 1:102:A:SER:H | 6                   | 0.66     | 0.35                | 0.52       |
| (1,4500) | 1:75:A:LYS:O  | 1:103:A:VAL:H | 6                   | 0.66     | 0.35                | 0.52       |
| (1,4500) | 1:69:A:ARG:H  | 1:75:A:LYS:O  | 6                   | 0.66     | 0.35                | 0.52       |
| (1,4500) | 1:75:A:LYS:O  | 1:100:A:GLU:H | 6                   | 0.66     | 0.35                | 0.52       |
| (1,4541) | 1:38:A:LEU:O  | 1:93:A:GLY:H  | 6                   | 0.58     | 0.34                | 0.5        |
| (1,4541) | 1:35:A:ILE:O  | 1:93:A:GLY:H  | 6                   | 0.58     | 0.34                | 0.5        |
| (1,4516) | 1:67:A:LEU:H  | 1:79:A:ARG:O  | 6                   | 0.5      | 0.31                | 0.39       |
| (1,4516) | 1:69:A:ARG:H  | 1:79:A:ARG:O  | 6                   | 0.5      | 0.31                | 0.39       |
| (1,4516) | 1:68:A:SER:H  | 1:79:A:ARG:O  | 6                   | 0.5      | 0.31                | 0.39       |
| (1,4516) | 1:79:A:ARG:O  | 1:105:A:SER:H | 6                   | 0.5      | 0.31                | 0.39       |

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| Key      | Atom-1        | Atom-2        | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|---------------|---------------|---------------------|----------|---------------------|------------|
| (1,4397) | 1:21:A:GLU:O  | 1:30:A:LYS:H  | 6                   | 0.47     | 0.16                | 0.53       |
| (1,4397) | 1:30:A:LYS:H  | 1:99:A:ILE:O  | 6                   | 0.47     | 0.16                | 0.53       |
| (1,36)   | 1:42:A:LEU:H  | 1:45:A:PHE:H  | 6                   | 0.46     | 0.16                | 0.44       |
| (1,36)   | 1:45:A:PHE:H  | 1:85:A:GLY:H  | 6                   | 0.46     | 0.16                | 0.44       |
| (1,4456) | 1:47:A:VAL:O  | 1:118:A:VAL:H | 6                   | 0.44     | 0.36                | 0.32       |
| (1,4569) | 1:75:A:LYS:O  | 1:101:A:ASP:H | 6                   | 0.4      | 0.2                 | 0.36       |
| (1,4569) | 1:29:A:VAL:O  | 1:101:A:ASP:H | 6                   | 0.4      | 0.2                 | 0.36       |
| (1,4561) | 1:31:A:VAL:O  | 1:99:A:ILE:H  | 6                   | 0.37     | 0.09                | 0.36       |
| (1,4561) | 1:86:A:ASN:O  | 1:99:A:ILE:H  | 6                   | 0.37     | 0.09                | 0.36       |
| (1,4497) | 1:69:A:ARG:H  | 1:79:A:ARG:O  | 6                   | 0.37     | 0.15                | 0.3        |
| (1,4497) | 1:69:A:ARG:H  | 1:78:A:GLU:O  | 6                   | 0.37     | 0.15                | 0.3        |
| (1,4497) | 1:69:A:ARG:H  | 1:76:A:ASP:O  | 6                   | 0.37     | 0.15                | 0.3        |
| (1,4437) | 1:41:A:GLY:H  | 1:121:A:GLU:O | 6                   | 0.35     | 0.12                | 0.32       |
| (1,4551) | 1:33:A:GLY:N  | 1:97:A:VAL:O  | 6                   | 0.3      | 0.14                | 0.3        |
| (1,4551) | 1:86:A:ASN:N  | 1:97:A:VAL:O  | 6                   | 0.3      | 0.14                | 0.3        |
| (1,162)  | 1:67:A:LEU:H  | 1:70:A:LYS:H  | 6                   | 0.23     | 0.08                | 0.24       |
| (1,146)  | 1:67:A:LEU:H  | 1:109:A:ASP:H | 6                   | 0.23     | 0.08                | 0.24       |
| (1,20)   | 1:89:A:ALA:H  | 1:95:A:ALA:H  | 6                   | 0.22     | 0.1                 | 0.22       |
| (1,4596) | 1:114:A:GLY:O | 1:149:A:ILE:H | 6                   | 0.21     | 0.12                | 0.18       |
| (3,194)  | 1:136:A:LYS:C | 2:201:A:CU:CU | 6                   | 0.19     | 0.02                | 0.18       |
| (1,4440) | 1:42:A:LEU:O  | 1:44:A:GLY:H  | 6                   | 0.16     | 0.06                | 0.15       |
| (1,208)  | 1:34:A:SER:H  | 1:95:A:ALA:H  | 6                   | 0.16     | 0.03                | 0.17       |
| (1,249)  | 1:50:A:PHE:H  | 1:109:A:ASP:H | 6                   | 0.16     | 0.06                | 0.15       |
| (1,195)  | 1:40:A:GLU:H  | 1:91:A:LYS:H  | 6                   | 0.16     | 0.07                | 0.12       |
| (1,4104) | 1:142:A:SER:C | 1:144:A:LEU:C | 6                   | 0.13     | 0.02                | 0.12       |
| (1,1267) | 1:39:A:THR:C  | 1:41:A:GLY:N  | 6                   | 0.11     | 0.01                | 0.11       |
| (1,4460) | 1:48:A:HIS:O  | 1:118:A:VAL:H | 5                   | 0.91     | 0.37                | 0.94       |
| (1,4460) | 1:48:A:HIS:O  | 1:116:A:THR:H | 5                   | 0.91     | 0.37                | 0.94       |
| (1,4460) | 1:48:A:HIS:O  | 1:68:A:SER:H  | 5                   | 0.91     | 0.37                | 0.94       |
| (1,4488) | 1:67:A:LEU:O  | 1:79:A:ARG:H  | 5                   | 0.87     | 0.48                | 0.8        |
| (1,4488) | 1:49:A:GLU:H  | 1:67:A:LEU:O  | 5                   | 0.87     | 0.48                | 0.8        |
| (1,4488) | 1:67:A:LEU:O  | 1:77:A:GLU:H  | 5                   | 0.87     | 0.48                | 0.8        |
| (1,4572) | 1:29:A:VAL:H  | 1:102:A:SER:O | 5                   | 0.73     | 0.45                | 0.58       |
| (1,4572) | 1:77:A:GLU:H  | 1:102:A:SER:O | 5                   | 0.73     | 0.45                | 0.58       |
| (1,4476) | 1:55:A:ALA:O  | 1:146:A:CYS:H | 5                   | 0.71     | 0.19                | 0.75       |
| (1,4503) | 1:76:A:ASP:O  | 1:104:A:ILE:N | 5                   | 0.61     | 0.11                | 0.66       |
| (1,4503) | 1:76:A:ASP:O  | 1:101:A:ASP:N | 5                   | 0.61     | 0.11                | 0.66       |
| (1,4503) | 1:76:A:ASP:O  | 1:103:A:VAL:N | 5                   | 0.61     | 0.11                | 0.66       |
| (1,4503) | 1:76:A:ASP:O  | 1:105:A:SER:N | 5                   | 0.61     | 0.11                | 0.66       |
| (1,84)   | 1:57:A:CYS:H  | 1:144:A:LEU:H | 5                   | 0.59     | 0.16                | 0.56       |
| (1,84)   | 1:120:A:HIS:H | 1:144:A:LEU:H | 5                   | 0.59     | 0.16                | 0.56       |
| (1,4457) | 1:47:A:VAL:H  | 1:118:A:VAL:O | 5                   | 0.56     | 0.17                | 0.58       |

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| Key      | Atom-1         | Atom-2        | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|----------------|---------------|---------------------|----------|---------------------|------------|
| (1,11)   | 1:48:A:HIS:H   | 1:84:A:LEU:H  | 5                   | 0.56     | 0.28                | 0.66       |
| (1,11)   | 1:48:A:HIS:H   | 1:83:A:ASP:H  | 5                   | 0.56     | 0.28                | 0.66       |
| (1,4490) | 1:67:A:LEU:N   | 1:77:A:GLU:O  | 5                   | 0.5      | 0.13                | 0.46       |
| (1,4490) | 1:67:A:LEU:N   | 1:79:A:ARG:O  | 5                   | 0.5      | 0.13                | 0.46       |
| (1,4490) | 1:67:A:LEU:N   | 1:78:A:GLU:O  | 5                   | 0.5      | 0.13                | 0.46       |
| (1,4575) | 1:77:A:GLU:N   | 1:103:A:VAL:O | 5                   | 0.45     | 0.22                | 0.39       |
| (1,4575) | 1:79:A:ARG:N   | 1:103:A:VAL:O | 5                   | 0.45     | 0.22                | 0.39       |
| (1,4575) | 1:22:A:GLN:N   | 1:103:A:VAL:O | 5                   | 0.45     | 0.22                | 0.39       |
| (1,4575) | 1:84:A:LEU:N   | 1:103:A:VAL:O | 5                   | 0.45     | 0.22                | 0.39       |
| (1,4575) | 1:29:A:VAL:N   | 1:103:A:VAL:O | 5                   | 0.45     | 0.22                | 0.39       |
| (1,4447) | 1:45:A:PHE:O   | 1:118:A:VAL:N | 5                   | 0.4      | 0.13                | 0.35       |
| (1,4447) | 1:45:A:PHE:O   | 1:84:A:LEU:N  | 5                   | 0.4      | 0.13                | 0.35       |
| (1,4447) | 1:45:A:PHE:O   | 1:86:A:ASN:N  | 5                   | 0.4      | 0.13                | 0.35       |
| (1,4400) | 1:31:A:VAL:O   | 1:99:A:ILE:H  | 5                   | 0.34     | 0.04                | 0.34       |
| (1,4400) | 1:31:A:VAL:O   | 1:100:A:GLU:H | 5                   | 0.34     | 0.04                | 0.34       |
| (1,4357) | 1:10:A:GLY:H   | 1:14:A:VAL:O  | 5                   | 0.3      | 0.09                | 0.31       |
| (1,4357) | 1:10:A:GLY:H   | 1:144:A:LEU:O | 5                   | 0.3      | 0.09                | 0.31       |
| (1,4357) | 1:10:A:GLY:H   | 1:146:A:CYS:O | 5                   | 0.3      | 0.09                | 0.31       |
| (1,4540) | 1:36:A:LYS:H   | 1:93:A:GLY:O  | 5                   | 0.28     | 0.1                 | 0.25       |
| (1,4424) | 1:14:A:VAL:H   | 1:38:A:LEU:O  | 5                   | 0.26     | 0.09                | 0.26       |
| (1,4424) | 1:38:A:LEU:O   | 1:93:A:GLY:H  | 5                   | 0.26     | 0.09                | 0.26       |
| (1,4424) | 1:38:A:LEU:O   | 1:121:A:GLU:H | 5                   | 0.26     | 0.09                | 0.26       |
| (1,267)  | 1:33:A:GLY:H   | 1:35:A:ILE:H  | 5                   | 0.26     | 0.1                 | 0.28       |
| (1,2954) | 1:105:A:SER:CA | 1:107:A:SER:N | 5                   | 0.25     | 0.01                | 0.26       |
| (3,144)  | 1:91:A:LYS:N   | 2:201:A:CU:CU | 5                   | 0.21     | 0.04                | 0.23       |
| (1,135)  | 1:79:A:ARG:H   | 1:82:A:GLY:H  | 5                   | 0.19     | 0.07                | 0.18       |
| (1,118)  | 1:47:A:VAL:H   | 1:84:A:LEU:H  | 5                   | 0.18     | 0.04                | 0.2        |
| (1,49)   | 1:47:A:VAL:H   | 1:118:A:VAL:H | 5                   | 0.17     | 0.07                | 0.16       |
| (1,191)  | 1:52:A:ASP:H   | 1:114:A:GLY:H | 5                   | 0.16     | 0.07                | 0.14       |
| (1,129)  | 1:60:A:ALA:H   | 1:63:A:HIS:H  | 5                   | 0.15     | 0.04                | 0.12       |
| (1,1689) | 1:57:A:CYS:CB  | 1:59:A:SER:CA | 5                   | 0.14     | 0.04                | 0.14       |
| (3,187)  | 1:118:A:VAL:C  | 2:201:A:CU:CU | 5                   | 0.14     | 0.03                | 0.13       |
| (1,161)  | 1:72:A:GLY:H   | 1:80:A:HIS:H  | 5                   | 0.14     | 0.04                | 0.12       |
| (1,252)  | 1:50:A:PHE:H   | 1:52:A:ASP:H  | 5                   | 0.13     | 0.02                | 0.14       |
| (1,73)   | 1:4:A:ALA:H    | 1:19:A:ASN:H  | 5                   | 0.13     | 0.01                | 0.13       |
| (1,112)  | 1:14:A:VAL:H   | 1:36:A:LYS:H  | 5                   | 0.12     | 0.01                | 0.12       |
| (1,4573) | 1:77:A:GLU:O   | 1:102:A:SER:H | 4                   | 0.82     | 0.31                | 0.78       |
| (1,4573) | 1:75:A:LYS:O   | 1:102:A:SER:H | 4                   | 0.82     | 0.31                | 0.78       |
| (1,4525) | 1:45:A:PHE:O   | 1:85:A:GLY:H  | 4                   | 0.72     | 0.09                | 0.69       |
| (1,4525) | 1:46:A:HIS:O   | 1:85:A:GLY:H  | 4                   | 0.72     | 0.09                | 0.69       |
| (1,4525) | 1:44:A:GLY:O   | 1:85:A:GLY:H  | 4                   | 0.72     | 0.09                | 0.69       |
| (1,4525) | 1:85:A:GLY:H   | 1:98:A:SER:O  | 4                   | 0.72     | 0.09                | 0.69       |

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| Key      | Atom-1        | Atom-2        | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|---------------|---------------|---------------------|----------|---------------------|------------|
| (1,4510) | 1:77:A:GLU:N  | 1:101:A:ASP:O | 4                   | 0.48     | 0.11                | 0.42       |
| (1,4510) | 1:68:A:SER:O  | 1:77:A:GLU:N  | 4                   | 0.48     | 0.11                | 0.42       |
| (1,4510) | 1:67:A:LEU:O  | 1:77:A:GLU:N  | 4                   | 0.48     | 0.11                | 0.42       |
| (1,4510) | 1:77:A:GLU:N  | 1:104:A:ILE:O | 4                   | 0.48     | 0.11                | 0.42       |
| (1,4538) | 1:39:A:THR:O  | 1:92:A:ASP:N  | 4                   | 0.41     | 0.05                | 0.42       |
| (1,4538) | 1:40:A:GLU:O  | 1:92:A:ASP:N  | 4                   | 0.41     | 0.05                | 0.42       |
| (1,4538) | 1:38:A:LEU:O  | 1:92:A:ASP:N  | 4                   | 0.41     | 0.05                | 0.42       |
| (1,4582) | 1:76:A:ASP:O  | 1:104:A:ILE:N | 4                   | 0.41     | 0.22                | 0.37       |
| (1,4582) | 1:75:A:LYS:O  | 1:104:A:ILE:N | 4                   | 0.41     | 0.22                | 0.37       |
| (1,4582) | 1:21:A:GLU:O  | 1:104:A:ILE:N | 4                   | 0.41     | 0.22                | 0.37       |
| (1,4582) | 1:77:A:GLU:O  | 1:104:A:ILE:N | 4                   | 0.41     | 0.22                | 0.37       |
| (1,4487) | 1:49:A:GLU:N  | 1:67:A:LEU:O  | 4                   | 0.38     | 0.07                | 0.36       |
| (1,4487) | 1:67:A:LEU:O  | 1:79:A:ARG:N  | 4                   | 0.38     | 0.07                | 0.36       |
| (1,4487) | 1:67:A:LEU:O  | 1:77:A:GLU:N  | 4                   | 0.38     | 0.07                | 0.36       |
| (1,4470) | 1:50:A:PHE:N  | 1:116:A:THR:O | 4                   | 0.34     | 0.16                | 0.28       |
| (1,4470) | 1:50:A:PHE:N  | 1:113:A:ILE:O | 4                   | 0.34     | 0.16                | 0.28       |
| (1,4470) | 1:50:A:PHE:N  | 1:114:A:GLY:O | 4                   | 0.34     | 0.16                | 0.28       |
| (1,4530) | 1:86:A:ASN:N  | 1:96:A:ASP:O  | 4                   | 0.33     | 0.15                | 0.34       |
| (1,4530) | 1:44:A:GLY:O  | 1:86:A:ASN:N  | 4                   | 0.33     | 0.15                | 0.34       |
| (1,4530) | 1:45:A:PHE:O  | 1:86:A:ASN:N  | 4                   | 0.33     | 0.15                | 0.34       |
| (1,4499) | 1:75:A:LYS:O  | 1:103:A:VAL:N | 4                   | 0.31     | 0.15                | 0.26       |
| (1,4499) | 1:75:A:LYS:O  | 1:101:A:ASP:N | 4                   | 0.31     | 0.15                | 0.26       |
| (1,4499) | 1:75:A:LYS:O  | 1:102:A:SER:N | 4                   | 0.31     | 0.15                | 0.26       |
| (1,4384) | 1:21:A:GLU:O  | 1:30:A:LYS:H  | 4                   | 0.29     | 0.19                | 0.23       |
| (1,4384) | 1:21:A:GLU:O  | 1:105:A:SER:H | 4                   | 0.29     | 0.19                | 0.23       |
| (1,4384) | 1:21:A:GLU:O  | 1:104:A:ILE:H | 4                   | 0.29     | 0.19                | 0.23       |
| (1,4406) | 1:18:A:ILE:O  | 1:32:A:TRP:N  | 4                   | 0.29     | 0.12                | 0.28       |
| (1,4406) | 1:17:A:ILE:O  | 1:32:A:TRP:N  | 4                   | 0.29     | 0.12                | 0.28       |
| (1,4486) | 1:57:A:CYS:N  | 1:116:A:THR:O | 4                   | 0.25     | 0.13                | 0.25       |
| (1,4486) | 1:57:A:CYS:N  | 1:146:A:CYS:O | 4                   | 0.25     | 0.13                | 0.25       |
| (1,4486) | 1:57:A:CYS:N  | 1:143:A:ARG:O | 4                   | 0.25     | 0.13                | 0.25       |
| (1,4486) | 1:57:A:CYS:N  | 1:145:A:ALA:O | 4                   | 0.25     | 0.13                | 0.25       |
| (1,4557) | 1:31:A:VAL:O  | 1:98:A:SER:H  | 4                   | 0.25     | 0.1                 | 0.26       |
| (1,4557) | 1:86:A:ASN:O  | 1:98:A:SER:H  | 4                   | 0.25     | 0.1                 | 0.26       |
| (1,4586) | 1:22:A:GLN:O  | 1:105:A:SER:N | 4                   | 0.25     | 0.1                 | 0.24       |
| (1,4586) | 1:76:A:ASP:O  | 1:105:A:SER:N | 4                   | 0.25     | 0.1                 | 0.24       |
| (1,4586) | 1:21:A:GLU:O  | 1:105:A:SER:N | 4                   | 0.25     | 0.1                 | 0.24       |
| (1,53)   | 1:48:A:HIS:H  | 1:118:A:VAL:H | 4                   | 0.24     | 0.05                | 0.22       |
| (1,127)  | 1:70:A:LYS:H  | 1:78:A:GLU:H  | 4                   | 0.24     | 0.11                | 0.2        |
| (1,4634) | 1:9:A:LYS:O   | 1:144:A:LEU:N | 4                   | 0.24     | 0.04                | 0.23       |
| (1,4634) | 1:55:A:ALA:O  | 1:144:A:LEU:N | 4                   | 0.24     | 0.04                | 0.23       |
| (1,4634) | 1:119:A:VAL:O | 1:144:A:LEU:N | 4                   | 0.24     | 0.04                | 0.23       |

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| Key      | Atom-1        | Atom-2        | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|---------------|---------------|---------------------|----------|---------------------|------------|
| (1,34)   | 1:34:A:SER:H  | 1:97:A:VAL:H  | 4                   | 0.22     | 0.05                | 0.24       |
| (1,137)  | 1:51:A:GLY:H  | 1:111:A:SER:H | 4                   | 0.2      | 0.05                | 0.21       |
| (3,196)  | 1:139:A:ASN:C | 2:201:A:CU:CU | 4                   | 0.18     | 0.07                | 0.18       |
| (1,183)  | 1:51:A:GLY:H  | 1:110:A:HIS:H | 4                   | 0.18     | 0.05                | 0.18       |
| (1,247)  | 1:37:A:GLY:H  | 1:39:A:THR:H  | 4                   | 0.16     | 0.02                | 0.16       |
| (1,1286) | 1:40:A:GLU:CB | 1:42:A:LEU:CB | 4                   | 0.14     | 0.03                | 0.14       |
| (1,177)  | 1:124:A:ASP:H | 1:126:A:LEU:H | 4                   | 0.14     | 0.03                | 0.13       |
| (1,223)  | 1:51:A:GLY:H  | 1:114:A:GLY:H | 4                   | 0.14     | 0.03                | 0.13       |
| (1,32)   | 1:52:A:ASP:H  | 1:149:A:ILE:H | 4                   | 0.13     | 0.04                | 0.12       |
| (1,122)  | 1:42:A:LEU:H  | 1:124:A:ASP:H | 4                   | 0.12     | 0.02                | 0.12       |
| (1,2034) | 1:67:A:LEU:C  | 1:69:A:ARG:N  | 4                   | 0.12     | 0.01                | 0.12       |
| (1,976)  | 1:27:A:GLY:CA | 1:30:A:LYS:CA | 4                   | 0.12     | 0.01                | 0.12       |
| (1,4579) | 1:78:A:GLU:N  | 1:104:A:ILE:O | 3                   | 1.11     | 0.66                | 0.65       |
| (1,4579) | 1:22:A:GLN:N  | 1:104:A:ILE:O | 3                   | 1.11     | 0.66                | 0.65       |
| (1,4579) | 1:79:A:ARG:N  | 1:104:A:ILE:O | 3                   | 1.11     | 0.66                | 0.65       |
| (1,4564) | 1:31:A:VAL:H  | 1:100:A:GLU:O | 3                   | 0.7      | 0.53                | 0.44       |
| (1,4564) | 1:76:A:ASP:H  | 1:100:A:GLU:O | 3                   | 0.7      | 0.53                | 0.44       |
| (1,4564) | 1:75:A:LYS:H  | 1:100:A:GLU:O | 3                   | 0.7      | 0.53                | 0.44       |
| (1,4449) | 1:45:A:PHE:H  | 1:120:A:HIS:O | 3                   | 0.59     | 0.46                | 0.43       |
| (1,4449) | 1:45:A:PHE:H  | 1:85:A:GLY:O  | 3                   | 0.59     | 0.46                | 0.43       |
| (1,4597) | 1:114:A:GLY:H | 1:151:A:ILE:O | 3                   | 0.58     | 0.4                 | 0.43       |
| (1,4597) | 1:114:A:GLY:H | 1:149:A:ILE:O | 3                   | 0.58     | 0.4                 | 0.43       |
| (1,4455) | 1:47:A:VAL:O  | 1:118:A:VAL:N | 3                   | 0.56     | 0.39                | 0.47       |
| (1,4455) | 1:47:A:VAL:O  | 1:117:A:LEU:N | 3                   | 0.56     | 0.39                | 0.47       |
| (1,4507) | 1:69:A:ARG:N  | 1:77:A:GLU:O  | 3                   | 0.52     | 0.17                | 0.63       |
| (1,4507) | 1:77:A:GLU:O  | 1:84:A:LEU:N  | 3                   | 0.52     | 0.17                | 0.63       |
| (1,4507) | 1:68:A:SER:N  | 1:77:A:GLU:O  | 3                   | 0.52     | 0.17                | 0.63       |
| (1,4396) | 1:21:A:GLU:H  | 1:30:A:LYS:O  | 3                   | 0.51     | 0.14                | 0.5        |
| (1,4511) | 1:78:A:GLU:O  | 1:105:A:SER:N | 3                   | 0.48     | 0.28                | 0.5        |
| (1,4511) | 1:69:A:ARG:N  | 1:78:A:GLU:O  | 3                   | 0.48     | 0.28                | 0.5        |
| (1,4491) | 1:68:A:SER:O  | 1:78:A:GLU:N  | 3                   | 0.46     | 0.06                | 0.49       |
| (1,4491) | 1:68:A:SER:O  | 1:79:A:ARG:N  | 3                   | 0.46     | 0.06                | 0.49       |
| (1,4578) | 1:75:A:LYS:O  | 1:103:A:VAL:N | 3                   | 0.36     | 0.24                | 0.28       |
| (1,4578) | 1:76:A:ASP:O  | 1:103:A:VAL:N | 3                   | 0.36     | 0.24                | 0.28       |
| (1,4392) | 1:29:A:VAL:O  | 1:101:A:ASP:H | 3                   | 0.33     | 0.17                | 0.27       |
| (1,4392) | 1:29:A:VAL:O  | 1:102:A:SER:H | 3                   | 0.33     | 0.17                | 0.27       |
| (1,4443) | 1:44:A:GLY:O  | 1:120:A:HIS:N | 3                   | 0.33     | 0.12                | 0.3        |
| (1,4443) | 1:44:A:GLY:O  | 1:85:A:GLY:N  | 3                   | 0.33     | 0.12                | 0.3        |
| (3,179)  | 1:46:A:HIS:C  | 2:201:A:CU:CU | 3                   | 0.3      | 0.07                | 0.34       |
| (1,4568) | 1:29:A:VAL:H  | 1:101:A:ASP:O | 3                   | 0.28     | 0.15                | 0.29       |
| (1,4568) | 1:75:A:LYS:H  | 1:101:A:ASP:O | 3                   | 0.28     | 0.15                | 0.29       |
| (1,4626) | 1:38:A:LEU:O  | 1:121:A:GLU:N | 3                   | 0.25     | 0.11                | 0.17       |

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| Key      | Atom-1         | Atom-2         | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|----------------|----------------|---------------------|----------|---------------------|------------|
| (1,4626) | 1:40:A:GLU:O   | 1:121:A:GLU:N  | 3                   | 0.25     | 0.11                | 0.17       |
| (1,4626) | 1:121:A:GLU:N  | 1:144:A:LEU:O  | 3                   | 0.25     | 0.11                | 0.17       |
| (3,137)  | 1:80:A:HIS:N   | 2:201:A:CU:CU  | 3                   | 0.24     | 0.07                | 0.22       |
| (1,2019) | 1:67:A:LEU:CA  | 1:70:A:LYS:CA  | 3                   | 0.21     | 0.07                | 0.17       |
| (3,160)  | 1:113:A:ILE:N  | 2:201:A:CU:CU  | 3                   | 0.21     | 0.05                | 0.24       |
| (1,197)  | 1:52:A:ASP:H   | 1:148:A:VAL:H  | 3                   | 0.19     | 0.07                | 0.22       |
| (1,100)  | 1:46:A:HIS:H   | 1:83:A:ASP:H   | 3                   | 0.18     | 0.06                | 0.22       |
| (3,178)  | 1:45:A:PHE:C   | 2:201:A:CU:CU  | 3                   | 0.18     | 0.04                | 0.2        |
| (1,145)  | 1:115:A:ARG:H  | 1:117:A:LEU:H  | 3                   | 0.17     | 0.01                | 0.16       |
| (1,263)  | 1:27:A:GLY:H   | 1:102:A:SER:H  | 3                   | 0.16     | 0.05                | 0.17       |
| (3,241)  | 1:59:A:SER:C   | 2:201:A:CU:CU  | 3                   | 0.16     | 0.05                | 0.13       |
| (1,151)  | 1:89:A:ALA:H   | 1:94:A:VAL:H   | 3                   | 0.15     | 0.05                | 0.12       |
| (1,4427) | 1:39:A:THR:O   | 1:91:A:LYS:N   | 3                   | 0.15     | 0.01                | 0.16       |
| (1,4427) | 1:39:A:THR:O   | 1:93:A:GLY:N   | 3                   | 0.15     | 0.01                | 0.16       |
| (1,4427) | 1:39:A:THR:O   | 1:92:A:ASP:N   | 3                   | 0.15     | 0.01                | 0.16       |
| (1,222)  | 1:72:A:GLY:H   | 1:127:A:GLY:H  | 3                   | 0.15     | 0.03                | 0.13       |
| (1,300)  | 1:72:A:GLY:H   | 1:127:A:GLY:H  | 3                   | 0.15     | 0.03                | 0.13       |
| (1,3292) | 1:118:A:VAL:CB | 1:120:A:HIS:CA | 3                   | 0.15     | 0.03                | 0.14       |
| (1,977)  | 1:27:A:GLY:CA  | 1:30:A:LYS:CB  | 3                   | 0.15     | 0.04                | 0.12       |
| (3,202)  | 1:48:A:HIS:H   | 2:201:A:CU:CU  | 3                   | 0.15     | 0.01                | 0.15       |
| (1,116)  | 1:42:A:LEU:H   | 1:123:A:ALA:H  | 3                   | 0.14     | 0.03                | 0.13       |
| (3,134)  | 1:77:A:GLU:N   | 2:201:A:CU:CU  | 3                   | 0.14     | 0.02                | 0.13       |
| (3,281)  | 1:135:A:THR:C  | 2:201:A:CU:CU  | 3                   | 0.14     | 0.03                | 0.14       |
| (1,4515) | 1:68:A:SER:N   | 1:79:A:ARG:O   | 3                   | 0.13     | 0.03                | 0.12       |
| (1,173)  | 1:73:A:GLY:H   | 1:126:A:LEU:H  | 3                   | 0.13     | 0.01                | 0.14       |
| (1,2975) | 1:106:A:LEU:N  | 1:108:A:GLY:CA | 3                   | 0.13     | 0.02                | 0.13       |
| (1,4107) | 1:142:A:SER:C  | 1:145:A:ALA:CB | 3                   | 0.13     | 0.0                 | 0.13       |
| (1,64)   | 1:90:A:ASP:H   | 1:95:A:ALA:H   | 3                   | 0.12     | 0.01                | 0.12       |
| (1,262)  | 1:17:A:ILE:H   | 1:33:A:GLY:H   | 3                   | 0.12     | 0.02                | 0.11       |
| (1,280)  | 1:108:A:GLY:H  | 1:112:A:ILE:H  | 3                   | 0.12     | 0.01                | 0.11       |
| (1,4459) | 1:48:A:HIS:O   | 1:118:A:VAL:N  | 2                   | 0.78     | 0.26                | 0.78       |
| (1,4459) | 1:48:A:HIS:O   | 1:68:A:SER:N   | 2                   | 0.78     | 0.26                | 0.78       |
| (3,333)  | 1:72:A:GLY:N   | 2:201:A:CU:CU  | 2                   | 0.68     | 0.57                | 0.68       |
| (1,4616) | 1:119:A:VAL:O  | 1:145:A:ALA:H  | 2                   | 0.56     | 0.38                | 0.56       |
| (1,4637) | 1:119:A:VAL:O  | 1:145:A:ALA:H  | 2                   | 0.56     | 0.38                | 0.56       |
| (1,4528) | 1:86:A:ASN:O   | 1:97:A:VAL:H   | 2                   | 0.54     | 0.2                 | 0.54       |
| (1,4528) | 1:44:A:GLY:H   | 1:86:A:ASN:O   | 2                   | 0.54     | 0.2                 | 0.54       |
| (1,4583) | 1:105:A:SER:O  | 1:112:A:ILE:N  | 2                   | 0.5      | 0.1                 | 0.5        |
| (1,182)  | 1:7:A:VAL:H    | 1:150:A:GLY:H  | 2                   | 0.48     | 0.24                | 0.48       |
| (1,4498) | 1:69:A:ARG:N   | 1:78:A:GLU:O   | 2                   | 0.46     | 0.0                 | 0.46       |
| (1,4498) | 1:69:A:ARG:N   | 1:79:A:ARG:O   | 2                   | 0.46     | 0.0                 | 0.46       |
| (1,4452) | 1:46:A:HIS:O   | 1:85:A:GLY:H   | 2                   | 0.46     | 0.23                | 0.46       |

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| Key       | Atom-1         | Atom-2        | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|-----------|----------------|---------------|---------------------|----------|---------------------|------------|
| (1,4452)  | 1:46:A:HIS:O   | 1:118:A:VAL:H | 2                   | 0.46     | 0.23                | 0.46       |
| (1,79)    | 1:119:A:VAL:H  | 1:144:A:LEU:H | 2                   | 0.44     | 0.16                | 0.44       |
| (1,160)   | 1:70:A:LYS:H   | 1:80:A:HIS:H  | 2                   | 0.44     | 0.26                | 0.44       |
| (1,4402)  | 1:31:A:VAL:N   | 1:100:A:GLU:O | 2                   | 0.43     | 0.3                 | 0.43       |
| (1,4402)  | 1:31:A:VAL:N   | 1:99:A:ILE:O  | 2                   | 0.43     | 0.3                 | 0.43       |
| (1,4590)  | 1:112:A:ILE:N  | 1:149:A:ILE:O | 2                   | 0.38     | 0.1                 | 0.38       |
| (1,132)   | 1:40:A:GLU:H   | 1:92:A:ASP:H  | 2                   | 0.35     | 0.06                | 0.35       |
| (1,4522)  | 1:45:A:PHE:O   | 1:84:A:LEU:N  | 2                   | 0.35     | 0.0                 | 0.35       |
| (1,4522)  | 1:46:A:HIS:O   | 1:84:A:LEU:N  | 2                   | 0.35     | 0.0                 | 0.35       |
| (1,96)    | 1:15:A:GLN:H   | 1:38:A:LEU:H  | 2                   | 0.34     | 0.2                 | 0.34       |
| (1,4526)  | 1:46:A:HIS:O   | 1:85:A:GLY:N  | 2                   | 0.34     | 0.19                | 0.34       |
| (1,4526)  | 1:44:A:GLY:O   | 1:85:A:GLY:N  | 2                   | 0.34     | 0.19                | 0.34       |
| (1,294)   | 1:37:A:GLY:H   | 1:40:A:GLU:H  | 2                   | 0.32     | 0.02                | 0.32       |
| (1,4502)  | 1:68:A:SER:O   | 1:75:A:LYS:N  | 2                   | 0.32     | 0.16                | 0.32       |
| (1,4502)  | 1:44:A:GLY:O   | 1:75:A:LYS:N  | 2                   | 0.32     | 0.16                | 0.32       |
| (1,4506)  | 1:76:A:ASP:N   | 1:101:A:ASP:O | 2                   | 0.3      | 0.01                | 0.3        |
| (1,4506)  | 1:76:A:ASP:N   | 1:84:A:LEU:O  | 2                   | 0.3      | 0.01                | 0.3        |
| (1,4348)  | 1:8:A:LEU:O    | 1:14:A:VAL:H  | 2                   | 0.24     | 0.01                | 0.24       |
| (1,4348)  | 1:8:A:LEU:O    | 1:16:A:GLY:H  | 2                   | 0.24     | 0.01                | 0.24       |
| (1,4475)  | 1:10:A:GLY:N   | 1:55:A:ALA:O  | 2                   | 0.23     | 0.08                | 0.23       |
| (1,4475)  | 1:55:A:ALA:O   | 1:143:A:ARG:N | 2                   | 0.23     | 0.08                | 0.23       |
| (1,4387)  | 1:2:A:THR:N    | 1:22:A:GLN:O  | 2                   | 0.22     | 0.11                | 0.22       |
| (1,4108)  | 1:142:A:SER:C  | 1:145:A:ALA:C | 2                   | 0.22     | 0.1                 | 0.22       |
| (1,220)   | 1:72:A:GLY:H   | 1:78:A:GLU:H  | 2                   | 0.21     | 0.01                | 0.21       |
| (3,265)   | 1:100:A:GLU:C  | 2:201:A:CU:CU | 2                   | 0.2      | 0.09                | 0.2        |
| (3,159)   | 1:112:A:ILE:N  | 2:201:A:CU:CU | 2                   | 0.2      | 0.05                | 0.2        |
| (1,117)   | 1:76:A:ASP:H   | 1:78:A:GLU:H  | 2                   | 0.2      | 0.02                | 0.2        |
| (1,289)   | 1:116:A:THR:H  | 1:147:A:GLY:H | 2                   | 0.2      | 0.01                | 0.2        |
| (1,138)   | 1:72:A:GLY:H   | 1:79:A:ARG:H  | 2                   | 0.18     | 0.05                | 0.18       |
| (1,139)   | 1:69:A:ARG:H   | 1:78:A:GLU:H  | 2                   | 0.18     | 0.04                | 0.18       |
| (1,218)   | 1:72:A:GLY:H   | 1:79:A:ARG:H  | 2                   | 0.18     | 0.05                | 0.18       |
| (3,203)   | 1:63:A:HIS:H   | 2:201:A:CU:CU | 2                   | 0.18     | 0.01                | 0.18       |
| (1,4445)  | 1:42:A:LEU:O   | 1:44:A:GLY:H  | 2                   | 0.18     | 0.06                | 0.18       |
| (3,195)   | 1:138:A:GLY:C  | 2:201:A:CU:CU | 2                   | 0.17     | 0.03                | 0.17       |
| (3,182)   | 1:62:A:PRO:C   | 2:201:A:CU:CU | 2                   | 0.17     | 0.01                | 0.17       |
| (3,193)   | 1:128:A:LYS:C  | 2:201:A:CU:CU | 2                   | 0.17     | 0.01                | 0.17       |
| (2,10700) | 1:86:A:ASN:C   | 1:89:A:ALA:C  | 2                   | 0.16     | 0.06                | 0.16       |
| (1,4514)  | 1:67:A:LEU:O   | 1:78:A:GLU:N  | 2                   | 0.16     | 0.04                | 0.16       |
| (1,235)   | 1:116:A:THR:H  | 1:118:A:VAL:H | 2                   | 0.16     | 0.03                | 0.16       |
| (1,3480)  | 1:126:A:LEU:CA | 1:128:A:LYS:C | 2                   | 0.16     | 0.02                | 0.16       |
| (2,158)   | 1:107:A:SER:N  | 1:109:A:ASP:N | 2                   | 0.16     | 0.02                | 0.16       |
| (1,2064)  | 1:68:A:SER:CB  | 1:70:A:LYS:C  | 2                   | 0.16     | 0.04                | 0.16       |

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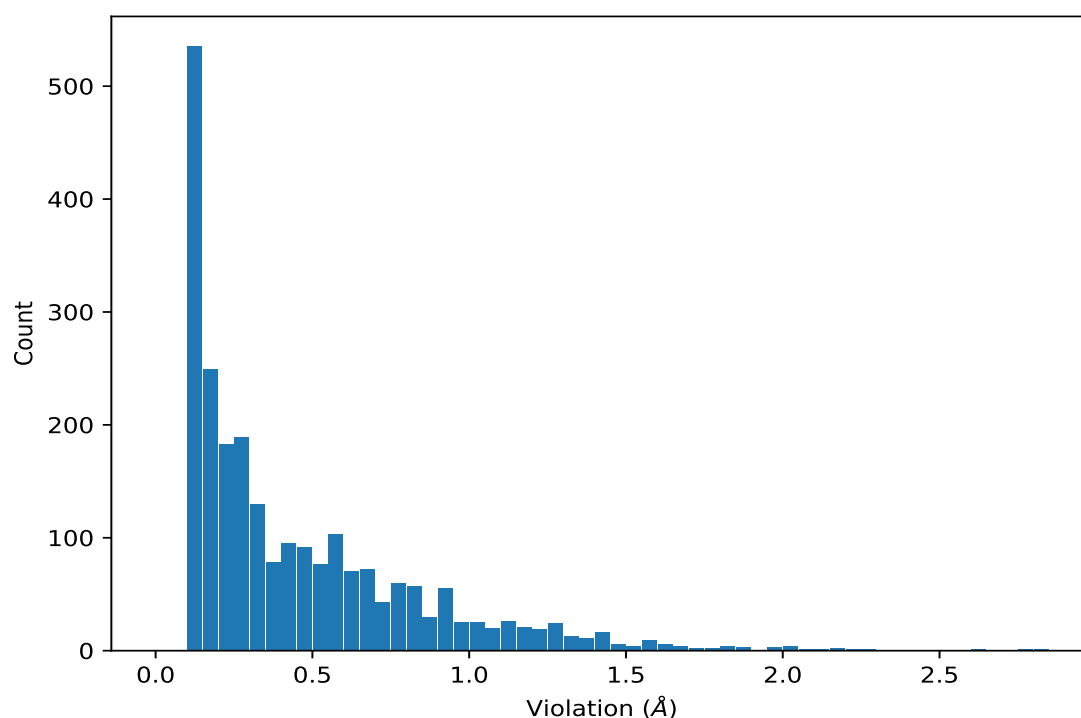
| Key       | Atom-1         | Atom-2        | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|-----------|----------------|---------------|---------------------|----------|---------------------|------------|
| (2,10545) | 1:86:A:ASN:N   | 1:89:A:ALA:C  | 2                   | 0.16     | 0.04                | 0.16       |
| (1,75)    | 1:35:A:ILE:H   | 1:97:A:VAL:H  | 2                   | 0.15     | 0.0                 | 0.15       |
| (2,10616) | 1:86:A:ASN:CB  | 1:89:A:ALA:C  | 2                   | 0.15     | 0.03                | 0.15       |
| (3,95)    | 1:12:A:GLY:N   | 2:201:A:CU:CU | 2                   | 0.14     | 0.03                | 0.14       |
| (1,133)   | 1:70:A:LYS:H   | 1:78:A:GLU:H  | 2                   | 0.14     | 0.01                | 0.14       |
| (1,2974)  | 1:105:A:SER:C  | 1:109:A:ASP:N | 2                   | 0.14     | 0.02                | 0.14       |
| (1,130)   | 1:53:A:ASN:H   | 1:60:A:ALA:H  | 2                   | 0.14     | 0.04                | 0.14       |
| (1,174)   | 1:53:A:ASN:H   | 1:57:A:CYS:H  | 2                   | 0.14     | 0.02                | 0.14       |
| (1,23)    | 1:23:A:LYS:H   | 1:106:A:LEU:H | 2                   | 0.13     | 0.01                | 0.13       |
| (1,1296)  | 1:40:A:GLU:C   | 1:42:A:LEU:CB | 2                   | 0.13     | 0.01                | 0.13       |
| (1,2576)  | 1:90:A:ASP:CB  | 1:92:A:ASP:CG | 2                   | 0.13     | 0.02                | 0.13       |
| (1,251)   | 1:111:A:SER:H  | 1:115:A:ARG:H | 2                   | 0.12     | 0.01                | 0.12       |
| (1,1099)  | 1:31:A:VAL:C   | 1:34:A:SER:CB | 2                   | 0.12     | 0.01                | 0.12       |
| (1,236)   | 1:60:A:ALA:H   | 1:116:A:THR:H | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,603)   | 1:13:A:PRO:CD  | 1:15:A:GLN:N  | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,255)   | 1:42:A:LEU:H   | 1:44:A:GLY:H  | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,266)   | 1:33:A:GLY:H   | 1:97:A:VAL:H  | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,219)   | 1:72:A:GLY:H   | 1:80:A:HIS:H  | 2                   | 0.11     | 0.01                | 0.11       |
| (1,3940)  | 1:136:A:LYS:CG | 1:138:A:GLY:C | 2                   | 0.11     | 0.01                | 0.11       |
| (2,1237)  | 1:4:A:ALA:CB   | 1:8:A:LEU:CA  | 2                   | 0.11     | 0.01                | 0.11       |
| (1,111)   | 1:17:A:ILE:H   | 1:33:A:GLY:H  | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1314)  | 1:41:A:GLY:C   | 1:43:A:HIS:CB | 2                   | 0.11     | 0.0                 | 0.11       |

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

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

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

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



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

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

| Key      | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|----------|---------------|---------------|----------|---------------|
| (1,4580) | 1:22:A:GLN:H  | 1:104:A:ILE:O | 2        | 2.81          |
| (1,4436) | 1:41:A:GLY:O  | 1:44:A:GLY:H  | 4        | 2.77          |
| (3,371)  | 1:132:A:GLU:N | 2:201:A:CU:CU | 18       | 2.6           |
| (3,371)  | 1:132:A:GLU:N | 2:201:A:CU:CU | 19       | 2.3           |
| (3,198)  | 1:143:A:ARG:C | 2:201:A:CU:CU | 11       | 2.2           |
| (1,4508) | 1:77:A:GLU:O  | 1:84:A:LEU:H  | 13       | 2.16          |
| (3,371)  | 1:132:A:GLU:N | 2:201:A:CU:CU | 6        | 2.15          |
| (3,371)  | 1:132:A:GLU:N | 2:201:A:CU:CU | 16       | 2.13          |
| (1,4496) | 1:69:A:ARG:O  | 1:77:A:GLU:H  | 3        | 2.09          |
| (1,4579) | 1:22:A:GLN:N  | 1:104:A:ILE:O | 2        | 2.04          |
| (1,4480) | 1:56:A:GLY:O  | 1:147:A:GLY:H | 1        | 2.02          |
| (1,4633) | 1:119:A:VAL:O | 1:144:A:LEU:H | 18       | 2.01          |
| (1,4436) | 1:41:A:GLY:O  | 1:91:A:LYS:H  | 5        | 2.01          |
| (1,4464) | 1:49:A:GLU:O  | 1:116:A:THR:H | 7        | 1.99          |
| (1,4489) | 1:67:A:LEU:H  | 1:79:A:ARG:O  | 16       | 1.97          |
| (1,4633) | 1:9:A:LYS:O   | 1:144:A:LEU:H | 13       | 1.96          |

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| Key      | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|----------|---------------|---------------|----------|---------------|
| (1,4480) | 1:56:A:GLY:O  | 1:146:A:CYS:H | 12       | 1.9           |
| (1,4620) | 1:46:A:HIS:H  | 1:120:A:HIS:O | 16       | 1.89          |
| (1,4489) | 1:67:A:LEU:H  | 1:105:A:SER:O | 6        | 1.85          |
| (1,4435) | 1:41:A:GLY:O  | 1:44:A:GLY:N  | 4        | 1.82          |
| (1,4473) | 1:54:A:THR:H  | 1:146:A:CYS:O | 17       | 1.81          |
| (1,4473) | 1:54:A:THR:H  | 1:147:A:GLY:O | 15       | 1.8           |
| (1,4388) | 1:2:A:THR:H   | 1:22:A:GLN:O  | 10       | 1.8           |
| (1,4480) | 1:56:A:GLY:O  | 1:146:A:CYS:H | 14       | 1.78          |
| (1,4509) | 1:77:A:GLU:H  | 1:104:A:ILE:O | 15       | 1.75          |
| (3,371)  | 1:132:A:GLU:N | 2:201:A:CU:CU | 1        | 1.74          |
| (1,4505) | 1:76:A:ASP:H  | 1:101:A:ASP:O | 19       | 1.73          |
| (1,4621) | 1:42:A:LEU:O  | 1:120:A:HIS:H | 19       | 1.69          |
| (1,4620) | 1:42:A:LEU:H  | 1:120:A:HIS:O | 8        | 1.69          |
| (1,4585) | 1:21:A:GLU:O  | 1:105:A:SER:H | 13       | 1.69          |
| (1,4480) | 1:56:A:GLY:O  | 1:147:A:GLY:H | 18       | 1.66          |
| (1,4473) | 1:54:A:THR:H  | 1:147:A:GLY:O | 3        | 1.65          |
| (1,4633) | 1:119:A:VAL:O | 1:144:A:LEU:H | 11       | 1.63          |
| (1,4480) | 1:56:A:GLY:O  | 1:146:A:CYS:H | 6        | 1.63          |
| (1,4577) | 1:84:A:LEU:O  | 1:103:A:VAL:H | 17       | 1.62          |
| (1,4521) | 1:46:A:HIS:O  | 1:84:A:LEU:H  | 15       | 1.62          |
| (1,4488) | 1:67:A:LEU:O  | 1:79:A:ARG:H  | 5        | 1.61          |
| (1,4480) | 1:56:A:GLY:O  | 1:146:A:CYS:H | 10       | 1.59          |
| (1,4473) | 1:54:A:THR:H  | 1:114:A:GLY:O | 8        | 1.59          |
| (1,4585) | 1:21:A:GLU:O  | 1:105:A:SER:H | 17       | 1.58          |
| (1,4589) | 1:112:A:ILE:H | 1:149:A:ILE:O | 9        | 1.57          |
| (1,4448) | 1:45:A:PHE:O  | 1:120:A:HIS:H | 15       | 1.57          |
| (1,4460) | 1:48:A:HIS:O  | 1:68:A:SER:H  | 17       | 1.56          |
| (1,4356) | 1:10:A:GLY:O  | 1:146:A:CYS:H | 7        | 1.56          |
| (1,4629) | 1:57:A:CYS:O  | 1:143:A:ARG:H | 13       | 1.55          |
| (1,4484) | 1:57:A:CYS:O  | 1:143:A:ARG:H | 13       | 1.55          |
| (1,4589) | 1:112:A:ILE:H | 1:151:A:ILE:O | 3        | 1.52          |
| (3,84)   | 1:150:A:GLY:C | 2:201:A:CU:CU | 8        | 1.5           |
| (1,4633) | 1:55:A:ALA:O  | 1:144:A:LEU:H | 6        | 1.5           |
| (1,4521) | 1:84:A:LEU:H  | 1:98:A:SER:O  | 19       | 1.5           |
| (1,4628) | 1:10:A:GLY:H  | 1:143:A:ARG:O | 14       | 1.48          |
| (1,4628) | 1:57:A:CYS:H  | 1:143:A:ARG:O | 15       | 1.48          |
| (1,4620) | 1:42:A:LEU:H  | 1:120:A:HIS:O | 1        | 1.48          |
| (1,4548) | 1:33:A:GLY:H  | 1:96:A:ASP:O  | 2        | 1.47          |
| (1,4620) | 1:42:A:LEU:H  | 1:120:A:HIS:O | 9        | 1.46          |
| (1,4493) | 1:68:A:SER:H  | 1:79:A:ARG:O  | 12       | 1.46          |
| (1,4480) | 1:56:A:GLY:O  | 1:146:A:CYS:H | 17       | 1.45          |
| (1,4473) | 1:54:A:THR:H  | 1:114:A:GLY:O | 9        | 1.45          |

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| Key      | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|----------|---------------|---------------|----------|---------------|
| (1,4469) | 1:50:A:PHE:H  | 1:116:A:THR:O | 3        | 1.45          |
| (1,4441) | 1:42:A:LEU:H  | 1:121:A:GLU:O | 9        | 1.45          |
| (1,4436) | 1:41:A:GLY:O  | 1:94:A:VAL:H  | 10       | 1.45          |
| (1,4572) | 1:77:A:GLU:H  | 1:102:A:SER:O | 9        | 1.44          |
| (1,4564) | 1:31:A:VAL:H  | 1:100:A:GLU:O | 9        | 1.44          |
| (1,4489) | 1:67:A:LEU:H  | 1:79:A:ARG:O  | 11       | 1.44          |
| (1,4529) | 1:86:A:ASN:H  | 1:98:A:SER:O  | 9        | 1.42          |
| (1,4500) | 1:75:A:LYS:O  | 1:100:A:GLU:H | 11       | 1.42          |
| (1,4469) | 1:50:A:PHE:H  | 1:116:A:THR:O | 17       | 1.42          |
| (1,4589) | 1:112:A:ILE:H | 1:149:A:ILE:O | 18       | 1.41          |
| (1,4565) | 1:84:A:LEU:O  | 1:100:A:GLU:H | 7        | 1.41          |
| (1,4501) | 1:75:A:LYS:H  | 1:84:A:LEU:O  | 13       | 1.41          |
| (1,4436) | 1:41:A:GLY:O  | 1:44:A:GLY:H  | 15       | 1.41          |
| (1,107)  | 1:46:A:HIS:H  | 1:119:A:VAL:H | 7        | 1.41          |
| (1,4464) | 1:49:A:GLU:O  | 1:116:A:THR:H | 8        | 1.4           |
| (1,4548) | 1:33:A:GLY:H  | 1:96:A:ASP:O  | 18       | 1.39          |
| (1,4589) | 1:48:A:HIS:O  | 1:112:A:ILE:H | 11       | 1.38          |
| (1,4560) | 1:31:A:VAL:H  | 1:99:A:ILE:O  | 1        | 1.38          |
| (1,4480) | 1:56:A:GLY:O  | 1:147:A:GLY:H | 2        | 1.37          |
| (1,4484) | 1:57:A:CYS:O  | 1:143:A:ARG:H | 2        | 1.36          |
| (1,4484) | 1:57:A:CYS:O  | 1:143:A:ARG:H | 3        | 1.36          |
| (1,4473) | 1:54:A:THR:H  | 1:114:A:GLY:O | 16       | 1.36          |
| (1,4473) | 1:7:A:VAL:O   | 1:54:A:THR:H  | 18       | 1.36          |
| (1,4589) | 1:105:A:SER:O | 1:112:A:ILE:H | 5        | 1.35          |
| (1,4584) | 1:105:A:SER:O | 1:112:A:ILE:H | 5        | 1.35          |
| (1,4501) | 1:75:A:LYS:H  | 1:85:A:GLY:O  | 11       | 1.34          |
| (1,4480) | 1:56:A:GLY:O  | 1:147:A:GLY:H | 7        | 1.33          |
| (1,4589) | 1:112:A:ILE:H | 1:149:A:ILE:O | 12       | 1.32          |
| (1,4536) | 1:36:A:LYS:H  | 1:92:A:ASP:O  | 19       | 1.32          |
| (1,4501) | 1:75:A:LYS:H  | 1:85:A:GLY:O  | 1        | 1.32          |
| (1,4480) | 1:56:A:GLY:O  | 1:147:A:GLY:H | 3        | 1.32          |
| (1,4480) | 1:56:A:GLY:O  | 1:116:A:THR:H | 8        | 1.32          |
| (1,4473) | 1:54:A:THR:H  | 1:114:A:GLY:O | 1        | 1.32          |
| (1,4576) | 1:29:A:VAL:H  | 1:103:A:VAL:O | 18       | 1.31          |
| (1,4480) | 1:56:A:GLY:O  | 1:147:A:GLY:H | 15       | 1.31          |
| (1,4592) | 1:113:A:ILE:O | 1:151:A:ILE:H | 13       | 1.3           |
| (1,4577) | 1:75:A:LYS:O  | 1:103:A:VAL:H | 13       | 1.3           |
| (1,4436) | 1:41:A:GLY:O  | 1:94:A:VAL:H  | 8        | 1.3           |
| (1,4589) | 1:112:A:ILE:H | 1:149:A:ILE:O | 1        | 1.29          |
| (1,4547) | 1:33:A:GLY:N  | 1:96:A:ASP:O  | 2        | 1.29          |
| (3,198)  | 1:143:A:ARG:C | 2:201:A:CU:CU | 3        | 1.28          |
| (1,4473) | 1:54:A:THR:H  | 1:146:A:CYS:O | 10       | 1.28          |

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| Key      | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|----------|---------------|---------------|----------|---------------|
| (1,4441) | 1:42:A:LEU:H  | 1:121:A:GLU:O | 16       | 1.28          |
| (1,4432) | 1:40:A:GLU:O  | 1:91:A:LYS:H  | 5        | 1.28          |
| (1,4593) | 1:113:A:ILE:H | 1:149:A:ILE:O | 5        | 1.27          |
| (1,4592) | 1:113:A:ILE:O | 1:149:A:ILE:H | 1        | 1.27          |
| (1,4589) | 1:112:A:ILE:H | 1:151:A:ILE:O | 15       | 1.27          |
| (1,4585) | 1:76:A:ASP:O  | 1:105:A:SER:H | 5        | 1.27          |
| (1,4559) | 1:31:A:VAL:N  | 1:99:A:ILE:O  | 1        | 1.27          |
| (1,4537) | 1:38:A:LEU:O  | 1:92:A:ASP:H  | 18       | 1.27          |
| (1,4504) | 1:76:A:ASP:O  | 1:105:A:SER:H | 12       | 1.27          |
| (3,333)  | 1:72:A:GLY:N  | 2:201:A:CU:CU | 6        | 1.26          |
| (1,4592) | 1:113:A:ILE:O | 1:149:A:ILE:H | 12       | 1.26          |
| (1,4589) | 1:112:A:ILE:H | 1:149:A:ILE:O | 8        | 1.26          |
| (1,4480) | 1:56:A:GLY:O  | 1:146:A:CYS:H | 13       | 1.26          |
| (1,4620) | 1:42:A:LEU:H  | 1:120:A:HIS:O | 15       | 1.25          |
| (1,4533) | 1:40:A:GLU:O  | 1:91:A:LYS:H  | 10       | 1.25          |
| (1,4480) | 1:56:A:GLY:O  | 1:147:A:GLY:H | 9        | 1.25          |
| (1,4473) | 1:54:A:THR:H  | 1:114:A:GLY:O | 12       | 1.25          |
| (1,4432) | 1:40:A:GLU:O  | 1:91:A:LYS:H  | 10       | 1.25          |
| (1,4428) | 1:39:A:THR:O  | 1:91:A:LYS:H  | 3        | 1.25          |
| (1,26)   | 1:48:A:HIS:H  | 1:149:A:ILE:H | 17       | 1.25          |
| (1,4629) | 1:57:A:CYS:O  | 1:143:A:ARG:H | 16       | 1.24          |
| (1,4576) | 1:84:A:LEU:H  | 1:103:A:VAL:O | 17       | 1.24          |
| (1,4547) | 1:33:A:GLY:N  | 1:96:A:ASP:O  | 18       | 1.24          |
| (1,4541) | 1:38:A:LEU:O  | 1:93:A:GLY:H  | 13       | 1.24          |
| (1,4536) | 1:36:A:LYS:H  | 1:92:A:ASP:O  | 16       | 1.24          |
| (1,4489) | 1:67:A:LEU:H  | 1:79:A:ARG:O  | 9        | 1.24          |
| (1,4484) | 1:57:A:CYS:O  | 1:143:A:ARG:H | 16       | 1.24          |
| (1,4480) | 1:56:A:GLY:O  | 1:147:A:GLY:H | 19       | 1.24          |
| (1,169)  | 1:49:A:GLU:H  | 1:111:A:SER:H | 12       | 1.24          |
| (1,4633) | 1:119:A:VAL:O | 1:144:A:LEU:H | 15       | 1.23          |
| (1,4573) | 1:75:A:LYS:O  | 1:102:A:SER:H | 13       | 1.23          |
| (1,4509) | 1:68:A:SER:O  | 1:77:A:GLU:H  | 9        | 1.23          |
| (1,4537) | 1:38:A:LEU:O  | 1:92:A:ASP:H  | 6        | 1.22          |
| (1,4536) | 1:39:A:THR:H  | 1:92:A:ASP:O  | 1        | 1.22          |
| (1,4449) | 1:45:A:PHE:H  | 1:85:A:GLY:O  | 19       | 1.22          |
| (1,4625) | 1:41:A:GLY:O  | 1:121:A:GLU:H | 11       | 1.21          |
| (1,4589) | 1:112:A:ILE:H | 1:149:A:ILE:O | 19       | 1.21          |
| (1,4504) | 1:76:A:ASP:O  | 1:104:A:ILE:H | 19       | 1.21          |
| (1,4473) | 1:54:A:THR:H  | 1:114:A:GLY:O | 19       | 1.21          |
| (1,4592) | 1:113:A:ILE:O | 1:151:A:ILE:H | 10       | 1.2           |
| (1,4537) | 1:38:A:LEU:O  | 1:92:A:ASP:H  | 17       | 1.2           |
| (1,4501) | 1:44:A:GLY:O  | 1:75:A:LYS:H  | 6        | 1.2           |

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| Key      | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|----------|---------------|---------------|----------|---------------|
| (1,4388) | 1:22:A:GLN:O  | 1:112:A:ILE:H | 13       | 1.2           |
| (1,4629) | 1:119:A:VAL:O | 1:143:A:ARG:H | 3        | 1.19          |
| (1,4592) | 1:113:A:ILE:O | 1:151:A:ILE:H | 19       | 1.19          |
| (1,4589) | 1:104:A:ILE:O | 1:112:A:ILE:H | 10       | 1.19          |
| (1,4401) | 1:21:A:GLU:O  | 1:31:A:VAL:H  | 15       | 1.19          |
| (1,4325) | 1:2:A:THR:H   | 1:20:A:PHE:O  | 9        | 1.19          |
| (1,4585) | 1:77:A:GLU:O  | 1:105:A:SER:H | 6        | 1.18          |
| (1,4576) | 1:84:A:LEU:H  | 1:103:A:VAL:O | 14       | 1.18          |
| (1,4548) | 1:86:A:ASN:H  | 1:96:A:ASP:O  | 6        | 1.18          |
| (1,4456) | 1:47:A:VAL:O  | 1:118:A:VAL:H | 16       | 1.18          |
| (1,4508) | 1:77:A:GLU:O  | 1:104:A:ILE:H | 19       | 1.17          |
| (1,4464) | 1:49:A:GLU:O  | 1:116:A:THR:H | 4        | 1.17          |
| (3,198)  | 1:143:A:ARG:C | 2:201:A:CU:CU | 7        | 1.16          |
| (1,4633) | 1:55:A:ALA:O  | 1:144:A:LEU:H | 12       | 1.16          |
| (1,4629) | 1:57:A:CYS:O  | 1:143:A:ARG:H | 15       | 1.16          |
| (1,4529) | 1:86:A:ASN:H  | 1:98:A:SER:O  | 18       | 1.16          |
| (1,4484) | 1:57:A:CYS:O  | 1:143:A:ARG:H | 15       | 1.16          |
| (1,4477) | 1:55:A:ALA:H  | 1:146:A:CYS:O | 16       | 1.16          |
| (1,4625) | 1:38:A:LEU:O  | 1:121:A:GLU:H | 8        | 1.15          |
| (1,4577) | 1:21:A:GLU:O  | 1:103:A:VAL:H | 11       | 1.15          |
| (1,4556) | 1:86:A:ASN:H  | 1:98:A:SER:O  | 17       | 1.15          |
| (1,4529) | 1:86:A:ASN:H  | 1:98:A:SER:O  | 17       | 1.15          |
| (1,4436) | 1:41:A:GLY:O  | 1:91:A:LYS:H  | 12       | 1.15          |
| (1,4589) | 1:112:A:ILE:H | 1:149:A:ILE:O | 14       | 1.14          |
| (1,4469) | 1:50:A:PHE:H  | 1:116:A:THR:O | 19       | 1.14          |
| (1,4620) | 1:44:A:GLY:H  | 1:120:A:HIS:O | 19       | 1.13          |
| (1,4597) | 1:114:A:GLY:H | 1:151:A:ILE:O | 2        | 1.13          |
| (1,4592) | 1:50:A:PHE:H  | 1:113:A:ILE:O | 11       | 1.13          |
| (1,4581) | 1:21:A:GLU:O  | 1:104:A:ILE:H | 13       | 1.13          |
| (1,4473) | 1:54:A:THR:H  | 1:115:A:ARG:O | 7        | 1.13          |
| (1,4469) | 1:50:A:PHE:H  | 1:113:A:ILE:O | 11       | 1.13          |
| (1,4448) | 1:45:A:PHE:O  | 1:85:A:GLY:H  | 19       | 1.13          |
| (1,4428) | 1:39:A:THR:O  | 1:93:A:GLY:H  | 6        | 1.13          |
| (1,4620) | 1:42:A:LEU:H  | 1:120:A:HIS:O | 2        | 1.12          |
| (1,4592) | 1:50:A:PHE:H  | 1:113:A:ILE:O | 8        | 1.12          |
| (1,4592) | 1:113:A:ILE:O | 1:151:A:ILE:H | 14       | 1.12          |
| (1,4536) | 1:36:A:LYS:H  | 1:92:A:ASP:O  | 8        | 1.12          |
| (1,4505) | 1:76:A:ASP:H  | 1:102:A:SER:O | 5        | 1.12          |
| (1,4488) | 1:49:A:GLU:H  | 1:67:A:LEU:O  | 8        | 1.12          |
| (1,4465) | 1:49:A:GLU:H  | 1:67:A:LEU:O  | 8        | 1.12          |
| (1,4388) | 1:2:A:THR:H   | 1:22:A:GLN:O  | 17       | 1.12          |
| (1,4513) | 1:78:A:GLU:H  | 1:102:A:SER:O | 11       | 1.1           |

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| Key      | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|----------|---------------|---------------|----------|---------------|
| (1,4480) | 1:56:A:GLY:O  | 1:147:A:GLY:H | 16       | 1.1           |
| (1,4477) | 1:55:A:ALA:H  | 1:146:A:CYS:O | 19       | 1.1           |
| (1,4584) | 1:84:A:LEU:H  | 1:105:A:SER:O | 10       | 1.09          |
| (1,4556) | 1:31:A:VAL:H  | 1:98:A:SER:O  | 11       | 1.09          |
| (1,4536) | 1:36:A:LYS:H  | 1:92:A:ASP:O  | 5        | 1.09          |
| (1,4388) | 1:2:A:THR:H   | 1:22:A:GLN:O  | 8        | 1.09          |
| (1,4325) | 1:2:A:THR:H   | 1:22:A:GLN:O  | 8        | 1.09          |
| (1,4537) | 1:39:A:THR:O  | 1:92:A:ASP:H  | 7        | 1.08          |
| (1,4455) | 1:47:A:VAL:O  | 1:118:A:VAL:N | 16       | 1.08          |
| (1,4428) | 1:39:A:THR:O  | 1:93:A:GLY:H  | 2        | 1.08          |
| (1,4428) | 1:39:A:THR:O  | 1:92:A:ASP:H  | 7        | 1.08          |
| (1,4584) | 1:79:A:ARG:H  | 1:105:A:SER:O | 9        | 1.07          |
| (1,4572) | 1:77:A:GLU:H  | 1:102:A:SER:O | 13       | 1.07          |
| (1,4556) | 1:31:A:VAL:H  | 1:98:A:SER:O  | 18       | 1.07          |
| (1,4508) | 1:77:A:GLU:O  | 1:104:A:ILE:H | 2        | 1.07          |
| (1,4428) | 1:39:A:THR:O  | 1:93:A:GLY:H  | 1        | 1.07          |
| (1,4619) | 1:42:A:LEU:N  | 1:120:A:HIS:O | 2        | 1.06          |
| (1,4580) | 1:78:A:GLU:H  | 1:104:A:ILE:O | 15       | 1.06          |
| (1,4556) | 1:86:A:ASN:H  | 1:98:A:SER:O  | 4        | 1.06          |
| (1,4548) | 1:33:A:GLY:H  | 1:96:A:ASP:O  | 3        | 1.06          |
| (1,4548) | 1:86:A:ASN:H  | 1:96:A:ASP:O  | 7        | 1.06          |
| (1,4428) | 1:39:A:THR:O  | 1:91:A:LYS:H  | 18       | 1.05          |
| (1,4556) | 1:31:A:VAL:H  | 1:98:A:SER:O  | 14       | 1.04          |
| (1,4529) | 1:86:A:ASN:H  | 1:96:A:ASP:O  | 8        | 1.04          |
| (1,4508) | 1:77:A:GLU:O  | 1:102:A:SER:H | 11       | 1.04          |
| (1,4589) | 1:105:A:SER:O | 1:112:A:ILE:H | 13       | 1.03          |
| (1,4589) | 1:49:A:GLU:O  | 1:112:A:ILE:H | 16       | 1.03          |
| (1,4584) | 1:105:A:SER:O | 1:112:A:ILE:H | 13       | 1.03          |
| (1,4555) | 1:86:A:ASN:N  | 1:98:A:SER:O  | 4        | 1.03          |
| (1,4459) | 1:48:A:HIS:O  | 1:68:A:SER:N  | 17       | 1.03          |
| (1,4433) | 1:40:A:GLU:H  | 1:121:A:GLU:O | 8        | 1.03          |
| (1,4628) | 1:57:A:CYS:H  | 1:143:A:ARG:O | 5        | 1.02          |
| (1,4580) | 1:79:A:ARG:H  | 1:104:A:ILE:O | 16       | 1.02          |
| (1,4573) | 1:77:A:GLU:O  | 1:102:A:SER:H | 9        | 1.02          |
| (1,4509) | 1:68:A:SER:O  | 1:77:A:GLU:H  | 3        | 1.02          |
| (1,4473) | 1:54:A:THR:H  | 1:114:A:GLY:O | 11       | 1.02          |
| (1,4436) | 1:41:A:GLY:O  | 1:121:A:GLU:H | 19       | 1.02          |
| (1,4428) | 1:39:A:THR:O  | 1:91:A:LYS:H  | 17       | 1.02          |
| (1,4628) | 1:57:A:CYS:H  | 1:143:A:ARG:O | 1        | 1.01          |
| (1,4536) | 1:36:A:LYS:H  | 1:92:A:ASP:O  | 4        | 1.01          |
| (1,4504) | 1:69:A:ARG:H  | 1:76:A:ASP:O  | 6        | 1.01          |
| (1,4516) | 1:67:A:LEU:H  | 1:79:A:ARG:O  | 3        | 1.0           |

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| Key      | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|----------|---------------|---------------|----------|---------------|
| (1,4512) | 1:69:A:ARG:H  | 1:78:A:GLU:O  | 2        | 1.0           |
| (1,4508) | 1:69:A:ARG:H  | 1:77:A:GLU:O  | 14       | 1.0           |
| (1,4505) | 1:76:A:ASP:H  | 1:101:A:ASP:O | 13       | 1.0           |
| (1,4492) | 1:68:A:SER:O  | 1:79:A:ARG:H  | 17       | 1.0           |
| (1,4469) | 1:50:A:PHE:H  | 1:112:A:ILE:O | 13       | 1.0           |
| (1,4629) | 1:57:A:CYS:O  | 1:143:A:ARG:H | 7        | 0.99          |
| (1,4629) | 1:57:A:CYS:O  | 1:143:A:ARG:H | 10       | 0.99          |
| (1,4533) | 1:38:A:LEU:O  | 1:91:A:LYS:H  | 15       | 0.99          |
| (1,4505) | 1:76:A:ASP:H  | 1:101:A:ASP:O | 1        | 0.99          |
| (1,4484) | 1:57:A:CYS:O  | 1:143:A:ARG:H | 7        | 0.99          |
| (1,4484) | 1:57:A:CYS:O  | 1:143:A:ARG:H | 10       | 0.99          |
| (1,4464) | 1:49:A:GLU:O  | 1:116:A:THR:H | 5        | 0.99          |
| (1,4405) | 1:18:A:ILE:O  | 1:32:A:TRP:H  | 13       | 0.99          |
| (1,169)  | 1:49:A:GLU:H  | 1:83:A:ASP:H  | 6        | 0.99          |
| (1,4592) | 1:49:A:GLU:H  | 1:113:A:ILE:O | 17       | 0.98          |
| (1,4584) | 1:22:A:GLN:H  | 1:105:A:SER:O | 16       | 0.98          |
| (1,4580) | 1:79:A:ARG:H  | 1:104:A:ILE:O | 3        | 0.98          |
| (1,4537) | 1:40:A:GLU:O  | 1:92:A:ASP:H  | 12       | 0.98          |
| (1,4480) | 1:56:A:GLY:O  | 1:147:A:GLY:H | 5        | 0.98          |
| (1,4389) | 1:22:A:GLN:H  | 1:105:A:SER:O | 16       | 0.98          |
| (1,4520) | 1:84:A:LEU:O  | 1:99:A:ILE:H  | 3        | 0.97          |
| (1,4495) | 1:69:A:ARG:O  | 1:78:A:GLU:N  | 3        | 0.97          |
| (1,4481) | 1:56:A:GLY:H  | 1:146:A:CYS:O | 16       | 0.97          |
| (1,4436) | 1:41:A:GLY:O  | 1:91:A:LYS:H  | 3        | 0.97          |
| (1,4632) | 1:9:A:LYS:H   | 1:144:A:LEU:O | 18       | 0.96          |
| (1,4555) | 1:86:A:ASN:N  | 1:98:A:SER:O  | 17       | 0.96          |
| (1,4536) | 1:40:A:GLU:H  | 1:92:A:ASP:O  | 10       | 0.96          |
| (1,4533) | 1:38:A:LEU:O  | 1:91:A:LYS:H  | 5        | 0.96          |
| (1,4505) | 1:76:A:ASP:H  | 1:101:A:ASP:O | 6        | 0.96          |
| (1,4473) | 1:54:A:THR:H  | 1:146:A:CYS:O | 6        | 0.96          |
| (3,198)  | 1:143:A:ARG:C | 2:201:A:CU:CU | 4        | 0.95          |
| (1,4580) | 1:79:A:ARG:H  | 1:104:A:ILE:O | 1        | 0.95          |
| (1,4580) | 1:77:A:GLU:H  | 1:104:A:ILE:O | 18       | 0.95          |
| (1,4577) | 1:75:A:LYS:O  | 1:103:A:VAL:H | 7        | 0.95          |
| (1,4536) | 1:36:A:LYS:H  | 1:92:A:ASP:O  | 9        | 0.95          |
| (1,4509) | 1:77:A:GLU:H  | 1:104:A:ILE:O | 18       | 0.95          |
| (1,4501) | 1:75:A:LYS:H  | 1:101:A:ASP:O | 2        | 0.95          |
| (1,4489) | 1:67:A:LEU:H  | 1:78:A:GLU:O  | 10       | 0.95          |
| (1,4476) | 1:55:A:ALA:O  | 1:146:A:CYS:H | 5        | 0.95          |
| (1,4473) | 1:7:A:VAL:O   | 1:54:A:THR:H  | 2        | 0.95          |
| (1,4460) | 1:48:A:HIS:O  | 1:116:A:THR:H | 11       | 0.95          |
| (1,4401) | 1:31:A:VAL:H  | 1:100:A:GLU:O | 1        | 0.95          |

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| Key      | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|----------|---------------|---------------|----------|---------------|
| (1,4388) | 1:2:A:THR:H   | 1:22:A:GLN:O  | 11       | 0.95          |
| (1,4356) | 1:10:A:GLY:O  | 1:14:A:VAL:H  | 4        | 0.95          |
| (1,4356) | 1:10:A:GLY:O  | 1:14:A:VAL:H  | 11       | 0.95          |
| (1,4637) | 1:119:A:VAL:O | 1:145:A:ALA:H | 12       | 0.94          |
| (1,4629) | 1:57:A:CYS:O  | 1:143:A:ARG:H | 5        | 0.94          |
| (1,4616) | 1:119:A:VAL:O | 1:145:A:ALA:H | 12       | 0.94          |
| (1,4592) | 1:113:A:ILE:O | 1:151:A:ILE:H | 9        | 0.94          |
| (1,4576) | 1:84:A:LEU:H  | 1:103:A:VAL:O | 4        | 0.94          |
| (1,4556) | 1:31:A:VAL:H  | 1:98:A:SER:O  | 3        | 0.94          |
| (1,4548) | 1:86:A:ASN:H  | 1:96:A:ASP:O  | 15       | 0.94          |
| (1,4547) | 1:33:A:GLY:N  | 1:96:A:ASP:O  | 3        | 0.94          |
| (1,4521) | 1:84:A:LEU:H  | 1:103:A:VAL:O | 4        | 0.94          |
| (1,4520) | 1:20:A:PHE:H  | 1:84:A:LEU:O  | 18       | 0.94          |
| (1,4501) | 1:75:A:LYS:H  | 1:102:A:SER:O | 12       | 0.94          |
| (1,4492) | 1:68:A:SER:O  | 1:79:A:ARG:H  | 16       | 0.94          |
| (1,4484) | 1:57:A:CYS:O  | 1:143:A:ARG:H | 5        | 0.94          |
| (1,4477) | 1:55:A:ALA:H  | 1:146:A:CYS:O | 5        | 0.94          |
| (1,4460) | 1:48:A:HIS:O  | 1:118:A:VAL:H | 1        | 0.94          |
| (1,4388) | 1:2:A:THR:H   | 1:22:A:GLN:O  | 4        | 0.94          |
| (1,4621) | 1:45:A:PHE:O  | 1:120:A:HIS:H | 5        | 0.93          |
| (1,4621) | 1:42:A:LEU:O  | 1:120:A:HIS:H | 10       | 0.93          |
| (1,4513) | 1:68:A:SER:O  | 1:78:A:GLU:H  | 5        | 0.93          |
| (1,4621) | 1:45:A:PHE:O  | 1:120:A:HIS:H | 7        | 0.92          |
| (1,4555) | 1:31:A:VAL:N  | 1:98:A:SER:O  | 11       | 0.92          |
| (1,4555) | 1:31:A:VAL:N  | 1:98:A:SER:O  | 14       | 0.92          |
| (1,4536) | 1:39:A:THR:H  | 1:92:A:ASP:O  | 3        | 0.92          |
| (1,4509) | 1:68:A:SER:O  | 1:77:A:GLU:H  | 8        | 0.92          |
| (1,176)  | 1:86:A:ASN:H  | 1:88:A:THR:H  | 7        | 0.92          |
| (1,169)  | 1:49:A:GLU:H  | 1:83:A:ASP:H  | 13       | 0.92          |
| (1,91)   | 1:119:A:VAL:H | 1:121:A:GLU:H | 3        | 0.92          |
| (1,4625) | 1:38:A:LEU:O  | 1:121:A:GLU:H | 2        | 0.91          |
| (1,4529) | 1:86:A:ASN:H  | 1:98:A:SER:O  | 12       | 0.91          |
| (1,4481) | 1:56:A:GLY:H  | 1:146:A:CYS:O | 5        | 0.91          |
| (1,4356) | 1:10:A:GLY:O  | 1:14:A:VAL:H  | 5        | 0.91          |
| (1,4324) | 1:2:A:THR:O   | 1:21:A:GLU:H  | 19       | 0.91          |
| (1,4592) | 1:50:A:PHE:H  | 1:113:A:ILE:O | 6        | 0.9           |
| (1,4521) | 1:84:A:LEU:H  | 1:101:A:ASP:O | 17       | 0.9           |
| (1,4521) | 1:84:A:LEU:H  | 1:149:A:ILE:O | 18       | 0.9           |
| (1,4509) | 1:68:A:SER:O  | 1:77:A:GLU:H  | 2        | 0.9           |
| (1,4494) | 1:68:A:SER:N  | 1:76:A:ASP:O  | 12       | 0.9           |
| (1,4405) | 1:18:A:ILE:O  | 1:32:A:TRP:H  | 18       | 0.9           |
| (1,4356) | 1:10:A:GLY:O  | 1:146:A:CYS:H | 16       | 0.9           |

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| Key      | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|----------|---------------|---------------|----------|---------------|
| (1,12)   | 1:117:A:LEU:H | 1:150:A:GLY:H | 4        | 0.9           |
| (1,4621) | 1:120:A:HIS:H | 1:145:A:ALA:O | 6        | 0.89          |
| (1,4576) | 1:21:A:GLU:H  | 1:103:A:VAL:O | 7        | 0.89          |
| (1,4537) | 1:38:A:LEU:O  | 1:92:A:ASP:H  | 10       | 0.89          |
| (1,4533) | 1:41:A:GLY:O  | 1:91:A:LYS:H  | 17       | 0.89          |
| (1,4513) | 1:67:A:LEU:O  | 1:78:A:GLU:H  | 18       | 0.89          |
| (1,4496) | 1:69:A:ARG:O  | 1:79:A:ARG:H  | 5        | 0.89          |
| (1,4465) | 1:49:A:GLU:H  | 1:116:A:THR:O | 14       | 0.89          |
| (1,4436) | 1:41:A:GLY:O  | 1:91:A:LYS:H  | 17       | 0.89          |
| (1,4576) | 1:21:A:GLU:H  | 1:103:A:VAL:O | 11       | 0.88          |
| (1,4512) | 1:69:A:ARG:H  | 1:78:A:GLU:O  | 14       | 0.88          |
| (1,4509) | 1:67:A:LEU:O  | 1:77:A:GLU:H  | 10       | 0.88          |
| (1,120)  | 1:149:A:ILE:H | 1:151:A:ILE:H | 5        | 0.88          |
| (1,12)   | 1:117:A:LEU:H | 1:150:A:GLY:H | 8        | 0.88          |
| (1,4577) | 1:76:A:ASP:O  | 1:103:A:VAL:H | 14       | 0.87          |
| (1,4556) | 1:31:A:VAL:H  | 1:98:A:SER:O  | 12       | 0.87          |
| (1,4548) | 1:33:A:GLY:H  | 1:96:A:ASP:O  | 11       | 0.87          |
| (1,4504) | 1:76:A:ASP:O  | 1:104:A:ILE:H | 8        | 0.87          |
| (1,4477) | 1:55:A:ALA:H  | 1:146:A:CYS:O | 8        | 0.87          |
| (1,4473) | 1:54:A:THR:H  | 1:146:A:CYS:O | 14       | 0.87          |
| (1,4468) | 1:50:A:PHE:O  | 1:116:A:THR:H | 19       | 0.87          |
| (1,4464) | 1:49:A:GLU:O  | 1:116:A:THR:H | 9        | 0.87          |
| (1,4444) | 1:44:A:GLY:O  | 1:85:A:GLY:H  | 18       | 0.87          |
| (1,4388) | 1:22:A:GLN:O  | 1:29:A:VAL:H  | 9        | 0.87          |
| (1,11)   | 1:48:A:HIS:H  | 1:83:A:ASP:H  | 12       | 0.87          |
| (1,4598) | 1:114:A:GLY:N | 1:151:A:ILE:O | 2        | 0.86          |
| (1,4536) | 1:39:A:THR:H  | 1:92:A:ASP:O  | 2        | 0.86          |
| (1,4525) | 1:45:A:PHE:O  | 1:85:A:GLY:H  | 16       | 0.86          |
| (1,4468) | 1:50:A:PHE:O  | 1:116:A:THR:H | 1        | 0.86          |
| (1,91)   | 1:119:A:VAL:H | 1:121:A:GLU:H | 2        | 0.86          |
| (1,91)   | 1:119:A:VAL:H | 1:121:A:GLU:H | 14       | 0.86          |
| (1,4576) | 1:78:A:GLU:H  | 1:103:A:VAL:O | 13       | 0.85          |
| (1,4513) | 1:78:A:GLU:H  | 1:103:A:VAL:O | 13       | 0.85          |
| (1,4496) | 1:69:A:ARG:O  | 1:79:A:ARG:H  | 10       | 0.85          |
| (1,4493) | 1:68:A:SER:H  | 1:78:A:GLU:O  | 19       | 0.85          |
| (1,4484) | 1:57:A:CYS:O  | 1:143:A:ARG:H | 8        | 0.85          |
| (1,4355) | 1:10:A:GLY:O  | 1:146:A:CYS:N | 16       | 0.85          |
| (1,12)   | 1:117:A:LEU:H | 1:150:A:GLY:H | 3        | 0.85          |
| (1,4593) | 1:113:A:ILE:H | 1:149:A:ILE:O | 3        | 0.84          |
| (1,4585) | 1:76:A:ASP:O  | 1:105:A:SER:H | 2        | 0.84          |
| (1,4512) | 1:69:A:ARG:H  | 1:78:A:GLU:O  | 13       | 0.84          |
| (1,4481) | 1:56:A:GLY:H  | 1:146:A:CYS:O | 19       | 0.84          |

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| Key      | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|----------|---------------|---------------|----------|---------------|
| (1,4476) | 1:55:A:ALA:O  | 1:146:A:CYS:H | 2        | 0.84          |
| (1,4436) | 1:41:A:GLY:O  | 1:91:A:LYS:H  | 18       | 0.84          |
| (1,4428) | 1:39:A:THR:O  | 1:93:A:GLY:H  | 12       | 0.84          |
| (1,4401) | 1:31:A:VAL:H  | 1:99:A:ILE:O  | 7        | 0.84          |
| (1,176)  | 1:86:A:ASN:H  | 1:88:A:THR:H  | 15       | 0.84          |
| (1,91)   | 1:12:A:GLY:H  | 1:121:A:GLU:H | 8        | 0.84          |
| (1,91)   | 1:119:A:VAL:H | 1:121:A:GLU:H | 9        | 0.84          |
| (1,4592) | 1:113:A:ILE:O | 1:151:A:ILE:H | 15       | 0.83          |
| (1,4585) | 1:21:A:GLU:O  | 1:105:A:SER:H | 11       | 0.83          |
| (1,4560) | 1:31:A:VAL:H  | 1:99:A:ILE:O  | 19       | 0.83          |
| (1,4505) | 1:76:A:ASP:H  | 1:102:A:SER:O | 3        | 0.83          |
| (1,4501) | 1:75:A:LYS:H  | 1:100:A:GLU:O | 17       | 0.83          |
| (1,4492) | 1:68:A:SER:O  | 1:79:A:ARG:H  | 15       | 0.83          |
| (1,4477) | 1:55:A:ALA:H  | 1:146:A:CYS:O | 7        | 0.83          |
| (1,4465) | 1:49:A:GLU:H  | 1:116:A:THR:O | 15       | 0.83          |
| (1,4448) | 1:45:A:PHE:O  | 1:84:A:LEU:H  | 7        | 0.83          |
| (1,169)  | 1:49:A:GLU:H  | 1:83:A:ASP:H  | 3        | 0.83          |
| (1,26)   | 1:51:A:GLY:H  | 1:149:A:ILE:H | 8        | 0.83          |
| (1,4625) | 1:38:A:LEU:O  | 1:121:A:GLU:H | 3        | 0.82          |
| (1,4581) | 1:77:A:GLU:O  | 1:104:A:ILE:H | 6        | 0.82          |
| (1,4533) | 1:41:A:GLY:O  | 1:91:A:LYS:H  | 6        | 0.82          |
| (1,4529) | 1:44:A:GLY:O  | 1:86:A:ASN:H  | 3        | 0.82          |
| (1,4529) | 1:86:A:ASN:H  | 1:96:A:ASP:O  | 4        | 0.82          |
| (1,4489) | 1:67:A:LEU:H  | 1:78:A:GLU:O  | 8        | 0.82          |
| (1,4469) | 1:50:A:PHE:H  | 1:116:A:THR:O | 1        | 0.82          |
| (1,4436) | 1:41:A:GLY:O  | 1:91:A:LYS:H  | 6        | 0.82          |
| (1,84)   | 1:57:A:CYS:H  | 1:144:A:LEU:H | 16       | 0.82          |
| (3,274)  | 1:120:A:HIS:C | 2:201:A:CU:CU | 19       | 0.81          |
| (1,4589) | 1:112:A:ILE:H | 1:149:A:ILE:O | 4        | 0.81          |
| (1,4516) | 1:67:A:LEU:H  | 1:79:A:ARG:O  | 19       | 0.81          |
| (1,4511) | 1:69:A:ARG:N  | 1:78:A:GLU:O  | 14       | 0.81          |
| (1,4489) | 1:67:A:LEU:H  | 1:79:A:ARG:O  | 2        | 0.81          |
| (1,4448) | 1:45:A:PHE:O  | 1:118:A:VAL:H | 3        | 0.81          |
| (1,4388) | 1:2:A:THR:H   | 1:22:A:GLN:O  | 6        | 0.81          |
| (1,4628) | 1:57:A:CYS:H  | 1:143:A:ARG:O | 11       | 0.8           |
| (1,4628) | 1:57:A:CYS:H  | 1:143:A:ARG:O | 16       | 0.8           |
| (1,4580) | 1:22:A:GLN:H  | 1:104:A:ILE:O | 6        | 0.8           |
| (1,4548) | 1:86:A:ASN:H  | 1:96:A:ASP:O  | 1        | 0.8           |
| (1,4536) | 1:39:A:THR:H  | 1:92:A:ASP:O  | 15       | 0.8           |
| (1,4509) | 1:67:A:LEU:O  | 1:77:A:GLU:H  | 12       | 0.8           |
| (1,4488) | 1:67:A:LEU:O  | 1:77:A:GLU:H  | 12       | 0.8           |
| (1,4485) | 1:57:A:CYS:H  | 1:145:A:ALA:O | 5        | 0.8           |

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| Key      | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|----------|---------------|---------------|----------|---------------|
| (1,4485) | 1:57:A:CYS:H  | 1:143:A:ARG:O | 11       | 0.8           |
| (1,4485) | 1:57:A:CYS:H  | 1:143:A:ARG:O | 16       | 0.8           |
| (1,4457) | 1:47:A:VAL:H  | 1:118:A:VAL:O | 17       | 0.8           |
| (1,11)   | 1:48:A:HIS:H  | 1:84:A:LEU:H  | 2        | 0.8           |
| (1,4629) | 1:119:A:VAL:O | 1:143:A:ARG:H | 8        | 0.79          |
| (1,4584) | 1:78:A:GLU:H  | 1:105:A:SER:O | 4        | 0.79          |
| (1,4581) | 1:21:A:GLU:O  | 1:104:A:ILE:H | 9        | 0.79          |
| (1,4575) | 1:29:A:VAL:N  | 1:103:A:VAL:O | 18       | 0.79          |
| (1,4560) | 1:31:A:VAL:H  | 1:99:A:ILE:O  | 2        | 0.79          |
| (1,4533) | 1:40:A:GLU:O  | 1:91:A:LYS:H  | 18       | 0.79          |
| (1,4532) | 1:39:A:THR:H  | 1:91:A:LYS:O  | 18       | 0.79          |
| (1,4513) | 1:78:A:GLU:H  | 1:105:A:SER:O | 4        | 0.79          |
| (1,4505) | 1:76:A:ASP:H  | 1:84:A:LEU:O  | 11       | 0.79          |
| (1,4465) | 1:49:A:GLU:H  | 1:116:A:THR:O | 4        | 0.79          |
| (1,4441) | 1:42:A:LEU:H  | 1:121:A:GLU:O | 1        | 0.79          |
| (1,4436) | 1:41:A:GLY:O  | 1:91:A:LYS:H  | 13       | 0.79          |
| (1,4436) | 1:41:A:GLY:O  | 1:91:A:LYS:H  | 14       | 0.79          |
| (1,4428) | 1:39:A:THR:O  | 1:93:A:GLY:H  | 14       | 0.79          |
| (1,98)   | 1:120:A:HIS:H | 1:123:A:ALA:H | 16       | 0.79          |
| (1,91)   | 1:119:A:VAL:H | 1:121:A:GLU:H | 16       | 0.79          |
| (1,4621) | 1:120:A:HIS:H | 1:145:A:ALA:O | 9        | 0.78          |
| (1,4591) | 1:50:A:PHE:N  | 1:113:A:ILE:O | 8        | 0.78          |
| (1,4591) | 1:113:A:ILE:O | 1:151:A:ILE:N | 14       | 0.78          |
| (1,4548) | 1:86:A:ASN:H  | 1:96:A:ASP:O  | 19       | 0.78          |
| (1,4512) | 1:78:A:GLU:O  | 1:105:A:SER:H | 4        | 0.78          |
| (1,4504) | 1:76:A:ASP:O  | 1:103:A:VAL:H | 18       | 0.78          |
| (1,4465) | 1:49:A:GLU:H  | 1:116:A:THR:O | 13       | 0.78          |
| (1,91)   | 1:119:A:VAL:H | 1:121:A:GLU:H | 5        | 0.78          |
| (1,63)   | 1:88:A:THR:H  | 1:90:A:ASP:H  | 4        | 0.78          |
| (1,4629) | 1:119:A:VAL:O | 1:143:A:ARG:H | 2        | 0.77          |
| (1,4620) | 1:42:A:LEU:H  | 1:120:A:HIS:O | 4        | 0.77          |
| (1,4593) | 1:50:A:PHE:O  | 1:113:A:ILE:H | 7        | 0.77          |
| (1,4593) | 1:49:A:GLU:O  | 1:113:A:ILE:H | 17       | 0.77          |
| (1,4556) | 1:86:A:ASN:H  | 1:98:A:SER:O  | 5        | 0.77          |
| (1,4464) | 1:49:A:GLU:O  | 1:116:A:THR:H | 1        | 0.77          |
| (1,4463) | 1:49:A:GLU:O  | 1:116:A:THR:N | 4        | 0.77          |
| (1,4428) | 1:39:A:THR:O  | 1:93:A:GLY:H  | 11       | 0.77          |
| (1,176)  | 1:86:A:ASN:H  | 1:88:A:THR:H  | 14       | 0.77          |
| (1,91)   | 1:119:A:VAL:H | 1:121:A:GLU:H | 13       | 0.77          |
| (1,4621) | 1:46:A:HIS:O  | 1:120:A:HIS:H | 15       | 0.76          |
| (1,4592) | 1:113:A:ILE:O | 1:151:A:ILE:H | 16       | 0.76          |
| (1,4532) | 1:39:A:THR:H  | 1:91:A:LYS:O  | 6        | 0.76          |

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| Key      | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|----------|---------------|---------------|----------|---------------|
| (1,4521) | 1:84:A:LEU:H  | 1:105:A:SER:O | 1        | 0.76          |
| (1,4496) | 1:69:A:ARG:O  | 1:77:A:GLU:H  | 1        | 0.76          |
| (1,4436) | 1:41:A:GLY:O  | 1:121:A:GLU:H | 9        | 0.76          |
| (1,4388) | 1:2:A:THR:H   | 1:22:A:GLN:O  | 3        | 0.76          |
| (1,4324) | 1:2:A:THR:O   | 1:21:A:GLU:H  | 2        | 0.76          |
| (1,120)  | 1:3:A:LYS:H   | 1:151:A:ILE:H | 10       | 0.76          |
| (1,98)   | 1:44:A:GLY:H  | 1:123:A:ALA:H | 15       | 0.76          |
| (1,4629) | 1:57:A:CYS:O  | 1:143:A:ARG:H | 14       | 0.75          |
| (1,4629) | 1:57:A:CYS:O  | 1:143:A:ARG:H | 18       | 0.75          |
| (1,4589) | 1:112:A:ILE:H | 1:151:A:ILE:O | 6        | 0.75          |
| (1,4556) | 1:86:A:ASN:H  | 1:98:A:SER:O  | 10       | 0.75          |
| (1,4529) | 1:86:A:ASN:H  | 1:98:A:SER:O  | 10       | 0.75          |
| (1,4519) | 1:84:A:LEU:O  | 1:99:A:ILE:N  | 3        | 0.75          |
| (1,4501) | 1:75:A:LYS:H  | 1:101:A:ASP:O | 8        | 0.75          |
| (1,4496) | 1:69:A:ARG:O  | 1:78:A:GLU:H  | 7        | 0.75          |
| (1,4484) | 1:57:A:CYS:O  | 1:143:A:ARG:H | 14       | 0.75          |
| (1,4484) | 1:57:A:CYS:O  | 1:143:A:ARG:H | 18       | 0.75          |
| (1,4479) | 1:56:A:GLY:O  | 1:116:A:THR:N | 8        | 0.75          |
| (1,4476) | 1:55:A:ALA:O  | 1:146:A:CYS:H | 16       | 0.75          |
| (1,4388) | 1:2:A:THR:H   | 1:22:A:GLN:O  | 5        | 0.75          |
| (1,4325) | 1:2:A:THR:H   | 1:20:A:PHE:O  | 6        | 0.75          |
| (1,91)   | 1:15:A:GLN:H  | 1:121:A:GLU:H | 7        | 0.75          |
| (1,4589) | 1:105:A:SER:O | 1:112:A:ILE:H | 17       | 0.74          |
| (1,4584) | 1:105:A:SER:O | 1:112:A:ILE:H | 17       | 0.74          |
| (1,4581) | 1:76:A:ASP:O  | 1:104:A:ILE:H | 5        | 0.74          |
| (1,4555) | 1:31:A:VAL:N  | 1:98:A:SER:O  | 3        | 0.74          |
| (1,4528) | 1:86:A:ASN:O  | 1:97:A:VAL:H  | 9        | 0.74          |
| (1,4503) | 1:76:A:ASP:O  | 1:104:A:ILE:N | 8        | 0.74          |
| (1,4495) | 1:69:A:ARG:O  | 1:78:A:GLU:N  | 7        | 0.74          |
| (1,4490) | 1:67:A:LEU:N  | 1:79:A:ARG:O  | 9        | 0.74          |
| (1,4388) | 1:2:A:THR:H   | 1:22:A:GLN:O  | 19       | 0.74          |
| (1,176)  | 1:86:A:ASN:H  | 1:88:A:THR:H  | 19       | 0.74          |
| (1,169)  | 1:49:A:GLU:H  | 1:83:A:ASP:H  | 14       | 0.74          |
| (1,63)   | 1:41:A:GLY:H  | 1:90:A:ASP:H  | 9        | 0.74          |
| (1,4621) | 1:45:A:PHE:O  | 1:120:A:HIS:H | 18       | 0.73          |
| (1,4620) | 1:42:A:LEU:H  | 1:120:A:HIS:O | 5        | 0.73          |
| (1,4576) | 1:22:A:GLN:H  | 1:103:A:VAL:O | 19       | 0.73          |
| (1,4559) | 1:31:A:VAL:N  | 1:99:A:ILE:O  | 19       | 0.73          |
| (1,4541) | 1:35:A:ILE:O  | 1:93:A:GLY:H  | 18       | 0.73          |
| (1,4504) | 1:76:A:ASP:O  | 1:103:A:VAL:H | 16       | 0.73          |
| (1,4501) | 1:75:A:LYS:H  | 1:101:A:ASP:O | 19       | 0.73          |
| (1,4402) | 1:31:A:VAL:N  | 1:99:A:ILE:O  | 7        | 0.73          |

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| Key      | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|----------|---------------|---------------|----------|---------------|
| (1,91)   | 1:119:A:VAL:H | 1:121:A:GLU:H | 4        | 0.73          |
| (1,91)   | 1:119:A:VAL:H | 1:121:A:GLU:H | 19       | 0.73          |
| (3,274)  | 1:120:A:HIS:C | 2:201:A:CU:CU | 14       | 0.72          |
| (1,4584) | 1:77:A:GLU:H  | 1:105:A:SER:O | 6        | 0.72          |
| (1,4582) | 1:77:A:GLU:O  | 1:104:A:ILE:N | 6        | 0.72          |
| (1,4560) | 1:31:A:VAL:H  | 1:99:A:ILE:O  | 6        | 0.72          |
| (1,4529) | 1:86:A:ASN:H  | 1:99:A:ILE:O  | 14       | 0.72          |
| (1,4473) | 1:7:A:VAL:O   | 1:54:A:THR:H  | 5        | 0.72          |
| (1,4435) | 1:41:A:GLY:O  | 1:44:A:GLY:N  | 15       | 0.72          |
| (1,192)  | 1:88:A:THR:H  | 1:122:A:LYS:H | 15       | 0.72          |
| (1,182)  | 1:7:A:VAL:H   | 1:150:A:GLY:H | 13       | 0.72          |
| (1,119)  | 1:46:A:HIS:H  | 1:84:A:LEU:H  | 2        | 0.72          |
| (1,91)   | 1:119:A:VAL:H | 1:121:A:GLU:H | 1        | 0.72          |
| (1,50)   | 1:120:A:HIS:H | 1:145:A:ALA:H | 18       | 0.72          |
| (1,36)   | 1:42:A:LEU:H  | 1:45:A:PHE:H  | 7        | 0.72          |
| (1,4633) | 1:119:A:VAL:O | 1:144:A:LEU:H | 9        | 0.71          |
| (1,4584) | 1:22:A:GLN:H  | 1:105:A:SER:O | 14       | 0.71          |
| (1,4563) | 1:29:A:VAL:N  | 1:100:A:GLU:O | 9        | 0.71          |
| (1,4555) | 1:86:A:ASN:N  | 1:98:A:SER:O  | 5        | 0.71          |
| (1,4537) | 1:38:A:LEU:O  | 1:92:A:ASP:H  | 16       | 0.71          |
| (1,4501) | 1:75:A:LYS:H  | 1:102:A:SER:O | 3        | 0.71          |
| (1,4463) | 1:49:A:GLU:O  | 1:116:A:THR:N | 5        | 0.71          |
| (1,63)   | 1:41:A:GLY:H  | 1:90:A:ASP:H  | 8        | 0.71          |
| (1,4632) | 1:10:A:GLY:H  | 1:144:A:LEU:O | 16       | 0.7           |
| (1,4591) | 1:113:A:ILE:O | 1:150:A:GLY:N | 13       | 0.7           |
| (1,4576) | 1:29:A:VAL:H  | 1:103:A:VAL:O | 2        | 0.7           |
| (1,4569) | 1:75:A:LYS:O  | 1:101:A:ASP:H | 15       | 0.7           |
| (1,4560) | 1:85:A:GLY:H  | 1:99:A:ILE:O  | 8        | 0.7           |
| (1,4537) | 1:38:A:LEU:O  | 1:92:A:ASP:H  | 8        | 0.7           |
| (1,4468) | 1:50:A:PHE:O  | 1:116:A:THR:H | 9        | 0.7           |
| (1,4463) | 1:49:A:GLU:O  | 1:114:A:GLY:N | 7        | 0.7           |
| (1,160)  | 1:70:A:LYS:H  | 1:80:A:HIS:H  | 2        | 0.7           |
| (1,63)   | 1:88:A:THR:H  | 1:90:A:ASP:H  | 16       | 0.7           |
| (1,12)   | 1:117:A:LEU:H | 1:150:A:GLY:H | 17       | 0.7           |
| (1,12)   | 1:117:A:LEU:H | 1:150:A:GLY:H | 19       | 0.7           |
| (1,4620) | 1:14:A:VAL:H  | 1:120:A:HIS:O | 7        | 0.69          |
| (1,4580) | 1:69:A:ARG:H  | 1:104:A:ILE:O | 8        | 0.69          |
| (1,4548) | 1:33:A:GLY:H  | 1:96:A:ASP:O  | 17       | 0.69          |
| (1,4537) | 1:40:A:GLU:O  | 1:92:A:ASP:H  | 1        | 0.69          |
| (1,4525) | 1:44:A:GLY:O  | 1:85:A:GLY:H  | 3        | 0.69          |
| (1,4525) | 1:46:A:HIS:O  | 1:85:A:GLY:H  | 18       | 0.69          |
| (1,4481) | 1:56:A:GLY:H  | 1:146:A:CYS:O | 8        | 0.69          |

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| Key      | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|----------|---------------|---------------|----------|---------------|
| (1,4452) | 1:46:A:HIS:O  | 1:85:A:GLY:H  | 18       | 0.69          |
| (1,4396) | 1:21:A:GLU:H  | 1:30:A:LYS:O  | 9        | 0.69          |
| (1,119)  | 1:45:A:PHE:H  | 1:84:A:LEU:H  | 4        | 0.69          |
| (1,88)   | 1:15:A:GLN:H  | 1:35:A:ILE:H  | 16       | 0.69          |
| (1,4633) | 1:119:A:VAL:O | 1:144:A:LEU:H | 17       | 0.68          |
| (1,4632) | 1:121:A:GLU:H | 1:144:A:LEU:O | 10       | 0.68          |
| (1,4625) | 1:121:A:GLU:H | 1:144:A:LEU:O | 10       | 0.68          |
| (1,4619) | 1:42:A:LEU:N  | 1:120:A:HIS:O | 4        | 0.68          |
| (1,4578) | 1:75:A:LYS:O  | 1:103:A:VAL:N | 13       | 0.68          |
| (1,4537) | 1:38:A:LEU:O  | 1:92:A:ASP:H  | 19       | 0.68          |
| (1,4521) | 1:46:A:HIS:O  | 1:84:A:LEU:H  | 11       | 0.68          |
| (1,4503) | 1:76:A:ASP:O  | 1:103:A:VAL:N | 18       | 0.68          |
| (1,98)   | 1:120:A:HIS:H | 1:123:A:ALA:H | 13       | 0.68          |
| (1,91)   | 1:119:A:VAL:H | 1:121:A:GLU:H | 12       | 0.68          |
| (1,85)   | 1:8:A:LEU:H   | 1:15:A:GLN:H  | 2        | 0.68          |
| (1,84)   | 1:57:A:CYS:H  | 1:144:A:LEU:H | 5        | 0.68          |
| (1,35)   | 1:43:A:HIS:H  | 1:45:A:PHE:H  | 15       | 0.68          |
| (1,4660) | 1:5:A:VAL:H   | 1:151:A:ILE:O | 13       | 0.67          |
| (1,4629) | 1:57:A:CYS:O  | 1:143:A:ARG:H | 11       | 0.67          |
| (1,4581) | 1:21:A:GLU:O  | 1:104:A:ILE:H | 17       | 0.67          |
| (1,4533) | 1:41:A:GLY:O  | 1:91:A:LYS:H  | 7        | 0.67          |
| (1,4512) | 1:69:A:ARG:H  | 1:78:A:GLU:O  | 17       | 0.67          |
| (1,4510) | 1:77:A:GLU:N  | 1:104:A:ILE:O | 15       | 0.67          |
| (1,4501) | 1:69:A:ARG:O  | 1:75:A:LYS:H  | 9        | 0.67          |
| (1,4496) | 1:69:A:ARG:O  | 1:75:A:LYS:H  | 9        | 0.67          |
| (1,4484) | 1:57:A:CYS:O  | 1:143:A:ARG:H | 11       | 0.67          |
| (1,4479) | 1:56:A:GLY:O  | 1:147:A:GLY:N | 18       | 0.67          |
| (1,4469) | 1:50:A:PHE:H  | 1:114:A:GLY:O | 10       | 0.67          |
| (1,4436) | 1:41:A:GLY:O  | 1:91:A:LYS:H  | 7        | 0.67          |
| (1,4432) | 1:40:A:GLU:O  | 1:121:A:GLU:H | 9        | 0.67          |
| (1,91)   | 1:119:A:VAL:H | 1:121:A:GLU:H | 17       | 0.67          |
| (1,12)   | 1:117:A:LEU:H | 1:150:A:GLY:H | 2        | 0.67          |
| (1,12)   | 1:117:A:LEU:H | 1:150:A:GLY:H | 16       | 0.67          |
| (1,4577) | 1:21:A:GLU:O  | 1:103:A:VAL:H | 12       | 0.66          |
| (1,4503) | 1:76:A:ASP:O  | 1:103:A:VAL:N | 16       | 0.66          |
| (1,4479) | 1:56:A:GLY:O  | 1:143:A:ARG:N | 14       | 0.66          |
| (1,4468) | 1:50:A:PHE:O  | 1:116:A:THR:H | 12       | 0.66          |
| (1,4401) | 1:31:A:VAL:H  | 1:100:A:GLU:O | 2        | 0.66          |
| (1,11)   | 1:48:A:HIS:H  | 1:83:A:ASP:H  | 13       | 0.66          |
| (1,4625) | 1:41:A:GLY:O  | 1:121:A:GLU:H | 16       | 0.65          |
| (1,4579) | 1:78:A:GLU:N  | 1:104:A:ILE:O | 18       | 0.65          |
| (1,4577) | 1:21:A:GLU:O  | 1:103:A:VAL:H | 3        | 0.65          |

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| Key      | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|----------|---------------|---------------|----------|---------------|
| (1,4560) | 1:31:A:VAL:H  | 1:99:A:ILE:O  | 18       | 0.65          |
| (1,4496) | 1:69:A:ARG:O  | 1:78:A:GLU:H  | 14       | 0.65          |
| (1,4447) | 1:45:A:PHE:O  | 1:86:A:ASN:N  | 15       | 0.65          |
| (1,4436) | 1:41:A:GLY:O  | 1:121:A:GLU:H | 16       | 0.65          |
| (1,4388) | 1:2:A:THR:H   | 1:22:A:GLN:O  | 14       | 0.65          |
| (1,4325) | 1:2:A:THR:H   | 1:152:A:ALA:O | 11       | 0.65          |
| (1,4325) | 1:2:A:THR:H   | 1:22:A:GLN:O  | 14       | 0.65          |
| (1,98)   | 1:44:A:GLY:H  | 1:123:A:ALA:H | 7        | 0.65          |
| (1,88)   | 1:15:A:GLN:H  | 1:35:A:ILE:H  | 4        | 0.65          |
| (1,50)   | 1:120:A:HIS:H | 1:145:A:ALA:H | 12       | 0.65          |
| (1,26)   | 1:51:A:GLY:H  | 1:149:A:ILE:H | 16       | 0.65          |
| (1,4579) | 1:79:A:ARG:N  | 1:104:A:ILE:O | 3        | 0.64          |
| (1,4565) | 1:84:A:LEU:O  | 1:100:A:GLU:H | 17       | 0.64          |
| (1,4559) | 1:31:A:VAL:N  | 1:99:A:ILE:O  | 2        | 0.64          |
| (1,4559) | 1:31:A:VAL:N  | 1:99:A:ILE:O  | 6        | 0.64          |
| (1,4537) | 1:40:A:GLU:O  | 1:92:A:ASP:H  | 3        | 0.64          |
| (1,4507) | 1:68:A:SER:N  | 1:77:A:GLU:O  | 14       | 0.64          |
| (1,4504) | 1:76:A:ASP:O  | 1:101:A:ASP:H | 13       | 0.64          |
| (1,4496) | 1:69:A:ARG:O  | 1:79:A:ARG:H  | 17       | 0.64          |
| (1,4469) | 1:50:A:PHE:H  | 1:114:A:GLY:O | 8        | 0.64          |
| (1,4457) | 1:47:A:VAL:H  | 1:118:A:VAL:O | 14       | 0.64          |
| (1,4448) | 1:45:A:PHE:O  | 1:85:A:GLY:H  | 17       | 0.64          |
| (1,4428) | 1:39:A:THR:O  | 1:91:A:LYS:H  | 13       | 0.64          |
| (1,4405) | 1:17:A:ILE:O  | 1:32:A:TRP:H  | 1        | 0.64          |
| (1,4356) | 1:10:A:GLY:O  | 1:14:A:VAL:H  | 3        | 0.64          |
| (1,303)  | 1:69:A:ARG:H  | 1:82:A:GLY:H  | 12       | 0.64          |
| (1,276)  | 1:47:A:VAL:H  | 1:85:A:GLY:H  | 4        | 0.64          |
| (1,107)  | 1:45:A:PHE:H  | 1:119:A:VAL:H | 11       | 0.64          |
| (1,98)   | 1:120:A:HIS:H | 1:123:A:ALA:H | 5        | 0.64          |
| (1,4569) | 1:75:A:LYS:O  | 1:101:A:ASP:H | 2        | 0.63          |
| (1,4548) | 1:33:A:GLY:H  | 1:96:A:ASP:O  | 5        | 0.63          |
| (1,4525) | 1:85:A:GLY:H  | 1:98:A:SER:O  | 15       | 0.63          |
| (1,4509) | 1:77:A:GLU:H  | 1:101:A:ASP:O | 13       | 0.63          |
| (1,4507) | 1:77:A:GLU:O  | 1:84:A:LEU:N  | 13       | 0.63          |
| (1,4500) | 1:75:A:LYS:O  | 1:101:A:ASP:H | 2        | 0.63          |
| (1,4488) | 1:67:A:LEU:O  | 1:79:A:ARG:H  | 2        | 0.63          |
| (1,4479) | 1:56:A:GLY:O  | 1:146:A:CYS:N | 17       | 0.63          |
| (1,4405) | 1:18:A:ILE:O  | 1:32:A:TRP:H  | 8        | 0.63          |
| (1,4397) | 1:21:A:GLU:O  | 1:30:A:LYS:H  | 18       | 0.63          |
| (1,91)   | 1:119:A:VAL:H | 1:121:A:GLU:H | 11       | 0.63          |
| (1,88)   | 1:15:A:GLN:H  | 1:35:A:ILE:H  | 8        | 0.63          |
| (1,50)   | 1:120:A:HIS:H | 1:145:A:ALA:H | 6        | 0.63          |

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| Key      | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|----------|---------------|---------------|----------|---------------|
| (1,28)   | 1:149:A:ILE:H | 1:151:A:ILE:H | 12       | 0.63          |
| (1,26)   | 1:48:A:HIS:H  | 1:149:A:ILE:H | 15       | 0.63          |
| (1,16)   | 1:48:A:HIS:H  | 1:50:A:PHE:H  | 16       | 0.63          |
| (1,4628) | 1:57:A:CYS:H  | 1:143:A:ARG:O | 8        | 0.62          |
| (1,4620) | 1:42:A:LEU:H  | 1:120:A:HIS:O | 14       | 0.62          |
| (1,4619) | 1:42:A:LEU:N  | 1:120:A:HIS:O | 7        | 0.62          |
| (1,4593) | 1:113:A:ILE:H | 1:151:A:ILE:O | 16       | 0.62          |
| (1,4584) | 1:22:A:GLN:H  | 1:105:A:SER:O | 11       | 0.62          |
| (1,4559) | 1:31:A:VAL:N  | 1:99:A:ILE:O  | 18       | 0.62          |
| (1,4555) | 1:31:A:VAL:N  | 1:98:A:SER:O  | 12       | 0.62          |
| (1,4541) | 1:38:A:LEU:O  | 1:93:A:GLY:H  | 7        | 0.62          |
| (1,4532) | 1:39:A:THR:H  | 1:91:A:LYS:O  | 12       | 0.62          |
| (1,4513) | 1:67:A:LEU:O  | 1:78:A:GLU:H  | 15       | 0.62          |
| (1,4492) | 1:68:A:SER:O  | 1:79:A:ARG:H  | 4        | 0.62          |
| (1,4489) | 1:67:A:LEU:H  | 1:79:A:ARG:O  | 4        | 0.62          |
| (1,4485) | 1:57:A:CYS:H  | 1:143:A:ARG:O | 8        | 0.62          |
| (1,4477) | 1:55:A:ALA:H  | 1:146:A:CYS:O | 18       | 0.62          |
| (1,4476) | 1:55:A:ALA:O  | 1:146:A:CYS:H | 19       | 0.62          |
| (1,4325) | 1:2:A:THR:H   | 1:20:A:PHE:O  | 10       | 0.62          |
| (1,91)   | 1:119:A:VAL:H | 1:121:A:GLU:H | 10       | 0.62          |
| (1,4632) | 1:121:A:GLU:H | 1:144:A:LEU:O | 19       | 0.61          |
| (1,4625) | 1:121:A:GLU:H | 1:144:A:LEU:O | 19       | 0.61          |
| (1,4619) | 1:46:A:HIS:N  | 1:120:A:HIS:O | 15       | 0.61          |
| (1,4536) | 1:39:A:THR:H  | 1:92:A:ASP:O  | 14       | 0.61          |
| (1,4532) | 1:39:A:THR:H  | 1:91:A:LYS:O  | 7        | 0.61          |
| (1,4505) | 1:76:A:ASP:H  | 1:102:A:SER:O | 7        | 0.61          |
| (1,4463) | 1:49:A:GLU:O  | 1:68:A:SER:N  | 8        | 0.61          |
| (1,4433) | 1:40:A:GLU:H  | 1:121:A:GLU:O | 16       | 0.61          |
| (1,4433) | 1:40:A:GLU:H  | 1:121:A:GLU:O | 19       | 0.61          |
| (1,4429) | 1:39:A:THR:H  | 1:91:A:LYS:O  | 7        | 0.61          |
| (1,4428) | 1:39:A:THR:O  | 1:91:A:LYS:H  | 4        | 0.61          |
| (1,4405) | 1:18:A:ILE:O  | 1:32:A:TRP:H  | 2        | 0.61          |
| (1,303)  | 1:49:A:GLU:H  | 1:82:A:GLY:H  | 17       | 0.61          |
| (1,176)  | 1:86:A:ASN:H  | 1:88:A:THR:H  | 9        | 0.61          |
| (1,98)   | 1:120:A:HIS:H | 1:123:A:ALA:H | 12       | 0.61          |
| (1,91)   | 1:119:A:VAL:H | 1:121:A:GLU:H | 6        | 0.61          |
| (1,79)   | 1:119:A:VAL:H | 1:144:A:LEU:H | 6        | 0.61          |
| (1,28)   | 1:149:A:ILE:H | 1:151:A:ILE:H | 17       | 0.61          |
| (1,28)   | 1:149:A:ILE:H | 1:151:A:ILE:H | 18       | 0.61          |
| (1,4629) | 1:57:A:CYS:O  | 1:143:A:ARG:H | 9        | 0.6           |
| (1,4619) | 1:42:A:LEU:N  | 1:120:A:HIS:O | 14       | 0.6           |
| (1,4583) | 1:105:A:SER:O | 1:112:A:ILE:N | 10       | 0.6           |

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| Key      | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|----------|---------------|---------------|----------|---------------|
| (1,4576) | 1:29:A:VAL:H  | 1:103:A:VAL:O | 15       | 0.6           |
| (1,4555) | 1:86:A:ASN:N  | 1:98:A:SER:O  | 10       | 0.6           |
| (1,4497) | 1:69:A:ARG:H  | 1:79:A:ARG:O  | 13       | 0.6           |
| (1,4484) | 1:57:A:CYS:O  | 1:143:A:ARG:H | 9        | 0.6           |
| (1,4479) | 1:56:A:GLY:O  | 1:147:A:GLY:N | 19       | 0.6           |
| (1,4470) | 1:50:A:PHE:N  | 1:113:A:ILE:O | 11       | 0.6           |
| (1,4460) | 1:48:A:HIS:O  | 1:116:A:THR:H | 18       | 0.6           |
| (1,4397) | 1:21:A:GLU:O  | 1:30:A:LYS:H  | 8        | 0.6           |
| (1,4384) | 1:21:A:GLU:O  | 1:30:A:LYS:H  | 8        | 0.6           |
| (1,176)  | 1:86:A:ASN:H  | 1:88:A:THR:H  | 16       | 0.6           |
| (1,107)  | 1:46:A:HIS:H  | 1:119:A:VAL:H | 5        | 0.6           |
| (1,36)   | 1:42:A:LEU:H  | 1:45:A:PHE:H  | 18       | 0.6           |
| (1,28)   | 1:149:A:ILE:H | 1:151:A:ILE:H | 4        | 0.6           |
| (1,16)   | 1:48:A:HIS:H  | 1:50:A:PHE:H  | 18       | 0.6           |
| (1,4629) | 1:57:A:CYS:O  | 1:143:A:ARG:H | 6        | 0.59          |
| (1,4621) | 1:120:A:HIS:H | 1:145:A:ALA:O | 2        | 0.59          |
| (1,4575) | 1:77:A:GLU:N  | 1:103:A:VAL:O | 4        | 0.59          |
| (1,4560) | 1:86:A:ASN:H  | 1:99:A:ILE:O  | 15       | 0.59          |
| (1,4547) | 1:33:A:GLY:N  | 1:96:A:ASP:O  | 17       | 0.59          |
| (1,4489) | 1:49:A:GLU:O  | 1:67:A:LEU:H  | 15       | 0.59          |
| (1,4484) | 1:57:A:CYS:O  | 1:143:A:ARG:H | 6        | 0.59          |
| (1,4477) | 1:55:A:ALA:H  | 1:146:A:CYS:O | 15       | 0.59          |
| (1,4464) | 1:49:A:GLU:O  | 1:67:A:LEU:H  | 15       | 0.59          |
| (1,4388) | 1:2:A:THR:H   | 1:22:A:GLN:O  | 16       | 0.59          |
| (1,4325) | 1:2:A:THR:H   | 1:20:A:PHE:O  | 13       | 0.59          |
| (1,176)  | 1:86:A:ASN:H  | 1:88:A:THR:H  | 8        | 0.59          |
| (1,120)  | 1:149:A:ILE:H | 1:151:A:ILE:H | 9        | 0.59          |
| (1,50)   | 1:120:A:HIS:H | 1:145:A:ALA:H | 19       | 0.59          |
| (1,28)   | 1:149:A:ILE:H | 1:151:A:ILE:H | 9        | 0.59          |
| (1,12)   | 1:53:A:ASN:H  | 1:117:A:LEU:H | 1        | 0.59          |
| (1,4625) | 1:38:A:LEU:O  | 1:121:A:GLU:H | 9        | 0.58          |
| (1,4585) | 1:76:A:ASP:O  | 1:105:A:SER:H | 3        | 0.58          |
| (1,4572) | 1:77:A:GLU:H  | 1:102:A:SER:O | 5        | 0.58          |
| (1,4512) | 1:78:A:GLU:O  | 1:105:A:SER:H | 7        | 0.58          |
| (1,4509) | 1:77:A:GLU:H  | 1:102:A:SER:O | 5        | 0.58          |
| (1,4508) | 1:69:A:ARG:H  | 1:77:A:GLU:O  | 12       | 0.58          |
| (1,4504) | 1:76:A:ASP:O  | 1:105:A:SER:H | 3        | 0.58          |
| (1,4496) | 1:69:A:ARG:O  | 1:79:A:ARG:H  | 15       | 0.58          |
| (1,4457) | 1:47:A:VAL:H  | 1:118:A:VAL:O | 16       | 0.58          |
| (1,4436) | 1:41:A:GLY:O  | 1:91:A:LYS:H  | 2        | 0.58          |
| (1,4436) | 1:41:A:GLY:O  | 1:91:A:LYS:H  | 11       | 0.58          |
| (1,4388) | 1:2:A:THR:H   | 1:22:A:GLN:O  | 7        | 0.58          |

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| Key      | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|----------|---------------|---------------|----------|---------------|
| (1,4325) | 1:2:A:THR:H   | 1:22:A:GLN:O  | 7        | 0.58          |
| (1,91)   | 1:119:A:VAL:H | 1:121:A:GLU:H | 18       | 0.58          |
| (1,28)   | 1:118:A:VAL:H | 1:149:A:ILE:H | 19       | 0.58          |
| (1,12)   | 1:117:A:LEU:H | 1:150:A:GLY:H | 5        | 0.58          |
| (1,4621) | 1:44:A:GLY:O  | 1:120:A:HIS:H | 3        | 0.57          |
| (1,4621) | 1:44:A:GLY:O  | 1:120:A:HIS:H | 16       | 0.57          |
| (1,4592) | 1:113:A:ILE:O | 1:151:A:ILE:H | 18       | 0.57          |
| (1,4581) | 1:75:A:LYS:O  | 1:104:A:ILE:H | 3        | 0.57          |
| (1,4552) | 1:33:A:GLY:H  | 1:97:A:VAL:O  | 13       | 0.57          |
| (1,4548) | 1:33:A:GLY:H  | 1:96:A:ASP:O  | 9        | 0.57          |
| (1,4547) | 1:33:A:GLY:N  | 1:96:A:ASP:O  | 5        | 0.57          |
| (1,4532) | 1:40:A:GLU:H  | 1:91:A:LYS:O  | 11       | 0.57          |
| (1,4532) | 1:39:A:THR:H  | 1:91:A:LYS:O  | 15       | 0.57          |
| (1,4532) | 1:39:A:THR:H  | 1:91:A:LYS:O  | 17       | 0.57          |
| (1,4509) | 1:69:A:ARG:O  | 1:77:A:GLU:H  | 16       | 0.57          |
| (1,4485) | 1:57:A:CYS:H  | 1:146:A:CYS:O | 15       | 0.57          |
| (1,4477) | 1:9:A:LYS:O   | 1:55:A:ALA:H  | 3        | 0.57          |
| (1,4448) | 1:45:A:PHE:O  | 1:118:A:VAL:H | 5        | 0.57          |
| (1,4444) | 1:44:A:GLY:O  | 1:120:A:HIS:H | 3        | 0.57          |
| (1,4444) | 1:44:A:GLY:O  | 1:120:A:HIS:H | 16       | 0.57          |
| (1,4433) | 1:40:A:GLU:H  | 1:91:A:LYS:O  | 11       | 0.57          |
| (1,4429) | 1:39:A:THR:H  | 1:91:A:LYS:O  | 15       | 0.57          |
| (1,4405) | 1:17:A:ILE:O  | 1:32:A:TRP:H  | 7        | 0.57          |
| (1,303)  | 1:49:A:GLU:H  | 1:82:A:GLY:H  | 4        | 0.57          |
| (1,176)  | 1:86:A:ASN:H  | 1:88:A:THR:H  | 6        | 0.57          |
| (1,26)   | 1:51:A:GLY:H  | 1:149:A:ILE:H | 10       | 0.57          |
| (1,4620) | 1:45:A:PHE:H  | 1:120:A:HIS:O | 11       | 0.56          |
| (1,4592) | 1:50:A:PHE:H  | 1:113:A:ILE:O | 4        | 0.56          |
| (1,4591) | 1:113:A:ILE:O | 1:150:A:GLY:N | 11       | 0.56          |
| (1,4559) | 1:86:A:ASN:N  | 1:99:A:ILE:O  | 15       | 0.56          |
| (1,4504) | 1:76:A:ASP:O  | 1:102:A:SER:H | 14       | 0.56          |
| (1,4499) | 1:75:A:LYS:O  | 1:101:A:ASP:N | 11       | 0.56          |
| (1,4481) | 1:56:A:GLY:H  | 1:146:A:CYS:O | 7        | 0.56          |
| (1,4479) | 1:56:A:GLY:O  | 1:147:A:GLY:N | 3        | 0.56          |
| (1,4437) | 1:41:A:GLY:H  | 1:121:A:GLU:O | 15       | 0.56          |
| (1,4435) | 1:41:A:GLY:O  | 1:91:A:LYS:N  | 12       | 0.56          |
| (1,4428) | 1:39:A:THR:O  | 1:91:A:LYS:H  | 9        | 0.56          |
| (1,4392) | 1:29:A:VAL:O  | 1:101:A:ASP:H | 7        | 0.56          |
| (1,4325) | 1:2:A:THR:H   | 1:20:A:PHE:O  | 15       | 0.56          |
| (1,169)  | 1:49:A:GLU:H  | 1:111:A:SER:H | 19       | 0.56          |
| (1,85)   | 1:8:A:LEU:H   | 1:15:A:GLN:H  | 9        | 0.56          |
| (1,84)   | 1:120:A:HIS:H | 1:144:A:LEU:H | 15       | 0.56          |

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| Key      | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|----------|---------------|---------------|----------|---------------|
| (1,84)   | 1:57:A:CYS:H  | 1:144:A:LEU:H | 19       | 0.56          |
| (1,50)   | 1:120:A:HIS:H | 1:145:A:ALA:H | 16       | 0.56          |
| (1,35)   | 1:43:A:HIS:H  | 1:45:A:PHE:H  | 14       | 0.56          |
| (1,28)   | 1:149:A:ILE:H | 1:151:A:ILE:H | 16       | 0.56          |
| (1,4561) | 1:31:A:VAL:O  | 1:99:A:ILE:H  | 8        | 0.55          |
| (1,4551) | 1:33:A:GLY:N  | 1:97:A:VAL:O  | 13       | 0.55          |
| (1,4520) | 1:75:A:LYS:H  | 1:84:A:LEU:O  | 5        | 0.55          |
| (1,4501) | 1:75:A:LYS:H  | 1:84:A:LEU:O  | 5        | 0.55          |
| (1,4501) | 1:75:A:LYS:H  | 1:101:A:ASP:O | 18       | 0.55          |
| (1,4492) | 1:68:A:SER:O  | 1:79:A:ARG:H  | 14       | 0.55          |
| (1,4428) | 1:39:A:THR:O  | 1:121:A:GLU:H | 5        | 0.55          |
| (1,4397) | 1:21:A:GLU:O  | 1:30:A:LYS:H  | 14       | 0.55          |
| (1,4356) | 1:10:A:GLY:O  | 1:14:A:VAL:H  | 15       | 0.55          |
| (1,169)  | 1:49:A:GLU:H  | 1:83:A:ASP:H  | 5        | 0.55          |
| (1,169)  | 1:49:A:GLU:H  | 1:111:A:SER:H | 8        | 0.55          |
| (1,85)   | 1:8:A:LEU:H   | 1:15:A:GLN:H  | 4        | 0.55          |
| (1,4629) | 1:57:A:CYS:O  | 1:143:A:ARG:H | 4        | 0.54          |
| (1,4625) | 1:121:A:GLU:H | 1:144:A:LEU:O | 14       | 0.54          |
| (1,4547) | 1:86:A:ASN:N  | 1:96:A:ASP:O  | 11       | 0.54          |
| (1,4537) | 1:38:A:LEU:O  | 1:92:A:ASP:H  | 9        | 0.54          |
| (1,4505) | 1:76:A:ASP:H  | 1:101:A:ASP:O | 2        | 0.54          |
| (1,4501) | 1:75:A:LYS:H  | 1:84:A:LEU:O  | 14       | 0.54          |
| (1,4484) | 1:57:A:CYS:O  | 1:143:A:ARG:H | 4        | 0.54          |
| (1,4464) | 1:49:A:GLU:O  | 1:116:A:THR:H | 2        | 0.54          |
| (1,4405) | 1:18:A:ILE:O  | 1:32:A:TRP:H  | 15       | 0.54          |
| (1,4405) | 1:17:A:ILE:O  | 1:32:A:TRP:H  | 19       | 0.54          |
| (1,176)  | 1:86:A:ASN:H  | 1:88:A:THR:H  | 5        | 0.54          |
| (1,120)  | 1:3:A:LYS:H   | 1:151:A:ILE:H | 18       | 0.54          |
| (1,96)   | 1:15:A:GLN:H  | 1:38:A:LEU:H  | 9        | 0.54          |
| (1,88)   | 1:15:A:GLN:H  | 1:35:A:ILE:H  | 7        | 0.54          |
| (1,28)   | 1:149:A:ILE:H | 1:151:A:ILE:H | 1        | 0.54          |
| (1,4659) | 1:5:A:VAL:N   | 1:151:A:ILE:O | 13       | 0.53          |
| (1,4625) | 1:40:A:GLU:O  | 1:121:A:GLU:H | 4        | 0.53          |
| (1,4591) | 1:113:A:ILE:O | 1:150:A:GLY:N | 1        | 0.53          |
| (1,4580) | 1:76:A:ASP:H  | 1:104:A:ILE:O | 12       | 0.53          |
| (1,4573) | 1:75:A:LYS:O  | 1:102:A:SER:H | 14       | 0.53          |
| (1,4530) | 1:44:A:GLY:O  | 1:86:A:ASN:N  | 9        | 0.53          |
| (1,4513) | 1:78:A:GLU:H  | 1:102:A:SER:O | 17       | 0.53          |
| (1,4505) | 1:76:A:ASP:H  | 1:104:A:ILE:O | 12       | 0.53          |
| (1,4500) | 1:75:A:LYS:O  | 1:102:A:SER:H | 14       | 0.53          |
| (1,4497) | 1:69:A:ARG:H  | 1:78:A:GLU:O  | 19       | 0.53          |
| (1,4479) | 1:56:A:GLY:O  | 1:147:A:GLY:N | 7        | 0.53          |

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| Key      | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|----------|---------------|---------------|----------|---------------|
| (1,4456) | 1:47:A:VAL:O  | 1:118:A:VAL:H | 1        | 0.53          |
| (1,4435) | 1:41:A:GLY:O  | 1:121:A:GLU:N | 5        | 0.53          |
| (1,4432) | 1:40:A:GLU:O  | 1:121:A:GLU:H | 4        | 0.53          |
| (1,4404) | 1:18:A:ILE:H  | 1:32:A:TRP:O  | 12       | 0.53          |
| (1,4404) | 1:18:A:ILE:H  | 1:32:A:TRP:O  | 16       | 0.53          |
| (1,4356) | 1:10:A:GLY:O  | 1:14:A:VAL:H  | 8        | 0.53          |
| (1,4356) | 1:10:A:GLY:O  | 1:14:A:VAL:H  | 14       | 0.53          |
| (1,176)  | 1:86:A:ASN:H  | 1:88:A:THR:H  | 13       | 0.53          |
| (1,91)   | 1:15:A:GLN:H  | 1:121:A:GLU:H | 15       | 0.53          |
| (1,50)   | 1:120:A:HIS:H | 1:145:A:ALA:H | 13       | 0.53          |
| (1,4577) | 1:75:A:LYS:O  | 1:103:A:VAL:H | 8        | 0.52          |
| (1,4526) | 1:46:A:HIS:O  | 1:85:A:GLY:N  | 18       | 0.52          |
| (1,4500) | 1:75:A:LYS:O  | 1:103:A:VAL:H | 8        | 0.52          |
| (1,4490) | 1:67:A:LEU:N  | 1:77:A:GLU:O  | 6        | 0.52          |
| (1,4464) | 1:49:A:GLU:O  | 1:116:A:THR:H | 11       | 0.52          |
| (1,4459) | 1:48:A:HIS:O  | 1:118:A:VAL:N | 1        | 0.52          |
| (1,4457) | 1:47:A:VAL:H  | 1:118:A:VAL:O | 4        | 0.52          |
| (1,4593) | 1:113:A:ILE:H | 1:151:A:ILE:O | 2        | 0.51          |
| (1,4582) | 1:21:A:GLU:O  | 1:104:A:ILE:N | 13       | 0.51          |
| (1,4573) | 1:75:A:LYS:O  | 1:102:A:SER:H | 12       | 0.51          |
| (1,4552) | 1:33:A:GLY:H  | 1:97:A:VAL:O  | 15       | 0.51          |
| (1,4552) | 1:33:A:GLY:H  | 1:97:A:VAL:O  | 19       | 0.51          |
| (1,4513) | 1:68:A:SER:O  | 1:78:A:GLU:H  | 9        | 0.51          |
| (1,4500) | 1:75:A:LYS:O  | 1:102:A:SER:H | 5        | 0.51          |
| (1,4491) | 1:68:A:SER:O  | 1:78:A:GLU:N  | 14       | 0.51          |
| (1,4397) | 1:30:A:LYS:H  | 1:99:A:ILE:O  | 11       | 0.51          |
| (1,4355) | 1:10:A:GLY:O  | 1:14:A:VAL:N  | 5        | 0.51          |
| (1,176)  | 1:86:A:ASN:H  | 1:88:A:THR:H  | 17       | 0.51          |
| (1,4633) | 1:119:A:VAL:O | 1:144:A:LEU:H | 7        | 0.5           |
| (1,4629) | 1:57:A:CYS:O  | 1:143:A:ARG:H | 1        | 0.5           |
| (1,4629) | 1:57:A:CYS:O  | 1:143:A:ARG:H | 19       | 0.5           |
| (1,4591) | 1:50:A:PHE:N  | 1:113:A:ILE:O | 6        | 0.5           |
| (1,4589) | 1:112:A:ILE:H | 1:151:A:ILE:O | 2        | 0.5           |
| (1,4577) | 1:84:A:LEU:O  | 1:103:A:VAL:H | 10       | 0.5           |
| (1,4560) | 1:85:A:GLY:H  | 1:99:A:ILE:O  | 13       | 0.5           |
| (1,4532) | 1:39:A:THR:H  | 1:91:A:LYS:O  | 13       | 0.5           |
| (1,4516) | 1:68:A:SER:H  | 1:79:A:ARG:O  | 8        | 0.5           |
| (1,4511) | 1:69:A:ARG:N  | 1:78:A:GLU:O  | 13       | 0.5           |
| (1,4501) | 1:75:A:LYS:H  | 1:102:A:SER:O | 4        | 0.5           |
| (1,4484) | 1:57:A:CYS:O  | 1:143:A:ARG:H | 1        | 0.5           |
| (1,4484) | 1:57:A:CYS:O  | 1:143:A:ARG:H | 19       | 0.5           |
| (1,4443) | 1:44:A:GLY:O  | 1:120:A:HIS:N | 16       | 0.5           |

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| Key      | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|----------|---------------|---------------|----------|---------------|
| (1,4429) | 1:39:A:THR:H  | 1:91:A:LYS:O  | 13       | 0.5           |
| (1,4405) | 1:18:A:ILE:O  | 1:32:A:TRP:H  | 6        | 0.5           |
| (1,4396) | 1:21:A:GLU:H  | 1:30:A:LYS:O  | 13       | 0.5           |
| (1,4388) | 1:2:A:THR:H   | 1:22:A:GLN:O  | 12       | 0.5           |
| (1,4356) | 1:10:A:GLY:O  | 1:14:A:VAL:H  | 10       | 0.5           |
| (1,4325) | 1:2:A:THR:H   | 1:22:A:GLN:O  | 12       | 0.5           |
| (1,276)  | 1:85:A:GLY:H  | 1:99:A:ILE:H  | 16       | 0.5           |
| (1,98)   | 1:120:A:HIS:H | 1:123:A:ALA:H | 18       | 0.5           |
| (1,50)   | 1:120:A:HIS:H | 1:145:A:ALA:H | 4        | 0.5           |
| (1,4621) | 1:44:A:GLY:O  | 1:120:A:HIS:H | 17       | 0.49          |
| (1,4620) | 1:42:A:LEU:H  | 1:120:A:HIS:O | 3        | 0.49          |
| (1,4576) | 1:29:A:VAL:H  | 1:103:A:VAL:O | 1        | 0.49          |
| (1,4548) | 1:33:A:GLY:H  | 1:96:A:ASP:O  | 14       | 0.49          |
| (1,4547) | 1:33:A:GLY:N  | 1:96:A:ASP:O  | 9        | 0.49          |
| (1,4508) | 1:77:A:GLU:O  | 1:102:A:SER:H | 17       | 0.49          |
| (1,4503) | 1:76:A:ASP:O  | 1:105:A:SER:N | 19       | 0.49          |
| (1,4493) | 1:68:A:SER:H  | 1:76:A:ASP:O  | 9        | 0.49          |
| (1,4491) | 1:68:A:SER:O  | 1:79:A:ARG:N  | 4        | 0.49          |
| (1,4487) | 1:67:A:LEU:O  | 1:79:A:ARG:N  | 5        | 0.49          |
| (1,4477) | 1:55:A:ALA:H  | 1:146:A:CYS:O | 2        | 0.49          |
| (1,4463) | 1:49:A:GLU:O  | 1:67:A:LEU:N  | 15       | 0.49          |
| (1,4460) | 1:48:A:HIS:O  | 1:116:A:THR:H | 10       | 0.49          |
| (1,4428) | 1:39:A:THR:O  | 1:91:A:LYS:H  | 8        | 0.49          |
| (1,4428) | 1:39:A:THR:O  | 1:91:A:LYS:H  | 16       | 0.49          |
| (1,239)  | 1:131:A:ASN:H | 1:138:A:GLY:H | 17       | 0.49          |
| (1,120)  | 1:3:A:LYS:H   | 1:151:A:ILE:H | 12       | 0.49          |
| (1,98)   | 1:120:A:HIS:H | 1:123:A:ALA:H | 9        | 0.49          |
| (1,16)   | 1:48:A:HIS:H  | 1:50:A:PHE:H  | 3        | 0.49          |
| (1,4632) | 1:121:A:GLU:H | 1:144:A:LEU:O | 1        | 0.48          |
| (1,4590) | 1:112:A:ILE:N | 1:149:A:ILE:O | 15       | 0.48          |
| (1,4517) | 1:67:A:LEU:O  | 1:79:A:ARG:H  | 3        | 0.48          |
| (1,4502) | 1:44:A:GLY:O  | 1:75:A:LYS:N  | 6        | 0.48          |
| (1,4492) | 1:68:A:SER:O  | 1:79:A:ARG:H  | 10       | 0.48          |
| (1,4469) | 1:50:A:PHE:H  | 1:116:A:THR:O | 16       | 0.48          |
| (1,4435) | 1:41:A:GLY:O  | 1:91:A:LYS:N  | 17       | 0.48          |
| (1,4388) | 1:2:A:THR:H   | 1:22:A:GLN:O  | 18       | 0.48          |
| (1,239)  | 1:131:A:ASN:H | 1:138:A:GLY:H | 10       | 0.48          |
| (1,120)  | 1:149:A:ILE:H | 1:151:A:ILE:H | 11       | 0.48          |
| (1,120)  | 1:149:A:ILE:H | 1:151:A:ILE:H | 14       | 0.48          |
| (1,98)   | 1:44:A:GLY:H  | 1:123:A:ALA:H | 3        | 0.48          |
| (1,88)   | 1:15:A:GLN:H  | 1:35:A:ILE:H  | 13       | 0.48          |
| (1,85)   | 1:8:A:LEU:H   | 1:15:A:GLN:H  | 5        | 0.48          |

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| Key      | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|----------|---------------|---------------|----------|---------------|
| (1,28)   | 1:149:A:ILE:H | 1:151:A:ILE:H | 11       | 0.48          |
| (1,28)   | 1:149:A:ILE:H | 1:151:A:ILE:H | 14       | 0.48          |
| (1,4628) | 1:57:A:CYS:H  | 1:143:A:ARG:O | 10       | 0.47          |
| (1,4538) | 1:38:A:LEU:O  | 1:92:A:ASP:N  | 6        | 0.47          |
| (1,4537) | 1:38:A:LEU:O  | 1:92:A:ASP:H  | 4        | 0.47          |
| (1,4536) | 1:39:A:THR:H  | 1:92:A:ASP:O  | 17       | 0.47          |
| (1,4496) | 1:69:A:ARG:O  | 1:79:A:ARG:H  | 11       | 0.47          |
| (1,4496) | 1:69:A:ARG:O  | 1:78:A:GLU:H  | 19       | 0.47          |
| (1,4495) | 1:69:A:ARG:O  | 1:75:A:LYS:N  | 9        | 0.47          |
| (1,4492) | 1:68:A:SER:O  | 1:78:A:GLU:H  | 3        | 0.47          |
| (1,4489) | 1:67:A:LEU:H  | 1:79:A:ARG:O  | 1        | 0.47          |
| (1,4481) | 1:56:A:GLY:H  | 1:146:A:CYS:O | 15       | 0.47          |
| (1,4455) | 1:47:A:VAL:O  | 1:118:A:VAL:N | 1        | 0.47          |
| (1,4429) | 1:39:A:THR:H  | 1:92:A:ASP:O  | 17       | 0.47          |
| (1,4401) | 1:31:A:VAL:H  | 1:100:A:GLU:O | 18       | 0.47          |
| (1,4388) | 1:22:A:GLN:O  | 1:105:A:SER:H | 15       | 0.47          |
| (1,120)  | 1:149:A:ILE:H | 1:151:A:ILE:H | 6        | 0.47          |
| (1,119)  | 1:45:A:PHE:H  | 1:84:A:LEU:H  | 1        | 0.47          |
| (1,85)   | 1:8:A:LEU:H   | 1:15:A:GLN:H  | 3        | 0.47          |
| (1,28)   | 1:149:A:ILE:H | 1:151:A:ILE:H | 6        | 0.47          |
| (1,26)   | 1:48:A:HIS:H  | 1:149:A:ILE:H | 2        | 0.47          |
| (1,26)   | 1:48:A:HIS:H  | 1:149:A:ILE:H | 6        | 0.47          |
| (1,26)   | 1:48:A:HIS:H  | 1:149:A:ILE:H | 11       | 0.47          |
| (1,16)   | 1:48:A:HIS:H  | 1:50:A:PHE:H  | 10       | 0.47          |
| (1,16)   | 1:48:A:HIS:H  | 1:149:A:ILE:H | 11       | 0.47          |
| (1,12)   | 1:117:A:LEU:H | 1:150:A:GLY:H | 12       | 0.47          |
| (3,371)  | 1:132:A:GLU:N | 2:201:A:CU:CU | 15       | 0.46          |
| (1,4580) | 1:22:A:GLN:H  | 1:104:A:ILE:O | 10       | 0.46          |
| (1,4576) | 1:29:A:VAL:H  | 1:103:A:VAL:O | 8        | 0.46          |
| (1,4568) | 1:29:A:VAL:H  | 1:101:A:ASP:O | 1        | 0.46          |
| (1,4508) | 1:69:A:ARG:H  | 1:77:A:GLU:O  | 5        | 0.46          |
| (1,4503) | 1:76:A:ASP:O  | 1:101:A:ASP:N | 13       | 0.46          |
| (1,4498) | 1:69:A:ARG:N  | 1:79:A:ARG:O  | 13       | 0.46          |
| (1,4498) | 1:69:A:ARG:N  | 1:78:A:GLU:O  | 19       | 0.46          |
| (1,4490) | 1:67:A:LEU:N  | 1:79:A:ARG:O  | 16       | 0.46          |
| (1,4437) | 1:41:A:GLY:H  | 1:121:A:GLU:O | 6        | 0.46          |
| (1,4389) | 1:22:A:GLN:H  | 1:104:A:ILE:O | 10       | 0.46          |
| (1,270)  | 1:56:A:GLY:H  | 1:148:A:VAL:H | 4        | 0.46          |
| (1,176)  | 1:86:A:ASN:H  | 1:88:A:THR:H  | 1        | 0.46          |
| (1,50)   | 1:120:A:HIS:H | 1:145:A:ALA:H | 17       | 0.46          |
| (1,36)   | 1:45:A:PHE:H  | 1:85:A:GLY:H  | 10       | 0.46          |
| (3,184)  | 1:82:A:GLY:C  | 2:201:A:CU:CU | 11       | 0.45          |

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| Key      | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|----------|---------------|---------------|----------|---------------|
| (1,4628) | 1:57:A:CYS:H  | 1:143:A:ARG:O | 19       | 0.45          |
| (1,4608) | 1:48:A:HIS:H  | 1:117:A:LEU:O | 4        | 0.45          |
| (1,4596) | 1:114:A:GLY:O | 1:149:A:ILE:H | 16       | 0.45          |
| (1,4548) | 1:35:A:ILE:H  | 1:96:A:ASP:O  | 13       | 0.45          |
| (1,4540) | 1:36:A:LYS:H  | 1:93:A:GLY:O  | 15       | 0.45          |
| (1,4490) | 1:67:A:LEU:N  | 1:78:A:GLU:O  | 15       | 0.45          |
| (1,4489) | 1:67:A:LEU:H  | 1:79:A:ARG:O  | 17       | 0.45          |
| (1,4485) | 1:57:A:CYS:H  | 1:143:A:ARG:O | 19       | 0.45          |
| (1,4479) | 1:56:A:GLY:O  | 1:147:A:GLY:N | 10       | 0.45          |
| (1,4456) | 1:47:A:VAL:O  | 1:118:A:VAL:H | 17       | 0.45          |
| (1,4435) | 1:41:A:GLY:O  | 1:121:A:GLU:N | 8        | 0.45          |
| (1,4428) | 1:39:A:THR:O  | 1:92:A:ASP:H  | 15       | 0.45          |
| (1,4406) | 1:18:A:ILE:O  | 1:32:A:TRP:N  | 2        | 0.45          |
| (1,4404) | 1:18:A:ILE:H  | 1:32:A:TRP:O  | 9        | 0.45          |
| (1,181)  | 1:18:A:ILE:H  | 1:150:A:GLY:H | 13       | 0.45          |
| (1,85)   | 1:8:A:LEU:H   | 1:15:A:GLN:H  | 13       | 0.45          |
| (1,26)   | 1:51:A:GLY:H  | 1:149:A:ILE:H | 3        | 0.45          |
| (1,4633) | 1:119:A:VAL:O | 1:144:A:LEU:H | 4        | 0.44          |
| (1,4629) | 1:57:A:CYS:O  | 1:143:A:ARG:H | 17       | 0.44          |
| (1,4620) | 1:42:A:LEU:H  | 1:120:A:HIS:O | 17       | 0.44          |
| (1,4564) | 1:76:A:ASP:H  | 1:100:A:GLU:O | 17       | 0.44          |
| (1,4548) | 1:33:A:GLY:H  | 1:96:A:ASP:O  | 12       | 0.44          |
| (1,4536) | 1:40:A:GLU:H  | 1:92:A:ASP:O  | 13       | 0.44          |
| (1,4510) | 1:77:A:GLU:N  | 1:101:A:ASP:O | 18       | 0.44          |
| (1,4505) | 1:76:A:ASP:H  | 1:100:A:GLU:O | 17       | 0.44          |
| (1,4492) | 1:68:A:SER:O  | 1:78:A:GLU:H  | 19       | 0.44          |
| (1,4484) | 1:57:A:CYS:O  | 1:143:A:ARG:H | 17       | 0.44          |
| (1,4479) | 1:56:A:GLY:O  | 1:147:A:GLY:N | 16       | 0.44          |
| (1,4468) | 1:50:A:PHE:O  | 1:116:A:THR:H | 13       | 0.44          |
| (1,4465) | 1:49:A:GLU:H  | 1:116:A:THR:O | 5        | 0.44          |
| (1,4465) | 1:49:A:GLU:H  | 1:116:A:THR:O | 10       | 0.44          |
| (1,4465) | 1:49:A:GLU:H  | 1:116:A:THR:O | 12       | 0.44          |
| (1,4444) | 1:44:A:GLY:O  | 1:86:A:ASN:H  | 15       | 0.44          |
| (1,4441) | 1:42:A:LEU:H  | 1:121:A:GLU:O | 8        | 0.44          |
| (1,4433) | 1:40:A:GLU:H  | 1:121:A:GLU:O | 4        | 0.44          |
| (1,4405) | 1:32:A:TRP:H  | 1:98:A:SER:O  | 16       | 0.44          |
| (1,4395) | 1:30:A:LYS:O  | 1:99:A:ILE:N  | 9        | 0.44          |
| (1,4357) | 1:10:A:GLY:H  | 1:146:A:CYS:O | 16       | 0.44          |
| (1,4356) | 1:10:A:GLY:O  | 1:14:A:VAL:H  | 17       | 0.44          |
| (1,276)  | 1:85:A:GLY:H  | 1:99:A:ILE:H  | 15       | 0.44          |
| (1,169)  | 1:49:A:GLU:H  | 1:83:A:ASP:H  | 10       | 0.44          |
| (1,28)   | 1:149:A:ILE:H | 1:151:A:ILE:H | 7        | 0.44          |

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| Key      | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|----------|---------------|---------------|----------|---------------|
| (3,371)  | 1:132:A:GLU:N | 2:201:A:CU:CU | 7        | 0.43          |
| (1,4597) | 1:114:A:GLY:H | 1:149:A:ILE:O | 5        | 0.43          |
| (1,4593) | 1:113:A:ILE:H | 1:149:A:ILE:O | 8        | 0.43          |
| (1,4591) | 1:113:A:ILE:O | 1:151:A:ILE:N | 16       | 0.43          |
| (1,4585) | 1:76:A:ASP:O  | 1:105:A:SER:H | 10       | 0.43          |
| (1,4584) | 1:22:A:GLN:H  | 1:105:A:SER:O | 15       | 0.43          |
| (1,4559) | 1:85:A:GLY:N  | 1:99:A:ILE:O  | 8        | 0.43          |
| (1,4504) | 1:76:A:ASP:O  | 1:105:A:SER:H | 10       | 0.43          |
| (1,4449) | 1:45:A:PHE:H  | 1:85:A:GLY:O  | 7        | 0.43          |
| (1,4433) | 1:40:A:GLU:H  | 1:121:A:GLU:O | 6        | 0.43          |
| (1,4389) | 1:22:A:GLN:H  | 1:105:A:SER:O | 15       | 0.43          |
| (1,4356) | 1:10:A:GLY:O  | 1:14:A:VAL:H  | 2        | 0.43          |
| (1,4324) | 1:2:A:THR:O   | 1:21:A:GLU:H  | 4        | 0.43          |
| (1,303)  | 1:49:A:GLU:H  | 1:82:A:GLY:H  | 9        | 0.43          |
| (1,176)  | 1:86:A:ASN:H  | 1:88:A:THR:H  | 10       | 0.43          |
| (1,131)  | 1:50:A:PHE:H  | 1:60:A:ALA:H  | 4        | 0.43          |
| (1,36)   | 1:45:A:PHE:H  | 1:85:A:GLY:H  | 15       | 0.43          |
| (1,4625) | 1:40:A:GLU:O  | 1:121:A:GLU:H | 17       | 0.42          |
| (1,4538) | 1:39:A:THR:O  | 1:92:A:ASP:N  | 17       | 0.42          |
| (1,4512) | 1:69:A:ARG:H  | 1:78:A:GLU:O  | 18       | 0.42          |
| (1,4441) | 1:42:A:LEU:H  | 1:120:A:HIS:O | 18       | 0.42          |
| (1,4432) | 1:40:A:GLU:O  | 1:121:A:GLU:H | 17       | 0.42          |
| (1,181)  | 1:18:A:ILE:H  | 1:150:A:GLY:H | 5        | 0.42          |
| (1,176)  | 1:86:A:ASN:H  | 1:88:A:THR:H  | 11       | 0.42          |
| (1,131)  | 1:50:A:PHE:H  | 1:60:A:ALA:H  | 7        | 0.42          |
| (1,63)   | 1:41:A:GLY:H  | 1:90:A:ASP:H  | 3        | 0.42          |
| (1,35)   | 1:43:A:HIS:H  | 1:45:A:PHE:H  | 11       | 0.42          |
| (3,274)  | 1:120:A:HIS:C | 2:201:A:CU:CU | 4        | 0.41          |
| (3,198)  | 1:143:A:ARG:C | 2:201:A:CU:CU | 8        | 0.41          |
| (3,198)  | 1:143:A:ARG:C | 2:201:A:CU:CU | 9        | 0.41          |
| (1,4621) | 1:44:A:GLY:O  | 1:120:A:HIS:H | 1        | 0.41          |
| (1,4593) | 1:113:A:ILE:H | 1:149:A:ILE:O | 18       | 0.41          |
| (1,4547) | 1:33:A:GLY:N  | 1:96:A:ASP:O  | 14       | 0.41          |
| (1,4538) | 1:40:A:GLU:O  | 1:92:A:ASP:N  | 12       | 0.41          |
| (1,4510) | 1:68:A:SER:O  | 1:77:A:GLU:N  | 3        | 0.41          |
| (1,4508) | 1:69:A:ARG:H  | 1:77:A:GLU:O  | 3        | 0.41          |
| (1,4496) | 1:69:A:ARG:O  | 1:79:A:ARG:H  | 13       | 0.41          |
| (1,4489) | 1:67:A:LEU:H  | 1:79:A:ARG:O  | 7        | 0.41          |
| (1,4476) | 1:55:A:ALA:O  | 1:146:A:CYS:H | 8        | 0.41          |
| (1,4473) | 1:54:A:THR:H  | 1:147:A:GLY:O | 13       | 0.41          |
| (1,4464) | 1:49:A:GLU:O  | 1:116:A:THR:H | 6        | 0.41          |
| (1,4444) | 1:44:A:GLY:O  | 1:120:A:HIS:H | 1        | 0.41          |

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| Key      | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|----------|---------------|---------------|----------|---------------|
| (1,4401) | 1:31:A:VAL:H  | 1:100:A:GLU:O | 6        | 0.41          |
| (1,276)  | 1:47:A:VAL:H  | 1:85:A:GLY:H  | 12       | 0.41          |
| (1,217)  | 1:87:A:VAL:H  | 1:122:A:LYS:H | 9        | 0.41          |
| (1,176)  | 1:86:A:ASN:H  | 1:88:A:THR:H  | 3        | 0.41          |
| (1,132)  | 1:40:A:GLU:H  | 1:92:A:ASP:H  | 16       | 0.41          |
| (1,50)   | 1:120:A:HIS:H | 1:145:A:ALA:H | 11       | 0.41          |
| (1,28)   | 1:118:A:VAL:H | 1:149:A:ILE:H | 5        | 0.41          |
| (1,12)   | 1:53:A:ASN:H  | 1:117:A:LEU:H | 9        | 0.41          |
| (1,4628) | 1:57:A:CYS:H  | 1:143:A:ARG:O | 7        | 0.4           |
| (1,4626) | 1:38:A:LEU:O  | 1:121:A:GLU:N | 8        | 0.4           |
| (1,4621) | 1:44:A:GLY:O  | 1:120:A:HIS:H | 4        | 0.4           |
| (1,4583) | 1:105:A:SER:O | 1:112:A:ILE:N | 13       | 0.4           |
| (1,4576) | 1:29:A:VAL:H  | 1:103:A:VAL:O | 6        | 0.4           |
| (1,4569) | 1:29:A:VAL:O  | 1:101:A:ASP:H | 19       | 0.4           |
| (1,4512) | 1:69:A:ARG:H  | 1:78:A:GLU:O  | 15       | 0.4           |
| (1,4510) | 1:67:A:LEU:O  | 1:77:A:GLU:N  | 12       | 0.4           |
| (1,4508) | 1:69:A:ARG:H  | 1:77:A:GLU:O  | 8        | 0.4           |
| (1,4487) | 1:67:A:LEU:O  | 1:77:A:GLU:N  | 12       | 0.4           |
| (1,4486) | 1:57:A:CYS:N  | 1:146:A:CYS:O | 16       | 0.4           |
| (1,4481) | 1:56:A:GLY:H  | 1:146:A:CYS:O | 3        | 0.4           |
| (1,4479) | 1:56:A:GLY:O  | 1:147:A:GLY:N | 2        | 0.4           |
| (1,4444) | 1:44:A:GLY:O  | 1:120:A:HIS:H | 4        | 0.4           |
| (1,4435) | 1:41:A:GLY:O  | 1:121:A:GLU:N | 10       | 0.4           |
| (1,4401) | 1:31:A:VAL:H  | 1:98:A:SER:O  | 8        | 0.4           |
| (1,267)  | 1:33:A:GLY:H  | 1:35:A:ILE:H  | 7        | 0.4           |
| (1,217)  | 1:87:A:VAL:H  | 1:122:A:LYS:H | 1        | 0.4           |
| (1,180)  | 1:114:A:GLY:H | 1:150:A:GLY:H | 13       | 0.4           |
| (1,127)  | 1:70:A:LYS:H  | 1:78:A:GLU:H  | 11       | 0.4           |
| (3,198)  | 1:143:A:ARG:C | 2:201:A:CU:CU | 17       | 0.39          |
| (1,4621) | 1:45:A:PHE:O  | 1:120:A:HIS:H | 11       | 0.39          |
| (1,4586) | 1:76:A:ASP:O  | 1:105:A:SER:N | 2        | 0.39          |
| (1,4585) | 1:21:A:GLU:O  | 1:105:A:SER:H | 7        | 0.39          |
| (1,4575) | 1:84:A:LEU:N  | 1:103:A:VAL:O | 17       | 0.39          |
| (1,4561) | 1:31:A:VAL:O  | 1:99:A:ILE:H  | 1        | 0.39          |
| (1,4541) | 1:38:A:LEU:O  | 1:93:A:GLY:H  | 17       | 0.39          |
| (1,4536) | 1:39:A:THR:H  | 1:92:A:ASP:O  | 18       | 0.39          |
| (1,4505) | 1:76:A:ASP:H  | 1:101:A:ASP:O | 15       | 0.39          |
| (1,4501) | 1:75:A:LYS:H  | 1:101:A:ASP:O | 16       | 0.39          |
| (1,4447) | 1:45:A:PHE:O  | 1:118:A:VAL:N | 3        | 0.39          |
| (1,4429) | 1:39:A:THR:H  | 1:92:A:ASP:O  | 18       | 0.39          |
| (1,4424) | 1:38:A:LEU:O  | 1:93:A:GLY:H  | 17       | 0.39          |
| (1,4400) | 1:31:A:VAL:O  | 1:99:A:ILE:H  | 1        | 0.39          |

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| Key      | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|----------|---------------|---------------|----------|---------------|
| (1,292)  | 1:37:A:GLY:H  | 1:39:A:THR:H  | 8        | 0.39          |
| (1,119)  | 1:46:A:HIS:H  | 1:84:A:LEU:H  | 17       | 0.39          |
| (3,371)  | 1:132:A:GLU:N | 2:201:A:CU:CU | 11       | 0.38          |
| (3,198)  | 1:143:A:ARG:C | 2:201:A:CU:CU | 14       | 0.38          |
| (1,4629) | 1:57:A:CYS:O  | 1:143:A:ARG:H | 12       | 0.38          |
| (1,4591) | 1:113:A:ILE:O | 1:151:A:ILE:N | 15       | 0.38          |
| (1,4591) | 1:113:A:ILE:O | 1:151:A:ILE:N | 18       | 0.38          |
| (1,4584) | 1:22:A:GLN:H  | 1:105:A:SER:O | 1        | 0.38          |
| (1,4581) | 1:77:A:GLU:O  | 1:104:A:ILE:H | 18       | 0.38          |
| (1,4551) | 1:86:A:ASN:N  | 1:97:A:VAL:O  | 15       | 0.38          |
| (1,4548) | 1:33:A:GLY:H  | 1:96:A:ASP:O  | 10       | 0.38          |
| (1,4547) | 1:33:A:GLY:N  | 1:96:A:ASP:O  | 12       | 0.38          |
| (1,4508) | 1:77:A:GLU:O  | 1:104:A:ILE:H | 18       | 0.38          |
| (1,4485) | 1:57:A:CYS:H  | 1:117:A:LEU:O | 7        | 0.38          |
| (1,4484) | 1:57:A:CYS:O  | 1:143:A:ARG:H | 12       | 0.38          |
| (1,4479) | 1:56:A:GLY:O  | 1:147:A:GLY:N | 5        | 0.38          |
| (1,4468) | 1:50:A:PHE:O  | 1:116:A:THR:H | 10       | 0.38          |
| (1,4417) | 1:15:A:GLN:O  | 1:35:A:ILE:H  | 8        | 0.38          |
| (1,292)  | 1:37:A:GLY:H  | 1:39:A:THR:H  | 16       | 0.38          |
| (1,276)  | 1:47:A:VAL:H  | 1:85:A:GLY:H  | 9        | 0.38          |
| (3,252)  | 1:79:A:ARG:C  | 2:201:A:CU:CU | 8        | 0.37          |
| (3,198)  | 1:143:A:ARG:C | 2:201:A:CU:CU | 2        | 0.37          |
| (3,198)  | 1:143:A:ARG:C | 2:201:A:CU:CU | 6        | 0.37          |
| (1,4632) | 1:10:A:GLY:H  | 1:144:A:LEU:O | 15       | 0.37          |
| (1,4591) | 1:113:A:ILE:O | 1:150:A:GLY:N | 9        | 0.37          |
| (1,4591) | 1:113:A:ILE:O | 1:150:A:GLY:N | 19       | 0.37          |
| (1,4561) | 1:31:A:VAL:O  | 1:99:A:ILE:H  | 7        | 0.37          |
| (1,4552) | 1:33:A:GLY:H  | 1:97:A:VAL:O  | 6        | 0.37          |
| (1,4492) | 1:68:A:SER:O  | 1:79:A:ARG:H  | 18       | 0.37          |
| (1,4491) | 1:68:A:SER:O  | 1:78:A:GLU:N  | 19       | 0.37          |
| (1,4485) | 1:57:A:CYS:H  | 1:117:A:LEU:O | 1        | 0.37          |
| (1,4479) | 1:56:A:GLY:O  | 1:143:A:ARG:N | 1        | 0.37          |
| (1,4479) | 1:56:A:GLY:O  | 1:147:A:GLY:N | 15       | 0.37          |
| (1,4405) | 1:32:A:TRP:H  | 1:97:A:VAL:O  | 9        | 0.37          |
| (1,4401) | 1:31:A:VAL:H  | 1:100:A:GLU:O | 19       | 0.37          |
| (1,4400) | 1:31:A:VAL:O  | 1:99:A:ILE:H  | 7        | 0.37          |
| (1,4397) | 1:21:A:GLU:O  | 1:30:A:LYS:H  | 9        | 0.37          |
| (1,4356) | 1:10:A:GLY:O  | 1:14:A:VAL:H  | 9        | 0.37          |
| (1,4355) | 1:10:A:GLY:O  | 1:14:A:VAL:N  | 3        | 0.37          |
| (1,4324) | 1:2:A:THR:O   | 1:21:A:GLU:H  | 15       | 0.37          |
| (1,176)  | 1:86:A:ASN:H  | 1:88:A:THR:H  | 4        | 0.37          |
| (1,123)  | 1:22:A:GLN:H  | 1:106:A:LEU:H | 3        | 0.37          |

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| Key      | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|----------|---------------|---------------|----------|---------------|
| (1,88)   | 1:15:A:GLN:H  | 1:35:A:ILE:H  | 5        | 0.37          |
| (1,85)   | 1:8:A:LEU:H   | 1:15:A:GLN:H  | 14       | 0.37          |
| (1,63)   | 1:88:A:THR:H  | 1:90:A:ASP:H  | 19       | 0.37          |
| (1,35)   | 1:43:A:HIS:H  | 1:45:A:PHE:H  | 12       | 0.37          |
| (1,4632) | 1:9:A:LYS:H   | 1:144:A:LEU:O | 2        | 0.36          |
| (1,4632) | 1:10:A:GLY:H  | 1:144:A:LEU:O | 17       | 0.36          |
| (1,4580) | 1:22:A:GLN:H  | 1:104:A:ILE:O | 9        | 0.36          |
| (1,4557) | 1:86:A:ASN:O  | 1:98:A:SER:H  | 17       | 0.36          |
| (1,4556) | 1:31:A:VAL:H  | 1:98:A:SER:O  | 9        | 0.36          |
| (1,4509) | 1:77:A:GLU:H  | 1:102:A:SER:O | 14       | 0.36          |
| (1,4496) | 1:69:A:ARG:O  | 1:79:A:ARG:H  | 18       | 0.36          |
| (1,4486) | 1:57:A:CYS:N  | 1:143:A:ARG:O | 19       | 0.36          |
| (1,4477) | 1:55:A:ALA:H  | 1:146:A:CYS:O | 1        | 0.36          |
| (1,4463) | 1:49:A:GLU:O  | 1:116:A:THR:N | 2        | 0.36          |
| (1,4389) | 1:22:A:GLN:H  | 1:104:A:ILE:O | 9        | 0.36          |
| (1,4356) | 1:10:A:GLY:O  | 1:14:A:VAL:H  | 19       | 0.36          |
| (1,4355) | 1:10:A:GLY:O  | 1:14:A:VAL:N  | 4        | 0.36          |
| (1,146)  | 1:67:A:LEU:H  | 1:109:A:ASP:H | 3        | 0.36          |
| (1,120)  | 1:149:A:ILE:H | 1:151:A:ILE:H | 8        | 0.36          |
| (1,35)   | 1:43:A:HIS:H  | 1:45:A:PHE:H  | 2        | 0.36          |
| (1,28)   | 1:149:A:ILE:H | 1:151:A:ILE:H | 8        | 0.36          |
| (1,16)   | 1:48:A:HIS:H  | 1:50:A:PHE:H  | 8        | 0.36          |
| (3,198)  | 1:143:A:ARG:C | 2:201:A:CU:CU | 1        | 0.35          |
| (3,179)  | 1:46:A:HIS:C  | 2:201:A:CU:CU | 9        | 0.35          |
| (1,4620) | 1:42:A:LEU:H  | 1:120:A:HIS:O | 6        | 0.35          |
| (1,4565) | 1:29:A:VAL:O  | 1:100:A:GLU:H | 11       | 0.35          |
| (1,4530) | 1:44:A:GLY:O  | 1:86:A:ASN:N  | 4        | 0.35          |
| (1,4522) | 1:46:A:HIS:O  | 1:84:A:LEU:N  | 15       | 0.35          |
| (1,4522) | 1:45:A:PHE:O  | 1:84:A:LEU:N  | 17       | 0.35          |
| (1,4520) | 1:84:A:LEU:O  | 1:99:A:ILE:H  | 4        | 0.35          |
| (1,4477) | 1:55:A:ALA:H  | 1:146:A:CYS:O | 11       | 0.35          |
| (1,4474) | 1:54:A:THR:N  | 1:114:A:GLY:O | 8        | 0.35          |
| (1,4447) | 1:45:A:PHE:O  | 1:84:A:LEU:N  | 17       | 0.35          |
| (1,4433) | 1:40:A:GLU:H  | 1:121:A:GLU:O | 2        | 0.35          |
| (1,4417) | 1:15:A:GLN:O  | 1:35:A:ILE:H  | 13       | 0.35          |
| (1,4406) | 1:18:A:ILE:O  | 1:32:A:TRP:N  | 6        | 0.35          |
| (1,162)  | 1:67:A:LEU:H  | 1:70:A:LYS:H  | 14       | 0.35          |
| (1,119)  | 1:46:A:HIS:H  | 1:84:A:LEU:H  | 18       | 0.35          |
| (1,98)   | 1:120:A:HIS:H | 1:123:A:ALA:H | 1        | 0.35          |
| (1,48)   | 1:6:A:ALA:H   | 1:8:A:LEU:H   | 9        | 0.35          |
| (1,28)   | 1:149:A:ILE:H | 1:151:A:ILE:H | 2        | 0.35          |
| (3,274)  | 1:120:A:HIS:C | 2:201:A:CU:CU | 2        | 0.34          |

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| Key      | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|----------|---------------|---------------|----------|---------------|
| (3,274)  | 1:120:A:HIS:C | 2:201:A:CU:CU | 10       | 0.34          |
| (3,198)  | 1:143:A:ARG:C | 2:201:A:CU:CU | 10       | 0.34          |
| (3,179)  | 1:46:A:HIS:C  | 2:201:A:CU:CU | 4        | 0.34          |
| (1,4660) | 1:5:A:VAL:H   | 1:151:A:ILE:O | 3        | 0.34          |
| (1,4561) | 1:31:A:VAL:O  | 1:99:A:ILE:H  | 6        | 0.34          |
| (1,4538) | 1:39:A:THR:O  | 1:92:A:ASP:N  | 18       | 0.34          |
| (1,4528) | 1:44:A:GLY:H  | 1:86:A:ASN:O  | 11       | 0.34          |
| (1,4521) | 1:45:A:PHE:O  | 1:84:A:LEU:H  | 14       | 0.34          |
| (1,4493) | 1:68:A:SER:H  | 1:77:A:GLU:O  | 6        | 0.34          |
| (1,4401) | 1:31:A:VAL:H  | 1:97:A:VAL:O  | 4        | 0.34          |
| (1,4400) | 1:31:A:VAL:O  | 1:99:A:ILE:H  | 6        | 0.34          |
| (1,4396) | 1:21:A:GLU:H  | 1:30:A:LYS:O  | 12       | 0.34          |
| (1,4388) | 1:2:A:THR:H   | 1:22:A:GLN:O  | 2        | 0.34          |
| (1,4356) | 1:10:A:GLY:O  | 1:14:A:VAL:H  | 6        | 0.34          |
| (1,4325) | 1:2:A:THR:H   | 1:22:A:GLN:O  | 2        | 0.34          |
| (1,294)  | 1:37:A:GLY:H  | 1:40:A:GLU:H  | 10       | 0.34          |
| (1,276)  | 1:47:A:VAL:H  | 1:85:A:GLY:H  | 11       | 0.34          |
| (1,217)  | 1:87:A:VAL:H  | 1:122:A:LYS:H | 7        | 0.34          |
| (1,107)  | 1:46:A:HIS:H  | 1:119:A:VAL:H | 15       | 0.34          |
| (1,50)   | 1:118:A:VAL:H | 1:145:A:ALA:H | 5        | 0.34          |
| (1,20)   | 1:89:A:ALA:H  | 1:95:A:ALA:H  | 16       | 0.34          |
| (3,371)  | 1:132:A:GLU:N | 2:201:A:CU:CU | 14       | 0.33          |
| (3,198)  | 1:143:A:ARG:C | 2:201:A:CU:CU | 16       | 0.33          |
| (3,137)  | 1:80:A:HIS:N  | 2:201:A:CU:CU | 13       | 0.33          |
| (2,156)  | 1:106:A:LEU:N | 1:108:A:GLY:N | 5        | 0.33          |
| (1,4627) | 1:57:A:CYS:N  | 1:143:A:ARG:O | 7        | 0.33          |
| (1,4569) | 1:29:A:VAL:O  | 1:101:A:ASP:H | 8        | 0.33          |
| (1,4547) | 1:33:A:GLY:N  | 1:96:A:ASP:O  | 10       | 0.33          |
| (1,4501) | 1:75:A:LYS:H  | 1:102:A:SER:O | 10       | 0.33          |
| (1,4496) | 1:69:A:ARG:O  | 1:79:A:ARG:H  | 4        | 0.33          |
| (1,4490) | 1:67:A:LEU:N  | 1:79:A:ARG:O  | 11       | 0.33          |
| (1,4464) | 1:49:A:GLU:O  | 1:116:A:THR:H | 10       | 0.33          |
| (1,4463) | 1:49:A:GLU:O  | 1:116:A:THR:N | 6        | 0.33          |
| (1,4448) | 1:45:A:PHE:O  | 1:118:A:VAL:H | 10       | 0.33          |
| (1,4387) | 1:2:A:THR:N   | 1:22:A:GLN:O  | 9        | 0.33          |
| (1,4326) | 1:2:A:THR:N   | 1:22:A:GLN:O  | 9        | 0.33          |
| (1,239)  | 1:131:A:ASN:H | 1:138:A:GLY:H | 5        | 0.33          |
| (1,234)  | 1:131:A:ASN:H | 1:139:A:ASN:H | 11       | 0.33          |
| (1,120)  | 1:149:A:ILE:H | 1:151:A:ILE:H | 13       | 0.33          |
| (1,88)   | 1:15:A:GLN:H  | 1:35:A:ILE:H  | 1        | 0.33          |
| (1,85)   | 1:8:A:LEU:H   | 1:15:A:GLN:H  | 17       | 0.33          |
| (1,28)   | 1:149:A:ILE:H | 1:151:A:ILE:H | 13       | 0.33          |

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| Key      | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|----------|---------------|---------------|----------|---------------|
| (1,20)   | 1:89:A:ALA:H  | 1:95:A:ALA:H  | 2        | 0.33          |
| (3,371)  | 1:132:A:GLU:N | 2:201:A:CU:CU | 10       | 0.32          |
| (3,295)  | 1:9:A:LYS:N   | 2:201:A:CU:CU | 12       | 0.32          |
| (1,4620) | 1:42:A:LEU:H  | 1:120:A:HIS:O | 12       | 0.32          |
| (1,4619) | 1:44:A:GLY:N  | 1:120:A:HIS:O | 17       | 0.32          |
| (1,4593) | 1:113:A:ILE:H | 1:149:A:ILE:O | 11       | 0.32          |
| (1,4581) | 1:76:A:ASP:O  | 1:104:A:ILE:H | 2        | 0.32          |
| (1,4565) | 1:29:A:VAL:O  | 1:100:A:GLU:H | 10       | 0.32          |
| (1,4561) | 1:31:A:VAL:O  | 1:99:A:ILE:H  | 15       | 0.32          |
| (1,4560) | 1:86:A:ASN:H  | 1:99:A:ILE:O  | 16       | 0.32          |
| (1,4557) | 1:31:A:VAL:O  | 1:98:A:SER:H  | 3        | 0.32          |
| (1,4537) | 1:38:A:LEU:O  | 1:92:A:ASP:H  | 11       | 0.32          |
| (1,4530) | 1:45:A:PHE:O  | 1:86:A:ASN:N  | 14       | 0.32          |
| (1,4508) | 1:77:A:GLU:O  | 1:103:A:VAL:H | 1        | 0.32          |
| (1,4500) | 1:69:A:ARG:H  | 1:75:A:LYS:O  | 9        | 0.32          |
| (1,4497) | 1:69:A:ARG:H  | 1:78:A:GLU:O  | 8        | 0.32          |
| (1,4495) | 1:69:A:ARG:O  | 1:79:A:ARG:N  | 11       | 0.32          |
| (1,4487) | 1:49:A:GLU:N  | 1:67:A:LEU:O  | 8        | 0.32          |
| (1,4479) | 1:56:A:GLY:O  | 1:143:A:ARG:N | 12       | 0.32          |
| (1,4447) | 1:45:A:PHE:O  | 1:84:A:LEU:N  | 7        | 0.32          |
| (1,4437) | 1:41:A:GLY:H  | 1:121:A:GLU:O | 17       | 0.32          |
| (1,4435) | 1:41:A:GLY:O  | 1:91:A:LYS:N  | 18       | 0.32          |
| (1,4428) | 1:39:A:THR:O  | 1:91:A:LYS:H  | 19       | 0.32          |
| (1,4404) | 1:18:A:ILE:H  | 1:32:A:TRP:O  | 11       | 0.32          |
| (1,4400) | 1:31:A:VAL:O  | 1:99:A:ILE:H  | 15       | 0.32          |
| (1,4357) | 1:10:A:GLY:H  | 1:14:A:VAL:O  | 5        | 0.32          |
| (1,4108) | 1:142:A:SER:C | 1:145:A:ALA:C | 13       | 0.32          |
| (1,276)  | 1:47:A:VAL:H  | 1:85:A:GLY:H  | 10       | 0.32          |
| (1,276)  | 1:47:A:VAL:H  | 1:85:A:GLY:H  | 19       | 0.32          |
| (1,234)  | 1:131:A:ASN:H | 1:139:A:ASN:H | 15       | 0.32          |
| (1,217)  | 1:87:A:VAL:H  | 1:122:A:LYS:H | 16       | 0.32          |
| (1,195)  | 1:40:A:GLU:H  | 1:91:A:LYS:H  | 7        | 0.32          |
| (1,88)   | 1:15:A:GLN:H  | 1:35:A:ILE:H  | 14       | 0.32          |
| (1,84)   | 1:57:A:CYS:H  | 1:144:A:LEU:H | 7        | 0.32          |
| (1,53)   | 1:48:A:HIS:H  | 1:118:A:VAL:H | 11       | 0.32          |
| (1,35)   | 1:43:A:HIS:H  | 1:45:A:PHE:H  | 5        | 0.32          |
| (1,11)   | 1:48:A:HIS:H  | 1:83:A:ASP:H  | 16       | 0.32          |
| (3,319)  | 1:41:A:GLY:N  | 2:201:A:CU:CU | 19       | 0.31          |
| (3,198)  | 1:143:A:ARG:C | 2:201:A:CU:CU | 12       | 0.31          |
| (1,4625) | 1:38:A:LEU:O  | 1:121:A:GLU:H | 5        | 0.31          |
| (1,4589) | 1:50:A:PHE:O  | 1:112:A:ILE:H | 7        | 0.31          |
| (1,4585) | 1:21:A:GLU:O  | 1:105:A:SER:H | 18       | 0.31          |

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| Key      | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|----------|---------------|---------------|----------|---------------|
| (1,4577) | 1:75:A:LYS:O  | 1:103:A:VAL:H | 16       | 0.31          |
| (1,4576) | 1:29:A:VAL:H  | 1:103:A:VAL:O | 16       | 0.31          |
| (1,4540) | 1:36:A:LYS:H  | 1:93:A:GLY:O  | 3        | 0.31          |
| (1,4537) | 1:40:A:GLU:O  | 1:92:A:ASP:H  | 2        | 0.31          |
| (1,4533) | 1:40:A:GLU:O  | 1:91:A:LYS:H  | 11       | 0.31          |
| (1,4512) | 1:67:A:LEU:H  | 1:78:A:GLU:O  | 19       | 0.31          |
| (1,4509) | 1:77:A:GLU:H  | 1:101:A:ASP:O | 6        | 0.31          |
| (1,4493) | 1:68:A:SER:H  | 1:79:A:ARG:O  | 13       | 0.31          |
| (1,4489) | 1:67:A:LEU:H  | 1:78:A:GLU:O  | 19       | 0.31          |
| (1,4487) | 1:67:A:LEU:O  | 1:79:A:ARG:N  | 2        | 0.31          |
| (1,4475) | 1:55:A:ALA:O  | 1:143:A:ARG:N | 2        | 0.31          |
| (1,4464) | 1:49:A:GLU:O  | 1:116:A:THR:H | 19       | 0.31          |
| (1,4437) | 1:41:A:GLY:H  | 1:121:A:GLU:O | 9        | 0.31          |
| (1,4432) | 1:40:A:GLU:O  | 1:91:A:LYS:H  | 11       | 0.31          |
| (1,4384) | 1:21:A:GLU:O  | 1:105:A:SER:H | 18       | 0.31          |
| (1,4357) | 1:10:A:GLY:H  | 1:14:A:VAL:O  | 14       | 0.31          |
| (1,4325) | 1:2:A:THR:H   | 1:20:A:PHE:O  | 17       | 0.31          |
| (1,2019) | 1:67:A:LEU:CA | 1:70:A:LYS:CA | 15       | 0.31          |
| (1,294)  | 1:37:A:GLY:H  | 1:40:A:GLU:H  | 5        | 0.31          |
| (1,267)  | 1:33:A:GLY:H  | 1:35:A:ILE:H  | 1        | 0.31          |
| (1,181)  | 1:18:A:ILE:H  | 1:150:A:GLY:H | 11       | 0.31          |
| (1,176)  | 1:86:A:ASN:H  | 1:88:A:THR:H  | 2        | 0.31          |
| (1,123)  | 1:22:A:GLN:H  | 1:106:A:LEU:H | 17       | 0.31          |
| (1,88)   | 1:15:A:GLN:H  | 1:35:A:ILE:H  | 9        | 0.31          |
| (1,85)   | 1:8:A:LEU:H   | 1:15:A:GLN:H  | 8        | 0.31          |
| (1,63)   | 1:41:A:GLY:H  | 1:90:A:ASP:H  | 13       | 0.31          |
| (3,319)  | 1:41:A:GLY:N  | 2:201:A:CU:CU | 12       | 0.3           |
| (3,310)  | 1:31:A:VAL:N  | 2:201:A:CU:CU | 8        | 0.3           |
| (3,265)  | 1:100:A:GLU:C | 2:201:A:CU:CU | 15       | 0.3           |
| (2,156)  | 1:106:A:LEU:N | 1:108:A:GLY:N | 17       | 0.3           |
| (1,4634) | 1:55:A:ALA:O  | 1:144:A:LEU:N | 11       | 0.3           |
| (1,4625) | 1:40:A:GLU:O  | 1:121:A:GLU:H | 15       | 0.3           |
| (1,4591) | 1:50:A:PHE:N  | 1:113:A:ILE:O | 4        | 0.3           |
| (1,4575) | 1:22:A:GLN:N  | 1:103:A:VAL:O | 14       | 0.3           |
| (1,4572) | 1:29:A:VAL:H  | 1:102:A:SER:O | 3        | 0.3           |
| (1,4551) | 1:86:A:ASN:N  | 1:97:A:VAL:O  | 19       | 0.3           |
| (1,4506) | 1:76:A:ASP:N  | 1:84:A:LEU:O  | 11       | 0.3           |
| (1,4470) | 1:50:A:PHE:N  | 1:114:A:GLY:O | 13       | 0.3           |
| (1,4463) | 1:49:A:GLU:O  | 1:116:A:THR:N | 10       | 0.3           |
| (1,4447) | 1:45:A:PHE:O  | 1:84:A:LEU:N  | 19       | 0.3           |
| (1,4443) | 1:44:A:GLY:O  | 1:120:A:HIS:N | 1        | 0.3           |
| (1,4437) | 1:41:A:GLY:H  | 1:121:A:GLU:O | 18       | 0.3           |

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| Key      | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|----------|---------------|---------------|----------|---------------|
| (1,4432) | 1:40:A:GLU:O  | 1:121:A:GLU:H | 15       | 0.3           |
| (1,4355) | 1:10:A:GLY:O  | 1:145:A:ALA:N | 7        | 0.3           |
| (1,234)  | 1:131:A:ASN:H | 1:139:A:ASN:H | 7        | 0.3           |
| (1,191)  | 1:52:A:ASP:H  | 1:114:A:GLY:H | 7        | 0.3           |
| (1,181)  | 1:18:A:ILE:H  | 1:150:A:GLY:H | 2        | 0.3           |
| (1,181)  | 1:18:A:ILE:H  | 1:150:A:GLY:H | 10       | 0.3           |
| (1,120)  | 1:3:A:LYS:H   | 1:151:A:ILE:H | 7        | 0.3           |
| (1,107)  | 1:45:A:PHE:H  | 1:119:A:VAL:H | 13       | 0.3           |
| (1,88)   | 1:15:A:GLN:H  | 1:35:A:ILE:H  | 3        | 0.3           |
| (1,88)   | 1:15:A:GLN:H  | 1:35:A:ILE:H  | 18       | 0.3           |
| (1,49)   | 1:47:A:VAL:H  | 1:118:A:VAL:H | 16       | 0.3           |
| (1,35)   | 1:43:A:HIS:H  | 1:45:A:PHE:H  | 6        | 0.3           |
| (1,16)   | 1:48:A:HIS:H  | 1:50:A:PHE:H  | 19       | 0.3           |
| (3,319)  | 1:41:A:GLY:N  | 2:201:A:CU:CU | 10       | 0.29          |
| (3,253)  | 1:83:A:ASP:C  | 2:201:A:CU:CU | 11       | 0.29          |
| (1,4633) | 1:119:A:VAL:O | 1:144:A:LEU:H | 10       | 0.29          |
| (1,4584) | 1:22:A:GLN:H  | 1:105:A:SER:O | 7        | 0.29          |
| (1,4568) | 1:75:A:LYS:H  | 1:101:A:ASP:O | 15       | 0.29          |
| (1,4551) | 1:33:A:GLY:N  | 1:97:A:VAL:O  | 6        | 0.29          |
| (1,4541) | 1:38:A:LEU:O  | 1:93:A:GLY:H  | 8        | 0.29          |
| (1,4508) | 1:77:A:GLU:O  | 1:102:A:SER:H | 7        | 0.29          |
| (1,4506) | 1:76:A:ASP:N  | 1:101:A:ASP:O | 19       | 0.29          |
| (1,4501) | 1:75:A:LYS:H  | 1:101:A:ASP:O | 15       | 0.29          |
| (1,4485) | 1:57:A:CYS:H  | 1:146:A:CYS:O | 10       | 0.29          |
| (1,4355) | 1:10:A:GLY:O  | 1:14:A:VAL:N  | 10       | 0.29          |
| (1,4324) | 1:2:A:THR:O   | 1:21:A:GLU:H  | 3        | 0.29          |
| (1,292)  | 1:37:A:GLY:H  | 1:39:A:THR:H  | 9        | 0.29          |
| (1,162)  | 1:67:A:LEU:H  | 1:70:A:LYS:H  | 15       | 0.29          |
| (1,132)  | 1:40:A:GLU:H  | 1:92:A:ASP:H  | 4        | 0.29          |
| (1,107)  | 1:46:A:HIS:H  | 1:119:A:VAL:H | 3        | 0.29          |
| (1,88)   | 1:15:A:GLN:H  | 1:35:A:ILE:H  | 2        | 0.29          |
| (1,36)   | 1:45:A:PHE:H  | 1:85:A:GLY:H  | 8        | 0.29          |
| (3,282)  | 1:142:A:SER:C | 2:201:A:CU:CU | 9        | 0.28          |
| (3,274)  | 1:120:A:HIS:C | 2:201:A:CU:CU | 17       | 0.28          |
| (3,253)  | 1:83:A:ASP:C  | 2:201:A:CU:CU | 13       | 0.28          |
| (3,236)  | 1:49:A:GLU:C  | 2:201:A:CU:CU | 7        | 0.28          |
| (3,196)  | 1:139:A:ASN:C | 2:201:A:CU:CU | 16       | 0.28          |
| (3,84)   | 1:150:A:GLY:C | 2:201:A:CU:CU | 10       | 0.28          |
| (1,4578) | 1:75:A:LYS:O  | 1:103:A:VAL:N | 8        | 0.28          |
| (1,4572) | 1:77:A:GLU:H  | 1:102:A:SER:O | 11       | 0.28          |
| (1,4520) | 1:45:A:PHE:H  | 1:84:A:LEU:O  | 16       | 0.28          |
| (1,4516) | 1:69:A:ARG:H  | 1:79:A:ARG:O  | 6        | 0.28          |

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| Key      | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|----------|---------------|---------------|----------|---------------|
| (1,4512) | 1:69:A:ARG:H  | 1:78:A:GLU:O  | 6        | 0.28          |
| (1,4509) | 1:77:A:GLU:H  | 1:102:A:SER:O | 11       | 0.28          |
| (1,4507) | 1:69:A:ARG:N  | 1:77:A:GLU:O  | 11       | 0.28          |
| (1,4504) | 1:69:A:ARG:H  | 1:76:A:ASP:O  | 9        | 0.28          |
| (1,4499) | 1:75:A:LYS:O  | 1:103:A:VAL:N | 8        | 0.28          |
| (1,4497) | 1:69:A:ARG:H  | 1:79:A:ARG:O  | 6        | 0.28          |
| (1,4497) | 1:69:A:ARG:H  | 1:76:A:ASP:O  | 9        | 0.28          |
| (1,4465) | 1:49:A:GLU:H  | 1:116:A:THR:O | 1        | 0.28          |
| (1,4465) | 1:49:A:GLU:H  | 1:116:A:THR:O | 2        | 0.28          |
| (1,4457) | 1:47:A:VAL:H  | 1:118:A:VAL:O | 19       | 0.28          |
| (1,4435) | 1:41:A:GLY:O  | 1:91:A:LYS:N  | 6        | 0.28          |
| (1,4400) | 1:31:A:VAL:O  | 1:100:A:GLU:H | 8        | 0.28          |
| (1,267)  | 1:33:A:GLY:H  | 1:35:A:ILE:H  | 2        | 0.28          |
| (1,217)  | 1:87:A:VAL:H  | 1:122:A:LYS:H | 17       | 0.28          |
| (1,181)  | 1:18:A:ILE:H  | 1:150:A:GLY:H | 1        | 0.28          |
| (1,181)  | 1:18:A:ILE:H  | 1:150:A:GLY:H | 15       | 0.28          |
| (1,176)  | 1:86:A:ASN:H  | 1:88:A:THR:H  | 12       | 0.28          |
| (1,169)  | 1:49:A:GLU:H  | 1:111:A:SER:H | 17       | 0.28          |
| (1,135)  | 1:79:A:ARG:H  | 1:82:A:GLY:H  | 18       | 0.28          |
| (1,131)  | 1:50:A:PHE:H  | 1:60:A:ALA:H  | 10       | 0.28          |
| (1,131)  | 1:50:A:PHE:H  | 1:60:A:ALA:H  | 14       | 0.28          |
| (1,123)  | 1:22:A:GLN:H  | 1:106:A:LEU:H | 8        | 0.28          |
| (1,79)   | 1:119:A:VAL:H | 1:144:A:LEU:H | 18       | 0.28          |
| (1,48)   | 1:6:A:ALA:H   | 1:8:A:LEU:H   | 3        | 0.28          |
| (1,34)   | 1:34:A:SER:H  | 1:97:A:VAL:H  | 6        | 0.28          |
| (1,28)   | 1:149:A:ILE:H | 1:151:A:ILE:H | 15       | 0.28          |
| (1,26)   | 1:51:A:GLY:H  | 1:149:A:ILE:H | 1        | 0.28          |
| (1,26)   | 1:51:A:GLY:H  | 1:149:A:ILE:H | 18       | 0.28          |
| (1,20)   | 1:89:A:ALA:H  | 1:95:A:ALA:H  | 8        | 0.28          |
| (3,213)  | 1:10:A:GLY:C  | 2:201:A:CU:CU | 15       | 0.27          |
| (3,198)  | 1:143:A:ARG:C | 2:201:A:CU:CU | 19       | 0.27          |
| (3,197)  | 1:140:A:ALA:C | 2:201:A:CU:CU | 15       | 0.27          |
| (3,144)  | 1:91:A:LYS:N  | 2:201:A:CU:CU | 16       | 0.27          |
| (2,156)  | 1:106:A:LEU:N | 1:108:A:GLY:N | 10       | 0.27          |
| (1,4590) | 1:112:A:ILE:N | 1:149:A:ILE:O | 13       | 0.27          |
| (1,4586) | 1:21:A:GLU:O  | 1:105:A:SER:N | 5        | 0.27          |
| (1,4565) | 1:84:A:LEU:O  | 1:100:A:GLU:H | 15       | 0.27          |
| (1,4556) | 1:86:A:ASN:H  | 1:98:A:SER:O  | 2        | 0.27          |
| (1,4504) | 1:76:A:ASP:O  | 1:102:A:SER:H | 17       | 0.27          |
| (1,4428) | 1:39:A:THR:O  | 1:93:A:GLY:H  | 10       | 0.27          |
| (1,4424) | 1:14:A:VAL:H  | 1:38:A:LEU:O  | 7        | 0.27          |
| (1,4392) | 1:29:A:VAL:O  | 1:102:A:SER:H | 15       | 0.27          |

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| Key      | Atom-1         | Atom-2        | Model ID | Violation (Å) |
|----------|----------------|---------------|----------|---------------|
| (1,2954) | 1:105:A:SER:CA | 1:107:A:SER:N | 18       | 0.27          |
| (1,276)  | 1:47:A:VAL:H   | 1:85:A:GLY:H  | 6        | 0.27          |
| (1,249)  | 1:50:A:PHE:H   | 1:109:A:ASP:H | 3        | 0.27          |
| (1,242)  | 1:91:A:LYS:H   | 1:93:A:GLY:H  | 13       | 0.27          |
| (1,217)  | 1:87:A:VAL:H   | 1:122:A:LYS:H | 8        | 0.27          |
| (1,181)  | 1:18:A:ILE:H   | 1:150:A:GLY:H | 18       | 0.27          |
| (1,169)  | 1:49:A:GLU:H   | 1:111:A:SER:H | 1        | 0.27          |
| (1,162)  | 1:67:A:LEU:H   | 1:70:A:LYS:H  | 8        | 0.27          |
| (1,135)  | 1:79:A:ARG:H   | 1:82:A:GLY:H  | 1        | 0.27          |
| (1,131)  | 1:50:A:PHE:H   | 1:60:A:ALA:H  | 3        | 0.27          |
| (1,120)  | 1:149:A:ILE:H  | 1:151:A:ILE:H | 3        | 0.27          |
| (1,88)   | 1:15:A:GLN:H   | 1:35:A:ILE:H  | 6        | 0.27          |
| (1,60)   | 1:3:A:LYS:H    | 1:22:A:GLN:H  | 9        | 0.27          |
| (1,36)   | 1:42:A:LEU:H   | 1:45:A:PHE:H  | 13       | 0.27          |
| (1,28)   | 1:149:A:ILE:H  | 1:151:A:ILE:H | 3        | 0.27          |
| (1,26)   | 1:51:A:GLY:H   | 1:149:A:ILE:H | 19       | 0.27          |
| (3,371)  | 1:132:A:GLU:N  | 2:201:A:CU:CU | 17       | 0.26          |
| (3,319)  | 1:41:A:GLY:N   | 2:201:A:CU:CU | 5        | 0.26          |
| (3,236)  | 1:49:A:GLU:C   | 2:201:A:CU:CU | 13       | 0.26          |
| (3,198)  | 1:143:A:ARG:C  | 2:201:A:CU:CU | 13       | 0.26          |
| (3,198)  | 1:143:A:ARG:C  | 2:201:A:CU:CU | 18       | 0.26          |
| (3,84)   | 1:150:A:GLY:C  | 2:201:A:CU:CU | 1        | 0.26          |
| (1,4660) | 1:5:A:VAL:H    | 1:151:A:ILE:O | 5        | 0.26          |
| (1,4660) | 1:5:A:VAL:H    | 1:151:A:ILE:O | 11       | 0.26          |
| (1,4632) | 1:10:A:GLY:H   | 1:144:A:LEU:O | 8        | 0.26          |
| (1,4619) | 1:42:A:LEU:N   | 1:120:A:HIS:O | 6        | 0.26          |
| (1,4619) | 1:42:A:LEU:N   | 1:120:A:HIS:O | 12       | 0.26          |
| (1,4580) | 1:22:A:GLN:H   | 1:104:A:ILE:O | 4        | 0.26          |
| (1,4537) | 1:38:A:LEU:O   | 1:92:A:ASP:H  | 5        | 0.26          |
| (1,4536) | 1:39:A:THR:H   | 1:92:A:ASP:O  | 6        | 0.26          |
| (1,4533) | 1:40:A:GLU:O   | 1:91:A:LYS:H  | 12       | 0.26          |
| (1,4529) | 1:86:A:ASN:H   | 1:97:A:VAL:O  | 16       | 0.26          |
| (1,4470) | 1:50:A:PHE:N   | 1:116:A:THR:O | 19       | 0.26          |
| (1,4432) | 1:40:A:GLU:O   | 1:91:A:LYS:H  | 16       | 0.26          |
| (1,4429) | 1:39:A:THR:H   | 1:92:A:ASP:O  | 6        | 0.26          |
| (1,4424) | 1:38:A:LEU:O   | 1:121:A:GLU:H | 13       | 0.26          |
| (1,4424) | 1:38:A:LEU:O   | 1:121:A:GLU:H | 18       | 0.26          |
| (1,4417) | 1:15:A:GLN:O   | 1:35:A:ILE:H  | 1        | 0.26          |
| (1,4389) | 1:22:A:GLN:H   | 1:104:A:ILE:O | 4        | 0.26          |
| (1,4357) | 1:10:A:GLY:H   | 1:144:A:LEU:O | 8        | 0.26          |
| (1,4324) | 1:2:A:THR:O    | 1:21:A:GLU:H  | 9        | 0.26          |
| (1,2954) | 1:105:A:SER:CA | 1:107:A:SER:N | 7        | 0.26          |

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| Key      | Atom-1         | Atom-2        | Model ID | Violation (Å) |
|----------|----------------|---------------|----------|---------------|
| (1,2954) | 1:105:A:SER:CA | 1:107:A:SER:N | 8        | 0.26          |
| (1,197)  | 1:52:A:ASP:H   | 1:148:A:VAL:H | 11       | 0.26          |
| (1,181)  | 1:18:A:ILE:H   | 1:150:A:GLY:H | 9        | 0.26          |
| (1,181)  | 1:18:A:ILE:H   | 1:150:A:GLY:H | 12       | 0.26          |
| (1,143)  | 1:36:A:LYS:H   | 1:94:A:VAL:H  | 9        | 0.26          |
| (1,137)  | 1:51:A:GLY:H   | 1:111:A:SER:H | 10       | 0.26          |
| (1,127)  | 1:70:A:LYS:H   | 1:78:A:GLU:H  | 9        | 0.26          |
| (1,48)   | 1:6:A:ALA:H    | 1:8:A:LEU:H   | 10       | 0.26          |
| (3,295)  | 1:9:A:LYS:N    | 2:201:A:CU:CU | 17       | 0.25          |
| (3,274)  | 1:120:A:HIS:C  | 2:201:A:CU:CU | 1        | 0.25          |
| (3,213)  | 1:10:A:GLY:C   | 2:201:A:CU:CU | 16       | 0.25          |
| (3,160)  | 1:113:A:ILE:N  | 2:201:A:CU:CU | 3        | 0.25          |
| (3,159)  | 1:112:A:ILE:N  | 2:201:A:CU:CU | 7        | 0.25          |
| (3,1)    | 1:2:A:THR:C    | 2:201:A:CU:CU | 9        | 0.25          |
| (1,4634) | 1:9:A:LYS:O    | 1:144:A:LEU:N | 13       | 0.25          |
| (1,4633) | 1:119:A:VAL:O  | 1:144:A:LEU:H | 2        | 0.25          |
| (1,4593) | 1:113:A:ILE:H  | 1:149:A:ILE:O | 14       | 0.25          |
| (1,4591) | 1:113:A:ILE:O  | 1:150:A:GLY:N | 12       | 0.25          |
| (1,4565) | 1:29:A:VAL:O   | 1:100:A:GLU:H | 14       | 0.25          |
| (1,4561) | 1:86:A:ASN:O   | 1:99:A:ILE:H  | 16       | 0.25          |
| (1,4540) | 1:36:A:LYS:H   | 1:93:A:GLY:O  | 13       | 0.25          |
| (1,4495) | 1:69:A:ARG:O   | 1:78:A:GLU:N  | 14       | 0.25          |
| (1,4480) | 1:56:A:GLY:O   | 1:146:A:CYS:H | 4        | 0.25          |
| (1,4463) | 1:49:A:GLU:O   | 1:116:A:THR:N | 11       | 0.25          |
| (1,4440) | 1:42:A:LEU:O   | 1:44:A:GLY:H  | 4        | 0.25          |
| (1,4417) | 1:15:A:GLN:O   | 1:35:A:ILE:H  | 7        | 0.25          |
| (1,4417) | 1:15:A:GLN:O   | 1:35:A:ILE:H  | 10       | 0.25          |
| (1,4404) | 1:18:A:ILE:H   | 1:32:A:TRP:O  | 10       | 0.25          |
| (1,4348) | 1:8:A:LEU:O    | 1:14:A:VAL:H  | 13       | 0.25          |
| (1,4324) | 1:2:A:THR:O    | 1:21:A:GLU:H  | 11       | 0.25          |
| (1,2874) | 1:102:A:SER:CB | 1:105:A:SER:C | 11       | 0.25          |
| (1,182)  | 1:7:A:VAL:H    | 1:150:A:GLY:H | 5        | 0.25          |
| (1,170)  | 1:69:A:ARG:H   | 1:80:A:HIS:H  | 12       | 0.25          |
| (1,168)  | 1:88:A:THR:H   | 1:94:A:VAL:H  | 15       | 0.25          |
| (1,157)  | 1:42:A:LEU:H   | 1:88:A:THR:H  | 11       | 0.25          |
| (1,146)  | 1:67:A:LEU:H   | 1:109:A:ASP:H | 5        | 0.25          |
| (1,141)  | 1:88:A:THR:H   | 1:94:A:VAL:H  | 15       | 0.25          |
| (1,107)  | 1:46:A:HIS:H   | 1:119:A:VAL:H | 8        | 0.25          |
| (1,88)   | 1:15:A:GLN:H   | 1:35:A:ILE:H  | 11       | 0.25          |
| (1,88)   | 1:15:A:GLN:H   | 1:35:A:ILE:H  | 12       | 0.25          |
| (1,88)   | 1:15:A:GLN:H   | 1:35:A:ILE:H  | 17       | 0.25          |
| (1,53)   | 1:48:A:HIS:H   | 1:118:A:VAL:H | 10       | 0.25          |

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| Key      | Atom-1         | Atom-2        | Model ID | Violation (Å) |
|----------|----------------|---------------|----------|---------------|
| (1,48)   | 1:6:A:ALA:H    | 1:8:A:LEU:H   | 18       | 0.25          |
| (1,43)   | 1:8:A:LEU:H    | 1:18:A:ILE:H  | 15       | 0.25          |
| (1,35)   | 1:43:A:HIS:H   | 1:45:A:PHE:H  | 17       | 0.25          |
| (1,24)   | 1:21:A:GLU:H   | 1:30:A:LYS:H  | 9        | 0.25          |
| (1,12)   | 1:117:A:LEU:H  | 1:150:A:GLY:H | 10       | 0.25          |
| (3,371)  | 1:132:A:GLU:N  | 2:201:A:CU:CU | 2        | 0.24          |
| (3,371)  | 1:132:A:GLU:N  | 2:201:A:CU:CU | 8        | 0.24          |
| (3,236)  | 1:49:A:GLU:C   | 2:201:A:CU:CU | 2        | 0.24          |
| (3,160)  | 1:113:A:ILE:N  | 2:201:A:CU:CU | 2        | 0.24          |
| (3,84)   | 1:150:A:GLY:C  | 2:201:A:CU:CU | 12       | 0.24          |
| (1,4660) | 1:5:A:VAL:H    | 1:151:A:ILE:O | 10       | 0.24          |
| (1,4633) | 1:119:A:VAL:O  | 1:144:A:LEU:H | 19       | 0.24          |
| (1,4625) | 1:40:A:GLU:O   | 1:121:A:GLU:H | 18       | 0.24          |
| (1,4580) | 1:22:A:GLN:H   | 1:104:A:ILE:O | 5        | 0.24          |
| (1,4555) | 1:86:A:ASN:N   | 1:98:A:SER:O  | 18       | 0.24          |
| (1,4540) | 1:36:A:LYS:H   | 1:93:A:GLY:O  | 8        | 0.24          |
| (1,4508) | 1:77:A:GLU:O   | 1:104:A:ILE:H | 16       | 0.24          |
| (1,4445) | 1:42:A:LEU:O   | 1:44:A:GLY:H  | 8        | 0.24          |
| (1,4440) | 1:42:A:LEU:O   | 1:44:A:GLY:H  | 8        | 0.24          |
| (1,4432) | 1:40:A:GLU:O   | 1:121:A:GLU:H | 18       | 0.24          |
| (1,4389) | 1:22:A:GLN:H   | 1:104:A:ILE:O | 5        | 0.24          |
| (1,4356) | 1:10:A:GLY:O   | 1:14:A:VAL:H  | 1        | 0.24          |
| (1,4356) | 1:10:A:GLY:O   | 1:14:A:VAL:H  | 18       | 0.24          |
| (1,2954) | 1:105:A:SER:CA | 1:107:A:SER:N | 6        | 0.24          |
| (1,218)  | 1:72:A:GLY:H   | 1:79:A:ARG:H  | 9        | 0.24          |
| (1,183)  | 1:51:A:GLY:H   | 1:110:A:HIS:H | 3        | 0.24          |
| (1,157)  | 1:42:A:LEU:H   | 1:88:A:THR:H  | 8        | 0.24          |
| (1,157)  | 1:42:A:LEU:H   | 1:88:A:THR:H  | 10       | 0.24          |
| (1,146)  | 1:67:A:LEU:H   | 1:109:A:ASP:H | 11       | 0.24          |
| (1,146)  | 1:67:A:LEU:H   | 1:109:A:ASP:H | 16       | 0.24          |
| (1,138)  | 1:72:A:GLY:H   | 1:79:A:ARG:H  | 9        | 0.24          |
| (1,131)  | 1:50:A:PHE:H   | 1:60:A:ALA:H  | 18       | 0.24          |
| (1,123)  | 1:22:A:GLN:H   | 1:106:A:LEU:H | 16       | 0.24          |
| (1,35)   | 1:43:A:HIS:H   | 1:45:A:PHE:H  | 4        | 0.24          |
| (1,34)   | 1:34:A:SER:H   | 1:97:A:VAL:H  | 15       | 0.24          |
| (1,19)   | 1:125:A:ASP:H  | 1:139:A:ASN:H | 15       | 0.24          |
| (3,310)  | 1:31:A:VAL:N   | 2:201:A:CU:CU | 1        | 0.23          |
| (3,305)  | 1:20:A:PHE:N   | 2:201:A:CU:CU | 9        | 0.23          |
| (3,295)  | 1:9:A:LYS:N    | 2:201:A:CU:CU | 4        | 0.23          |
| (3,295)  | 1:9:A:LYS:N    | 2:201:A:CU:CU | 18       | 0.23          |
| (3,241)  | 1:59:A:SER:C   | 2:201:A:CU:CU | 7        | 0.23          |
| (3,213)  | 1:10:A:GLY:C   | 2:201:A:CU:CU | 7        | 0.23          |

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| Key       | Atom-1         | Atom-2        | Model ID | Violation (Å) |
|-----------|----------------|---------------|----------|---------------|
| (3,213)   | 1:10:A:GLY:C   | 2:201:A:CU:CU | 13       | 0.23          |
| (3,194)   | 1:136:A:LYS:C  | 2:201:A:CU:CU | 14       | 0.23          |
| (3,144)   | 1:91:A:LYS:N   | 2:201:A:CU:CU | 8        | 0.23          |
| (3,144)   | 1:91:A:LYS:N   | 2:201:A:CU:CU | 19       | 0.23          |
| (1,4660)  | 1:5:A:VAL:H    | 1:151:A:ILE:O | 7        | 0.23          |
| (1,4585)  | 1:79:A:ARG:O   | 1:105:A:SER:H | 9        | 0.23          |
| (1,4582)  | 1:75:A:LYS:O   | 1:104:A:ILE:N | 3        | 0.23          |
| (1,4547)  | 1:86:A:ASN:N   | 1:96:A:ASP:O  | 1        | 0.23          |
| (1,4520)  | 1:46:A:HIS:H   | 1:84:A:LEU:O  | 15       | 0.23          |
| (1,4516)  | 1:79:A:ARG:O   | 1:105:A:SER:H | 9        | 0.23          |
| (1,4499)  | 1:75:A:LYS:O   | 1:102:A:SER:N | 14       | 0.23          |
| (1,4495)  | 1:69:A:ARG:O   | 1:78:A:GLU:N  | 19       | 0.23          |
| (1,4489)  | 1:67:A:LEU:H   | 1:79:A:ARG:O  | 5        | 0.23          |
| (1,4479)  | 1:56:A:GLY:O   | 1:143:A:ARG:N | 6        | 0.23          |
| (1,4463)  | 1:49:A:GLU:O   | 1:116:A:THR:N | 1        | 0.23          |
| (1,4452)  | 1:46:A:HIS:O   | 1:118:A:VAL:H | 11       | 0.23          |
| (1,4441)  | 1:42:A:LEU:H   | 1:121:A:GLU:O | 2        | 0.23          |
| (1,4417)  | 1:15:A:GLN:O   | 1:35:A:ILE:H  | 11       | 0.23          |
| (1,4404)  | 1:18:A:ILE:H   | 1:32:A:TRP:O  | 13       | 0.23          |
| (1,4404)  | 1:18:A:ILE:H   | 1:32:A:TRP:O  | 14       | 0.23          |
| (1,4348)  | 1:8:A:LEU:O    | 1:16:A:GLY:H  | 5        | 0.23          |
| (1,2954)  | 1:105:A:SER:CA | 1:107:A:SER:N | 3        | 0.23          |
| (1,293)   | 1:119:A:VAL:H  | 1:141:A:GLY:H | 15       | 0.23          |
| (1,211)   | 1:41:A:GLY:H   | 1:89:A:ALA:H  | 8        | 0.23          |
| (1,181)   | 1:18:A:ILE:H   | 1:150:A:GLY:H | 8        | 0.23          |
| (1,181)   | 1:18:A:ILE:H   | 1:150:A:GLY:H | 19       | 0.23          |
| (1,151)   | 1:89:A:ALA:H   | 1:94:A:VAL:H  | 9        | 0.23          |
| (1,139)   | 1:69:A:ARG:H   | 1:78:A:GLU:H  | 17       | 0.23          |
| (1,137)   | 1:51:A:GLY:H   | 1:111:A:SER:H | 5        | 0.23          |
| (1,131)   | 1:50:A:PHE:H   | 1:60:A:ALA:H  | 8        | 0.23          |
| (1,129)   | 1:60:A:ALA:H   | 1:63:A:HIS:H  | 12       | 0.23          |
| (1,123)   | 1:22:A:GLN:H   | 1:106:A:LEU:H | 7        | 0.23          |
| (1,85)    | 1:8:A:LEU:H    | 1:15:A:GLN:H  | 16       | 0.23          |
| (1,34)    | 1:34:A:SER:H   | 1:97:A:VAL:H  | 19       | 0.23          |
| (3,310)   | 1:31:A:VAL:N   | 2:201:A:CU:CU | 2        | 0.22          |
| (3,236)   | 1:49:A:GLU:C   | 2:201:A:CU:CU | 8        | 0.22          |
| (3,178)   | 1:45:A:PHE:C   | 2:201:A:CU:CU | 18       | 0.22          |
| (3,137)   | 1:80:A:HIS:N   | 2:201:A:CU:CU | 6        | 0.22          |
| (3,84)    | 1:150:A:GLY:C  | 2:201:A:CU:CU | 13       | 0.22          |
| (3,40)    | 1:66:A:PRO:C   | 2:201:A:CU:CU | 7        | 0.22          |
| (2,10700) | 1:86:A:ASN:C   | 1:89:A:ALA:C  | 17       | 0.22          |
| (1,4664)  | 1:5:A:VAL:H    | 1:152:A:ALA:O | 7        | 0.22          |

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| Key      | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|----------|---------------|---------------|----------|---------------|
| (1,4632) | 1:14:A:VAL:H  | 1:144:A:LEU:O | 14       | 0.22          |
| (1,4596) | 1:114:A:GLY:O | 1:149:A:ILE:H | 10       | 0.22          |
| (1,4548) | 1:33:A:GLY:H  | 1:96:A:ASP:O  | 4        | 0.22          |
| (1,4547) | 1:86:A:ASN:N  | 1:96:A:ASP:O  | 6        | 0.22          |
| (1,4541) | 1:38:A:LEU:O  | 1:93:A:GLY:H  | 19       | 0.22          |
| (1,4512) | 1:69:A:ARG:H  | 1:78:A:GLU:O  | 11       | 0.22          |
| (1,4480) | 1:56:A:GLY:O  | 1:116:A:THR:H | 11       | 0.22          |
| (1,4404) | 1:18:A:ILE:H  | 1:32:A:TRP:O  | 4        | 0.22          |
| (1,4404) | 1:18:A:ILE:H  | 1:32:A:TRP:O  | 5        | 0.22          |
| (1,4404) | 1:18:A:ILE:H  | 1:32:A:TRP:O  | 15       | 0.22          |
| (1,4325) | 1:2:A:THR:H   | 1:20:A:PHE:O  | 18       | 0.22          |
| (1,271)  | 1:33:A:GLY:H  | 1:99:A:ILE:H  | 19       | 0.22          |
| (1,261)  | 1:129:A:GLY:H | 1:136:A:LYS:H | 15       | 0.22          |
| (1,239)  | 1:131:A:ASN:H | 1:138:A:GLY:H | 7        | 0.22          |
| (1,220)  | 1:72:A:GLY:H  | 1:78:A:GLU:H  | 6        | 0.22          |
| (1,197)  | 1:52:A:ASP:H  | 1:148:A:VAL:H | 7        | 0.22          |
| (1,181)  | 1:18:A:ILE:H  | 1:150:A:GLY:H | 14       | 0.22          |
| (1,162)  | 1:67:A:LEU:H  | 1:70:A:LYS:H  | 4        | 0.22          |
| (1,120)  | 1:3:A:LYS:H   | 1:151:A:ILE:H | 1        | 0.22          |
| (1,118)  | 1:47:A:VAL:H  | 1:84:A:LEU:H  | 3        | 0.22          |
| (1,107)  | 1:46:A:HIS:H  | 1:119:A:VAL:H | 19       | 0.22          |
| (1,100)  | 1:46:A:HIS:H  | 1:83:A:ASP:H  | 3        | 0.22          |
| (1,100)  | 1:46:A:HIS:H  | 1:83:A:ASP:H  | 15       | 0.22          |
| (1,85)   | 1:8:A:LEU:H   | 1:15:A:GLN:H  | 7        | 0.22          |
| (1,43)   | 1:8:A:LEU:H   | 1:18:A:ILE:H  | 3        | 0.22          |
| (1,12)   | 1:47:A:VAL:H  | 1:117:A:LEU:H | 14       | 0.22          |
| (3,371)  | 1:132:A:GLU:N | 2:201:A:CU:CU | 3        | 0.21          |
| (3,236)  | 1:49:A:GLU:C  | 2:201:A:CU:CU | 5        | 0.21          |
| (3,213)  | 1:10:A:GLY:C  | 2:201:A:CU:CU | 8        | 0.21          |
| (3,213)  | 1:10:A:GLY:C  | 2:201:A:CU:CU | 10       | 0.21          |
| (3,213)  | 1:10:A:GLY:C  | 2:201:A:CU:CU | 18       | 0.21          |
| (3,196)  | 1:139:A:ASN:C | 2:201:A:CU:CU | 7        | 0.21          |
| (3,84)   | 1:150:A:GLY:C | 2:201:A:CU:CU | 4        | 0.21          |
| (3,84)   | 1:150:A:GLY:C | 2:201:A:CU:CU | 16       | 0.21          |
| (1,4634) | 1:119:A:VAL:O | 1:144:A:LEU:N | 15       | 0.21          |
| (1,4593) | 1:113:A:ILE:H | 1:149:A:ILE:O | 13       | 0.21          |
| (1,4565) | 1:29:A:VAL:O  | 1:100:A:GLU:H | 3        | 0.21          |
| (1,4564) | 1:75:A:LYS:H  | 1:100:A:GLU:O | 7        | 0.21          |
| (1,4559) | 1:86:A:ASN:N  | 1:99:A:ILE:O  | 16       | 0.21          |
| (1,4557) | 1:31:A:VAL:O  | 1:98:A:SER:H  | 9        | 0.21          |
| (1,4535) | 1:40:A:GLU:N  | 1:92:A:ASP:O  | 13       | 0.21          |
| (1,4529) | 1:44:A:GLY:O  | 1:86:A:ASN:H  | 5        | 0.21          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,4514) | 1:67:A:LEU:O   | 1:78:A:GLU:N   | 18       | 0.21          |
| (1,4501) | 1:75:A:LYS:H   | 1:100:A:GLU:O  | 7        | 0.21          |
| (1,4417) | 1:15:A:GLN:O   | 1:35:A:ILE:H   | 15       | 0.21          |
| (1,4406) | 1:17:A:ILE:O   | 1:32:A:TRP:N   | 18       | 0.21          |
| (1,4404) | 1:18:A:ILE:H   | 1:32:A:TRP:O   | 18       | 0.21          |
| (1,4086) | 1:142:A:SER:CA | 1:145:A:ALA:CB | 4        | 0.21          |
| (1,1689) | 1:57:A:CYS:CB  | 1:59:A:SER:CA  | 8        | 0.21          |
| (1,1278) | 1:40:A:GLU:CA  | 1:42:A:LEU:CB  | 19       | 0.21          |
| (1,977)  | 1:27:A:GLY:CA  | 1:30:A:LYS:CB  | 9        | 0.21          |
| (1,263)  | 1:27:A:GLY:H   | 1:102:A:SER:H  | 2        | 0.21          |
| (1,211)  | 1:41:A:GLY:H   | 1:89:A:ALA:H   | 19       | 0.21          |
| (1,201)  | 1:16:A:GLY:H   | 1:34:A:SER:H   | 15       | 0.21          |
| (1,169)  | 1:49:A:GLU:H   | 1:83:A:ASP:H   | 7        | 0.21          |
| (1,118)  | 1:47:A:VAL:H   | 1:84:A:LEU:H   | 10       | 0.21          |
| (1,117)  | 1:76:A:ASP:H   | 1:78:A:GLU:H   | 7        | 0.21          |
| (1,103)  | 1:77:A:GLU:H   | 1:79:A:ARG:H   | 13       | 0.21          |
| (1,48)   | 1:6:A:ALA:H    | 1:8:A:LEU:H    | 16       | 0.21          |
| (1,48)   | 1:6:A:ALA:H    | 1:8:A:LEU:H    | 19       | 0.21          |
| (1,43)   | 1:8:A:LEU:H    | 1:18:A:ILE:H   | 16       | 0.21          |
| (1,43)   | 1:8:A:LEU:H    | 1:18:A:ILE:H   | 17       | 0.21          |
| (1,35)   | 1:43:A:HIS:H   | 1:45:A:PHE:H   | 10       | 0.21          |
| (1,35)   | 1:43:A:HIS:H   | 1:45:A:PHE:H   | 19       | 0.21          |
| (3,319)  | 1:41:A:GLY:N   | 2:201:A:CU:CU  | 3        | 0.2           |
| (3,310)  | 1:31:A:VAL:N   | 2:201:A:CU:CU  | 10       | 0.2           |
| (3,274)  | 1:120:A:HIS:C  | 2:201:A:CU:CU  | 18       | 0.2           |
| (3,232)  | 1:40:A:GLU:C   | 2:201:A:CU:CU  | 15       | 0.2           |
| (3,213)  | 1:10:A:GLY:C   | 2:201:A:CU:CU  | 2        | 0.2           |
| (3,195)  | 1:138:A:GLY:C  | 2:201:A:CU:CU  | 18       | 0.2           |
| (3,179)  | 1:46:A:HIS:C   | 2:201:A:CU:CU  | 12       | 0.2           |
| (3,178)  | 1:45:A:PHE:C   | 2:201:A:CU:CU  | 10       | 0.2           |
| (1,4613) | 1:47:A:VAL:O   | 1:118:A:VAL:H  | 10       | 0.2           |
| (1,4596) | 1:114:A:GLY:O  | 1:149:A:ILE:H  | 9        | 0.2           |
| (1,4586) | 1:76:A:ASP:O   | 1:105:A:SER:N  | 10       | 0.2           |
| (1,4584) | 1:22:A:GLN:H   | 1:105:A:SER:O  | 3        | 0.2           |
| (1,4576) | 1:22:A:GLN:H   | 1:103:A:VAL:O  | 3        | 0.2           |
| (1,4495) | 1:69:A:ARG:O   | 1:79:A:ARG:N   | 4        | 0.2           |
| (1,4465) | 1:49:A:GLU:H   | 1:116:A:THR:O  | 9        | 0.2           |
| (1,4456) | 1:47:A:VAL:O   | 1:118:A:VAL:H  | 10       | 0.2           |
| (1,4443) | 1:44:A:GLY:O   | 1:85:A:GLY:N   | 4        | 0.2           |
| (1,4389) | 1:22:A:GLN:H   | 1:103:A:VAL:O  | 3        | 0.2           |
| (1,4355) | 1:10:A:GLY:O   | 1:145:A:ALA:N  | 11       | 0.2           |
| (1,303)  | 1:49:A:GLU:H   | 1:82:A:GLY:H   | 19       | 0.2           |

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| Key       | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|-----------|---------------|---------------|----------|---------------|
| (1,292)   | 1:37:A:GLY:H  | 1:39:A:THR:H  | 4        | 0.2           |
| (1,289)   | 1:116:A:THR:H | 1:147:A:GLY:H | 4        | 0.2           |
| (1,234)   | 1:131:A:ASN:H | 1:139:A:ASN:H | 14       | 0.2           |
| (1,232)   | 1:116:A:THR:H | 1:148:A:VAL:H | 6        | 0.2           |
| (1,232)   | 1:116:A:THR:H | 1:148:A:VAL:H | 10       | 0.2           |
| (1,220)   | 1:72:A:GLY:H  | 1:78:A:GLU:H  | 10       | 0.2           |
| (1,208)   | 1:34:A:SER:H  | 1:95:A:ALA:H  | 12       | 0.2           |
| (1,201)   | 1:16:A:GLY:H  | 1:34:A:SER:H  | 5        | 0.2           |
| (1,201)   | 1:16:A:GLY:H  | 1:34:A:SER:H  | 6        | 0.2           |
| (1,201)   | 1:16:A:GLY:H  | 1:34:A:SER:H  | 13       | 0.2           |
| (1,171)   | 1:57:A:CYS:H  | 1:147:A:GLY:H | 12       | 0.2           |
| (1,159)   | 1:49:A:GLU:H  | 1:118:A:VAL:H | 4        | 0.2           |
| (1,159)   | 1:49:A:GLU:H  | 1:118:A:VAL:H | 14       | 0.2           |
| (1,146)   | 1:67:A:LEU:H  | 1:109:A:ASP:H | 19       | 0.2           |
| (1,131)   | 1:50:A:PHE:H  | 1:60:A:ALA:H  | 2        | 0.2           |
| (1,118)   | 1:47:A:VAL:H  | 1:84:A:LEU:H  | 5        | 0.2           |
| (1,95)    | 1:9:A:LYS:H   | 1:145:A:ALA:H | 12       | 0.2           |
| (1,63)    | 1:88:A:THR:H  | 1:90:A:ASP:H  | 11       | 0.2           |
| (1,53)    | 1:48:A:HIS:H  | 1:118:A:VAL:H | 18       | 0.2           |
| (1,42)    | 1:19:A:ASN:H  | 1:31:A:VAL:H  | 6        | 0.2           |
| (3,319)   | 1:41:A:GLY:N  | 2:201:A:CU:CU | 16       | 0.19          |
| (3,310)   | 1:31:A:VAL:N  | 2:201:A:CU:CU | 6        | 0.19          |
| (3,295)   | 1:9:A:LYS:N   | 2:201:A:CU:CU | 14       | 0.19          |
| (3,282)   | 1:142:A:SER:C | 2:201:A:CU:CU | 8        | 0.19          |
| (3,282)   | 1:142:A:SER:C | 2:201:A:CU:CU | 16       | 0.19          |
| (3,274)   | 1:120:A:HIS:C | 2:201:A:CU:CU | 8        | 0.19          |
| (3,274)   | 1:120:A:HIS:C | 2:201:A:CU:CU | 11       | 0.19          |
| (3,203)   | 1:63:A:HIS:H  | 2:201:A:CU:CU | 5        | 0.19          |
| (3,198)   | 1:143:A:ARG:C | 2:201:A:CU:CU | 5        | 0.19          |
| (3,194)   | 1:136:A:LYS:C | 2:201:A:CU:CU | 10       | 0.19          |
| (3,194)   | 1:136:A:LYS:C | 2:201:A:CU:CU | 16       | 0.19          |
| (2,10545) | 1:86:A:ASN:N  | 1:89:A:ALA:C  | 17       | 0.19          |
| (2,156)   | 1:106:A:LEU:N | 1:108:A:GLY:N | 13       | 0.19          |
| (2,156)   | 1:106:A:LEU:N | 1:108:A:GLY:N | 14       | 0.19          |
| (1,4597)  | 1:114:A:GLY:H | 1:151:A:ILE:O | 6        | 0.19          |
| (1,4591)  | 1:113:A:ILE:O | 1:150:A:GLY:N | 10       | 0.19          |
| (1,4577)  | 1:76:A:ASP:O  | 1:103:A:VAL:H | 4        | 0.19          |
| (1,4552)  | 1:33:A:GLY:H  | 1:97:A:VAL:O  | 1        | 0.19          |
| (1,4493)  | 1:68:A:SER:H  | 1:79:A:ARG:O  | 15       | 0.19          |
| (1,4488)  | 1:67:A:LEU:O  | 1:79:A:ARG:H  | 11       | 0.19          |
| (1,4481)  | 1:56:A:GLY:H  | 1:146:A:CYS:O | 2        | 0.19          |
| (1,4470)  | 1:50:A:PHE:N  | 1:116:A:THR:O | 1        | 0.19          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,4468) | 1:50:A:PHE:O   | 1:116:A:THR:H  | 14       | 0.19          |
| (1,4456) | 1:47:A:VAL:O   | 1:118:A:VAL:H  | 8        | 0.19          |
| (1,4444) | 1:44:A:GLY:O   | 1:85:A:GLY:H   | 9        | 0.19          |
| (1,4432) | 1:40:A:GLU:O   | 1:91:A:LYS:H   | 19       | 0.19          |
| (1,4035) | 1:141:A:GLY:N  | 1:144:A:LEU:CB | 13       | 0.19          |
| (1,3292) | 1:118:A:VAL:CB | 1:120:A:HIS:CA | 14       | 0.19          |
| (1,2064) | 1:68:A:SER:CB  | 1:70:A:LYS:C   | 17       | 0.19          |
| (1,1286) | 1:40:A:GLU:CB  | 1:42:A:LEU:CB  | 19       | 0.19          |
| (1,300)  | 1:72:A:GLY:H   | 1:127:A:GLY:H  | 8        | 0.19          |
| (1,289)  | 1:116:A:THR:H  | 1:147:A:GLY:H  | 13       | 0.19          |
| (1,271)  | 1:33:A:GLY:H   | 1:99:A:ILE:H   | 1        | 0.19          |
| (1,271)  | 1:33:A:GLY:H   | 1:99:A:ILE:H   | 6        | 0.19          |
| (1,235)  | 1:116:A:THR:H  | 1:118:A:VAL:H  | 3        | 0.19          |
| (1,222)  | 1:72:A:GLY:H   | 1:127:A:GLY:H  | 8        | 0.19          |
| (1,217)  | 1:87:A:VAL:H   | 1:122:A:LYS:H  | 5        | 0.19          |
| (1,211)  | 1:41:A:GLY:H   | 1:89:A:ALA:H   | 2        | 0.19          |
| (1,208)  | 1:34:A:SER:H   | 1:95:A:ALA:H   | 7        | 0.19          |
| (1,201)  | 1:16:A:GLY:H   | 1:34:A:SER:H   | 12       | 0.19          |
| (1,187)  | 1:46:A:HIS:H   | 1:48:A:HIS:H   | 5        | 0.19          |
| (1,181)  | 1:18:A:ILE:H   | 1:150:A:GLY:H  | 7        | 0.19          |
| (1,181)  | 1:18:A:ILE:H   | 1:150:A:GLY:H  | 16       | 0.19          |
| (1,169)  | 1:49:A:GLU:H   | 1:111:A:SER:H  | 4        | 0.19          |
| (1,161)  | 1:72:A:GLY:H   | 1:80:A:HIS:H   | 1        | 0.19          |
| (1,145)  | 1:115:A:ARG:H  | 1:117:A:LEU:H  | 7        | 0.19          |
| (1,143)  | 1:36:A:LYS:H   | 1:94:A:VAL:H   | 4        | 0.19          |
| (1,137)  | 1:51:A:GLY:H   | 1:111:A:SER:H  | 18       | 0.19          |
| (1,131)  | 1:50:A:PHE:H   | 1:60:A:ALA:H   | 13       | 0.19          |
| (1,53)   | 1:48:A:HIS:H   | 1:118:A:VAL:H  | 17       | 0.19          |
| (1,49)   | 1:47:A:VAL:H   | 1:118:A:VAL:H  | 4        | 0.19          |
| (1,43)   | 1:8:A:LEU:H    | 1:18:A:ILE:H   | 8        | 0.19          |
| (1,32)   | 1:52:A:ASP:H   | 1:149:A:ILE:H  | 6        | 0.19          |
| (1,28)   | 1:118:A:VAL:H  | 1:149:A:ILE:H  | 10       | 0.19          |
| (1,17)   | 1:48:A:HIS:H   | 1:116:A:THR:H  | 11       | 0.19          |
| (1,14)   | 1:46:A:HIS:H   | 1:48:A:HIS:H   | 5        | 0.19          |
| (1,12)   | 1:117:A:LEU:H  | 1:150:A:GLY:H  | 18       | 0.19          |
| (1,5)    | 1:20:A:PHE:H   | 1:152:A:ALA:H  | 15       | 0.19          |
| (3,319)  | 1:41:A:GLY:N   | 2:201:A:CU:CU  | 13       | 0.18          |
| (3,310)  | 1:31:A:VAL:N   | 2:201:A:CU:CU  | 16       | 0.18          |
| (3,295)  | 1:9:A:LYS:N    | 2:201:A:CU:CU  | 10       | 0.18          |
| (3,282)  | 1:142:A:SER:C  | 2:201:A:CU:CU  | 17       | 0.18          |
| (3,274)  | 1:120:A:HIS:C  | 2:201:A:CU:CU  | 6        | 0.18          |
| (3,236)  | 1:49:A:GLU:C   | 2:201:A:CU:CU  | 4        | 0.18          |

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| Key       | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|-----------|---------------|---------------|----------|---------------|
| (3,236)   | 1:49:A:GLU:C  | 2:201:A:CU:CU | 15       | 0.18          |
| (3,203)   | 1:63:A:HIS:H  | 2:201:A:CU:CU | 16       | 0.18          |
| (3,194)   | 1:136:A:LYS:C | 2:201:A:CU:CU | 7        | 0.18          |
| (3,193)   | 1:128:A:LYS:C | 2:201:A:CU:CU | 4        | 0.18          |
| (3,187)   | 1:118:A:VAL:C | 2:201:A:CU:CU | 2        | 0.18          |
| (3,182)   | 1:62:A:PRO:C  | 2:201:A:CU:CU | 19       | 0.18          |
| (3,181)   | 1:60:A:ALA:C  | 2:201:A:CU:CU | 6        | 0.18          |
| (3,144)   | 1:91:A:LYS:N  | 2:201:A:CU:CU | 15       | 0.18          |
| (3,95)    | 1:12:A:GLY:N  | 2:201:A:CU:CU | 7        | 0.18          |
| (3,1)     | 1:2:A:THR:C   | 2:201:A:CU:CU | 1        | 0.18          |
| (3,1)     | 1:2:A:THR:C   | 2:201:A:CU:CU | 15       | 0.18          |
| (2,10616) | 1:86:A:ASN:CB | 1:89:A:ALA:C  | 8        | 0.18          |
| (2,156)   | 1:106:A:LEU:N | 1:108:A:GLY:N | 7        | 0.18          |
| (1,4637)  | 1:119:A:VAL:O | 1:145:A:ALA:H | 13       | 0.18          |
| (1,4634)  | 1:9:A:LYS:O   | 1:144:A:LEU:N | 18       | 0.18          |
| (1,4616)  | 1:119:A:VAL:O | 1:145:A:ALA:H | 13       | 0.18          |
| (1,4580)  | 1:22:A:GLN:H  | 1:104:A:ILE:O | 17       | 0.18          |
| (1,4576)  | 1:22:A:GLN:H  | 1:103:A:VAL:O | 12       | 0.18          |
| (1,4569)  | 1:75:A:LYS:O  | 1:101:A:ASP:H | 18       | 0.18          |
| (1,4551)  | 1:33:A:GLY:N  | 1:97:A:VAL:O  | 1        | 0.18          |
| (1,4533)  | 1:40:A:GLU:O  | 1:91:A:LYS:H  | 13       | 0.18          |
| (1,4532)  | 1:39:A:THR:H  | 1:91:A:LYS:O  | 2        | 0.18          |
| (1,4515)  | 1:68:A:SER:N  | 1:79:A:ARG:O  | 19       | 0.18          |
| (1,4497)  | 1:69:A:ARG:H  | 1:79:A:ARG:O  | 1        | 0.18          |
| (1,4441)  | 1:42:A:LEU:H  | 1:121:A:GLU:O | 5        | 0.18          |
| (1,4429)  | 1:39:A:THR:H  | 1:91:A:LYS:O  | 2        | 0.18          |
| (1,4389)  | 1:2:A:THR:O   | 1:22:A:GLN:H  | 1        | 0.18          |
| (1,4389)  | 1:22:A:GLN:H  | 1:104:A:ILE:O | 17       | 0.18          |
| (1,4356)  | 1:10:A:GLY:O  | 1:14:A:VAL:H  | 12       | 0.18          |
| (1,4355)  | 1:10:A:GLY:O  | 1:14:A:VAL:N  | 2        | 0.18          |
| (1,4355)  | 1:10:A:GLY:O  | 1:14:A:VAL:N  | 15       | 0.18          |
| (1,292)   | 1:37:A:GLY:H  | 1:39:A:THR:H  | 3        | 0.18          |
| (1,271)   | 1:33:A:GLY:H  | 1:99:A:ILE:H  | 2        | 0.18          |
| (1,267)   | 1:33:A:GLY:H  | 1:35:A:ILE:H  | 4        | 0.18          |
| (1,249)   | 1:50:A:PHE:H  | 1:109:A:ASP:H | 7        | 0.18          |
| (1,247)   | 1:37:A:GLY:H  | 1:39:A:THR:H  | 3        | 0.18          |
| (1,223)   | 1:51:A:GLY:H  | 1:114:A:GLY:H | 10       | 0.18          |
| (1,217)   | 1:87:A:VAL:H  | 1:122:A:LYS:H | 10       | 0.18          |
| (1,208)   | 1:34:A:SER:H  | 1:95:A:ALA:H  | 3        | 0.18          |
| (1,201)   | 1:16:A:GLY:H  | 1:34:A:SER:H  | 16       | 0.18          |
| (1,201)   | 1:16:A:GLY:H  | 1:34:A:SER:H  | 18       | 0.18          |
| (1,183)   | 1:51:A:GLY:H  | 1:110:A:HIS:H | 6        | 0.18          |

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| Key      | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|----------|---------------|---------------|----------|---------------|
| (1,181)  | 1:18:A:ILE:H  | 1:150:A:GLY:H | 3        | 0.18          |
| (1,177)  | 1:124:A:ASP:H | 1:126:A:LEU:H | 19       | 0.18          |
| (1,168)  | 1:88:A:THR:H  | 1:94:A:VAL:H  | 14       | 0.18          |
| (1,161)  | 1:72:A:GLY:H  | 1:80:A:HIS:H  | 13       | 0.18          |
| (1,157)  | 1:42:A:LEU:H  | 1:88:A:THR:H  | 5        | 0.18          |
| (1,157)  | 1:42:A:LEU:H  | 1:88:A:THR:H  | 19       | 0.18          |
| (1,143)  | 1:36:A:LYS:H  | 1:94:A:VAL:H  | 11       | 0.18          |
| (1,143)  | 1:36:A:LYS:H  | 1:94:A:VAL:H  | 12       | 0.18          |
| (1,141)  | 1:88:A:THR:H  | 1:94:A:VAL:H  | 14       | 0.18          |
| (1,135)  | 1:79:A:ARG:H  | 1:82:A:GLY:H  | 10       | 0.18          |
| (1,131)  | 1:50:A:PHE:H  | 1:60:A:ALA:H  | 11       | 0.18          |
| (1,123)  | 1:22:A:GLN:H  | 1:106:A:LEU:H | 18       | 0.18          |
| (1,117)  | 1:76:A:ASP:H  | 1:78:A:GLU:H  | 19       | 0.18          |
| (1,116)  | 1:42:A:LEU:H  | 1:123:A:ALA:H | 9        | 0.18          |
| (1,42)   | 1:19:A:ASN:H  | 1:31:A:VAL:H  | 4        | 0.18          |
| (1,38)   | 1:6:A:ALA:H   | 1:152:A:ALA:H | 2        | 0.18          |
| (3,319)  | 1:41:A:GLY:N  | 2:201:A:CU:CU | 4        | 0.17          |
| (3,319)  | 1:41:A:GLY:N  | 2:201:A:CU:CU | 11       | 0.17          |
| (3,319)  | 1:41:A:GLY:N  | 2:201:A:CU:CU | 14       | 0.17          |
| (3,310)  | 1:31:A:VAL:N  | 2:201:A:CU:CU | 3        | 0.17          |
| (3,281)  | 1:135:A:THR:C | 2:201:A:CU:CU | 18       | 0.17          |
| (3,253)  | 1:83:A:ASP:C  | 2:201:A:CU:CU | 18       | 0.17          |
| (3,244)  | 1:67:A:LEU:C  | 2:201:A:CU:CU | 4        | 0.17          |
| (3,213)  | 1:10:A:GLY:C  | 2:201:A:CU:CU | 5        | 0.17          |
| (3,213)  | 1:10:A:GLY:C  | 2:201:A:CU:CU | 14       | 0.17          |
| (3,194)  | 1:136:A:LYS:C | 2:201:A:CU:CU | 17       | 0.17          |
| (3,187)  | 1:118:A:VAL:C | 2:201:A:CU:CU | 17       | 0.17          |
| (3,132)  | 1:75:A:LYS:N  | 2:201:A:CU:CU | 8        | 0.17          |
| (3,84)   | 1:150:A:GLY:C | 2:201:A:CU:CU | 11       | 0.17          |
| (3,1)    | 1:2:A:THR:C   | 2:201:A:CU:CU | 5        | 0.17          |
| (3,1)    | 1:2:A:THR:C   | 2:201:A:CU:CU | 6        | 0.17          |
| (2,158)  | 1:107:A:SER:N | 1:109:A:ASP:N | 3        | 0.17          |
| (1,4660) | 1:5:A:VAL:H   | 1:151:A:ILE:O | 2        | 0.17          |
| (1,4626) | 1:40:A:GLU:O  | 1:121:A:GLU:N | 2        | 0.17          |
| (1,4626) | 1:121:A:GLU:N | 1:144:A:LEU:O | 14       | 0.17          |
| (1,4584) | 1:22:A:GLN:H  | 1:105:A:SER:O | 19       | 0.17          |
| (1,4582) | 1:76:A:ASP:O  | 1:104:A:ILE:N | 2        | 0.17          |
| (1,4575) | 1:79:A:ARG:N  | 1:103:A:VAL:O | 13       | 0.17          |
| (1,4569) | 1:29:A:VAL:O  | 1:101:A:ASP:H | 17       | 0.17          |
| (1,4548) | 1:33:A:GLY:H  | 1:96:A:ASP:O  | 8        | 0.17          |
| (1,4521) | 1:46:A:HIS:O  | 1:84:A:LEU:H  | 3        | 0.17          |
| (1,4467) | 1:50:A:PHE:O  | 1:116:A:THR:N | 13       | 0.17          |

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| Key      | Atom-1         | Atom-2        | Model ID | Violation (Å) |
|----------|----------------|---------------|----------|---------------|
| (1,4437) | 1:41:A:GLY:H   | 1:121:A:GLU:O | 4        | 0.17          |
| (1,4392) | 1:29:A:VAL:O   | 1:101:A:ASP:H | 17       | 0.17          |
| (1,4389) | 1:22:A:GLN:H   | 1:105:A:SER:O | 19       | 0.17          |
| (1,3480) | 1:126:A:LEU:CA | 1:128:A:LYS:C | 6        | 0.17          |
| (1,2187) | 1:74:A:PRO:CD  | 1:76:A:ASP:CB | 14       | 0.17          |
| (1,2019) | 1:67:A:LEU:CA  | 1:70:A:LYS:CA | 14       | 0.17          |
| (1,1914) | 1:65:A:ASN:N   | 1:68:A:SER:C  | 5        | 0.17          |
| (1,292)  | 1:37:A:GLY:H   | 1:39:A:THR:H  | 2        | 0.17          |
| (1,276)  | 1:85:A:GLY:H   | 1:99:A:ILE:H  | 13       | 0.17          |
| (1,263)  | 1:27:A:GLY:H   | 1:102:A:SER:H | 16       | 0.17          |
| (1,261)  | 1:129:A:GLY:H  | 1:136:A:LYS:H | 11       | 0.17          |
| (1,247)  | 1:37:A:GLY:H   | 1:39:A:THR:H  | 2        | 0.17          |
| (1,239)  | 1:131:A:ASN:H  | 1:138:A:GLY:H | 14       | 0.17          |
| (1,234)  | 1:131:A:ASN:H  | 1:139:A:ASN:H | 8        | 0.17          |
| (1,234)  | 1:131:A:ASN:H  | 1:139:A:ASN:H | 10       | 0.17          |
| (1,225)  | 1:114:A:GLY:H  | 1:150:A:GLY:H | 2        | 0.17          |
| (1,198)  | 1:52:A:ASP:H   | 1:56:A:GLY:H  | 7        | 0.17          |
| (1,198)  | 1:52:A:ASP:H   | 1:56:A:GLY:H  | 12       | 0.17          |
| (1,183)  | 1:51:A:GLY:H   | 1:110:A:HIS:H | 14       | 0.17          |
| (1,160)  | 1:70:A:LYS:H   | 1:80:A:HIS:H  | 16       | 0.17          |
| (1,159)  | 1:49:A:GLU:H   | 1:118:A:VAL:H | 2        | 0.17          |
| (1,159)  | 1:49:A:GLU:H   | 1:118:A:VAL:H | 7        | 0.17          |
| (1,159)  | 1:49:A:GLU:H   | 1:118:A:VAL:H | 10       | 0.17          |
| (1,157)  | 1:42:A:LEU:H   | 1:88:A:THR:H  | 12       | 0.17          |
| (1,157)  | 1:42:A:LEU:H   | 1:88:A:THR:H  | 13       | 0.17          |
| (1,143)  | 1:36:A:LYS:H   | 1:94:A:VAL:H  | 3        | 0.17          |
| (1,130)  | 1:53:A:ASN:H   | 1:60:A:ALA:H  | 8        | 0.17          |
| (1,123)  | 1:22:A:GLN:H   | 1:106:A:LEU:H | 2        | 0.17          |
| (1,123)  | 1:22:A:GLN:H   | 1:106:A:LEU:H | 11       | 0.17          |
| (1,115)  | 1:20:A:PHE:H   | 1:151:A:ILE:H | 8        | 0.17          |
| (1,115)  | 1:20:A:PHE:H   | 1:151:A:ILE:H | 18       | 0.17          |
| (1,107)  | 1:46:A:HIS:H   | 1:119:A:VAL:H | 9        | 0.17          |
| (1,50)   | 1:120:A:HIS:H  | 1:145:A:ALA:H | 10       | 0.17          |
| (1,43)   | 1:8:A:LEU:H    | 1:18:A:ILE:H  | 6        | 0.17          |
| (1,42)   | 1:19:A:ASN:H   | 1:31:A:VAL:H  | 11       | 0.17          |
| (1,42)   | 1:19:A:ASN:H   | 1:31:A:VAL:H  | 14       | 0.17          |
| (1,42)   | 1:19:A:ASN:H   | 1:31:A:VAL:H  | 16       | 0.17          |
| (1,26)   | 1:48:A:HIS:H   | 1:149:A:ILE:H | 14       | 0.17          |
| (3,371)  | 1:132:A:GLU:N  | 2:201:A:CU:CU | 4        | 0.16          |
| (3,310)  | 1:31:A:VAL:N   | 2:201:A:CU:CU | 15       | 0.16          |
| (3,295)  | 1:9:A:LYS:N    | 2:201:A:CU:CU | 6        | 0.16          |
| (3,221)  | 1:21:A:GLU:C   | 2:201:A:CU:CU | 9        | 0.16          |

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| Key      | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|----------|---------------|---------------|----------|---------------|
| (3,213)  | 1:10:A:GLY:C  | 2:201:A:CU:CU | 17       | 0.16          |
| (3,202)  | 1:48:A:HIS:H  | 2:201:A:CU:CU | 8        | 0.16          |
| (3,194)  | 1:136:A:LYS:C | 2:201:A:CU:CU | 8        | 0.16          |
| (3,193)  | 1:128:A:LYS:C | 2:201:A:CU:CU | 9        | 0.16          |
| (3,182)  | 1:62:A:PRO:C  | 2:201:A:CU:CU | 1        | 0.16          |
| (3,144)  | 1:91:A:LYS:N  | 2:201:A:CU:CU | 12       | 0.16          |
| (3,137)  | 1:80:A:HIS:N  | 2:201:A:CU:CU | 14       | 0.16          |
| (3,134)  | 1:77:A:GLU:N  | 2:201:A:CU:CU | 15       | 0.16          |
| (3,84)   | 1:150:A:GLY:C | 2:201:A:CU:CU | 14       | 0.16          |
| (3,46)   | 1:74:A:PRO:C  | 2:201:A:CU:CU | 8        | 0.16          |
| (2,156)  | 1:106:A:LEU:N | 1:108:A:GLY:N | 11       | 0.16          |
| (1,4552) | 1:33:A:GLY:H  | 1:97:A:VAL:O  | 7        | 0.16          |
| (1,4536) | 1:39:A:THR:H  | 1:92:A:ASP:O  | 12       | 0.16          |
| (1,4520) | 1:46:A:HIS:H  | 1:84:A:LEU:O  | 7        | 0.16          |
| (1,4516) | 1:67:A:LEU:H  | 1:79:A:ARG:O  | 13       | 0.16          |
| (1,4513) | 1:67:A:LEU:O  | 1:78:A:GLU:H  | 14       | 0.16          |
| (1,4502) | 1:68:A:SER:O  | 1:75:A:LYS:N  | 9        | 0.16          |
| (1,4489) | 1:67:A:LEU:H  | 1:79:A:ARG:O  | 13       | 0.16          |
| (1,4453) | 1:46:A:HIS:H  | 1:84:A:LEU:O  | 7        | 0.16          |
| (1,4440) | 1:42:A:LEU:O  | 1:44:A:GLY:H  | 17       | 0.16          |
| (1,4435) | 1:41:A:GLY:O  | 1:91:A:LYS:N  | 3        | 0.16          |
| (1,4433) | 1:40:A:GLU:H  | 1:91:A:LYS:O  | 3        | 0.16          |
| (1,4429) | 1:39:A:THR:H  | 1:92:A:ASP:O  | 12       | 0.16          |
| (1,4427) | 1:39:A:THR:O  | 1:93:A:GLY:N  | 11       | 0.16          |
| (1,4427) | 1:39:A:THR:O  | 1:92:A:ASP:N  | 14       | 0.16          |
| (1,4356) | 1:10:A:GLY:O  | 1:14:A:VAL:H  | 13       | 0.16          |
| (1,4104) | 1:142:A:SER:C | 1:144:A:LEU:C | 2        | 0.16          |
| (1,4104) | 1:142:A:SER:C | 1:144:A:LEU:C | 8        | 0.16          |
| (1,2974) | 1:105:A:SER:C | 1:109:A:ASP:N | 8        | 0.16          |
| (1,2019) | 1:67:A:LEU:CA | 1:70:A:LYS:CA | 18       | 0.16          |
| (1,292)  | 1:37:A:GLY:H  | 1:39:A:THR:H  | 19       | 0.16          |
| (1,271)  | 1:33:A:GLY:H  | 1:99:A:ILE:H  | 18       | 0.16          |
| (1,252)  | 1:50:A:PHE:H  | 1:52:A:ASP:H  | 10       | 0.16          |
| (1,243)  | 1:39:A:THR:H  | 1:93:A:GLY:H  | 5        | 0.16          |
| (1,239)  | 1:131:A:ASN:H | 1:138:A:GLY:H | 8        | 0.16          |
| (1,234)  | 1:131:A:ASN:H | 1:139:A:ASN:H | 2        | 0.16          |
| (1,217)  | 1:87:A:VAL:H  | 1:122:A:LYS:H | 14       | 0.16          |
| (1,208)  | 1:34:A:SER:H  | 1:95:A:ALA:H  | 1        | 0.16          |
| (1,201)  | 1:16:A:GLY:H  | 1:34:A:SER:H  | 4        | 0.16          |
| (1,198)  | 1:52:A:ASP:H  | 1:56:A:GLY:H  | 10       | 0.16          |
| (1,198)  | 1:52:A:ASP:H  | 1:56:A:GLY:H  | 19       | 0.16          |
| (1,172)  | 1:86:A:ASN:H  | 1:98:A:SER:H  | 9        | 0.16          |

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| Key      | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|----------|---------------|---------------|----------|---------------|
| (1,164)  | 1:115:A:ARG:H | 1:151:A:ILE:H | 7        | 0.16          |
| (1,145)  | 1:115:A:ARG:H | 1:117:A:LEU:H | 6        | 0.16          |
| (1,145)  | 1:115:A:ARG:H | 1:117:A:LEU:H | 17       | 0.16          |
| (1,144)  | 1:115:A:ARG:H | 1:151:A:ILE:H | 7        | 0.16          |
| (1,143)  | 1:36:A:LYS:H  | 1:94:A:VAL:H  | 5        | 0.16          |
| (1,129)  | 1:60:A:ALA:H  | 1:63:A:HIS:H  | 14       | 0.16          |
| (1,115)  | 1:20:A:PHE:H  | 1:151:A:ILE:H | 19       | 0.16          |
| (1,49)   | 1:47:A:VAL:H  | 1:118:A:VAL:H | 12       | 0.16          |
| (1,43)   | 1:8:A:LEU:H   | 1:18:A:ILE:H  | 1        | 0.16          |
| (1,43)   | 1:8:A:LEU:H   | 1:18:A:ILE:H  | 2        | 0.16          |
| (1,43)   | 1:8:A:LEU:H   | 1:18:A:ILE:H  | 4        | 0.16          |
| (1,42)   | 1:19:A:ASN:H  | 1:31:A:VAL:H  | 8        | 0.16          |
| (1,38)   | 1:6:A:ALA:H   | 1:152:A:ALA:H | 3        | 0.16          |
| (1,35)   | 1:43:A:HIS:H  | 1:45:A:PHE:H  | 1        | 0.16          |
| (1,26)   | 1:48:A:HIS:H  | 1:149:A:ILE:H | 13       | 0.16          |
| (1,16)   | 1:48:A:HIS:H  | 1:149:A:ILE:H | 13       | 0.16          |
| (1,16)   | 1:48:A:HIS:H  | 1:50:A:PHE:H  | 14       | 0.16          |
| (3,371)  | 1:132:A:GLU:N | 2:201:A:CU:CU | 9        | 0.15          |
| (3,371)  | 1:132:A:GLU:N | 2:201:A:CU:CU | 13       | 0.15          |
| (3,282)  | 1:142:A:SER:C | 2:201:A:CU:CU | 4        | 0.15          |
| (3,282)  | 1:142:A:SER:C | 2:201:A:CU:CU | 18       | 0.15          |
| (3,274)  | 1:120:A:HIS:C | 2:201:A:CU:CU | 9        | 0.15          |
| (3,253)  | 1:83:A:ASP:C  | 2:201:A:CU:CU | 5        | 0.15          |
| (3,236)  | 1:49:A:GLU:C  | 2:201:A:CU:CU | 12       | 0.15          |
| (3,236)  | 1:49:A:GLU:C  | 2:201:A:CU:CU | 17       | 0.15          |
| (3,202)  | 1:48:A:HIS:H  | 2:201:A:CU:CU | 13       | 0.15          |
| (3,159)  | 1:112:A:ILE:N | 2:201:A:CU:CU | 5        | 0.15          |
| (3,150)  | 1:97:A:VAL:N  | 2:201:A:CU:CU | 16       | 0.15          |
| (3,135)  | 1:78:A:GLU:N  | 2:201:A:CU:CU | 1        | 0.15          |
| (3,1)    | 1:2:A:THR:C   | 2:201:A:CU:CU | 10       | 0.15          |
| (2,156)  | 1:106:A:LEU:N | 1:108:A:GLY:N | 2        | 0.15          |
| (2,156)  | 1:106:A:LEU:N | 1:108:A:GLY:N | 9        | 0.15          |
| (1,4660) | 1:5:A:VAL:H   | 1:151:A:ILE:O | 19       | 0.15          |
| (1,4625) | 1:40:A:GLU:O  | 1:121:A:GLU:H | 6        | 0.15          |
| (1,4621) | 1:45:A:PHE:O  | 1:120:A:HIS:H | 13       | 0.15          |
| (1,4596) | 1:114:A:GLY:O | 1:149:A:ILE:H | 15       | 0.15          |
| (1,4584) | 1:22:A:GLN:H  | 1:105:A:SER:O | 12       | 0.15          |
| (1,4577) | 1:77:A:GLU:O  | 1:103:A:VAL:H | 9        | 0.15          |
| (1,4574) | 1:77:A:GLU:O  | 1:102:A:SER:N | 9        | 0.15          |
| (1,4552) | 1:33:A:GLY:H  | 1:97:A:VAL:O  | 2        | 0.15          |
| (1,4540) | 1:36:A:LYS:H  | 1:93:A:GLY:O  | 17       | 0.15          |
| (1,4533) | 1:40:A:GLU:O  | 1:91:A:LYS:H  | 2        | 0.15          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,4529) | 1:86:A:ASN:H   | 1:98:A:SER:O   | 13       | 0.15          |
| (1,4526) | 1:44:A:GLY:O   | 1:85:A:GLY:N   | 3        | 0.15          |
| (1,4508) | 1:77:A:GLU:O   | 1:103:A:VAL:H  | 9        | 0.15          |
| (1,4499) | 1:75:A:LYS:O   | 1:102:A:SER:N  | 5        | 0.15          |
| (1,4481) | 1:56:A:GLY:H   | 1:146:A:CYS:O  | 18       | 0.15          |
| (1,4475) | 1:10:A:GLY:N   | 1:55:A:ALA:O   | 16       | 0.15          |
| (1,4465) | 1:49:A:GLU:H   | 1:116:A:THR:O  | 6        | 0.15          |
| (1,4444) | 1:44:A:GLY:O   | 1:86:A:ASN:H   | 2        | 0.15          |
| (1,4441) | 1:42:A:LEU:H   | 1:121:A:GLU:O  | 19       | 0.15          |
| (1,4432) | 1:40:A:GLU:O   | 1:121:A:GLU:H  | 6        | 0.15          |
| (1,4397) | 1:21:A:GLU:O   | 1:30:A:LYS:H   | 17       | 0.15          |
| (1,4389) | 1:22:A:GLN:H   | 1:105:A:SER:O  | 12       | 0.15          |
| (1,4384) | 1:21:A:GLU:O   | 1:30:A:LYS:H   | 17       | 0.15          |
| (1,4357) | 1:10:A:GLY:H   | 1:14:A:VAL:O   | 15       | 0.15          |
| (1,3027) | 1:108:A:GLY:CA | 1:110:A:HIS:N  | 7        | 0.15          |
| (1,3001) | 1:107:A:SER:N  | 1:109:A:ASP:CA | 3        | 0.15          |
| (1,2975) | 1:106:A:LEU:N  | 1:108:A:GLY:CA | 4        | 0.15          |
| (1,2973) | 1:105:A:SER:C  | 1:108:A:GLY:C  | 18       | 0.15          |
| (1,2576) | 1:90:A:ASP:CB  | 1:92:A:ASP:CG  | 18       | 0.15          |
| (1,2010) | 1:67:A:LEU:N   | 1:70:A:LYS:CA  | 14       | 0.15          |
| (1,1689) | 1:57:A:CYS:CB  | 1:59:A:SER:CA  | 11       | 0.15          |
| (1,271)  | 1:33:A:GLY:H   | 1:99:A:ILE:H   | 13       | 0.15          |
| (1,261)  | 1:129:A:GLY:H  | 1:136:A:LYS:H  | 6        | 0.15          |
| (1,249)  | 1:50:A:PHE:H   | 1:109:A:ASP:H  | 17       | 0.15          |
| (1,223)  | 1:51:A:GLY:H   | 1:114:A:GLY:H  | 12       | 0.15          |
| (1,211)  | 1:41:A:GLY:H   | 1:89:A:ALA:H   | 13       | 0.15          |
| (1,201)  | 1:16:A:GLY:H   | 1:34:A:SER:H   | 8        | 0.15          |
| (1,201)  | 1:16:A:GLY:H   | 1:34:A:SER:H   | 14       | 0.15          |
| (1,187)  | 1:46:A:HIS:H   | 1:48:A:HIS:H   | 13       | 0.15          |
| (1,174)  | 1:53:A:ASN:H   | 1:57:A:CYS:H   | 16       | 0.15          |
| (1,162)  | 1:67:A:LEU:H   | 1:70:A:LYS:H   | 18       | 0.15          |
| (1,133)  | 1:70:A:LYS:H   | 1:78:A:GLU:H   | 8        | 0.15          |
| (1,127)  | 1:70:A:LYS:H   | 1:78:A:GLU:H   | 8        | 0.15          |
| (1,123)  | 1:22:A:GLN:H   | 1:106:A:LEU:H  | 19       | 0.15          |
| (1,118)  | 1:47:A:VAL:H   | 1:84:A:LEU:H   | 11       | 0.15          |
| (1,115)  | 1:20:A:PHE:H   | 1:151:A:ILE:H  | 12       | 0.15          |
| (1,95)   | 1:9:A:LYS:H    | 1:145:A:ALA:H  | 2        | 0.15          |
| (1,95)   | 1:9:A:LYS:H    | 1:145:A:ALA:H  | 6        | 0.15          |
| (1,95)   | 1:9:A:LYS:H    | 1:145:A:ALA:H  | 17       | 0.15          |
| (1,86)   | 1:11:A:ASP:H   | 1:144:A:LEU:H  | 15       | 0.15          |
| (1,75)   | 1:35:A:ILE:H   | 1:97:A:VAL:H   | 8        | 0.15          |
| (1,75)   | 1:35:A:ILE:H   | 1:97:A:VAL:H   | 16       | 0.15          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,73)   | 1:4:A:ALA:H    | 1:19:A:ASN:H   | 18       | 0.15          |
| (1,63)   | 1:41:A:GLY:H   | 1:90:A:ASP:H   | 2        | 0.15          |
| (1,48)   | 1:6:A:ALA:H    | 1:8:A:LEU:H    | 11       | 0.15          |
| (1,43)   | 1:8:A:LEU:H    | 1:18:A:ILE:H   | 13       | 0.15          |
| (1,42)   | 1:19:A:ASN:H   | 1:31:A:VAL:H   | 2        | 0.15          |
| (1,42)   | 1:19:A:ASN:H   | 1:31:A:VAL:H   | 5        | 0.15          |
| (1,42)   | 1:19:A:ASN:H   | 1:31:A:VAL:H   | 15       | 0.15          |
| (1,34)   | 1:34:A:SER:H   | 1:97:A:VAL:H   | 16       | 0.15          |
| (1,26)   | 1:51:A:GLY:H   | 1:149:A:ILE:H  | 4        | 0.15          |
| (1,20)   | 1:89:A:ALA:H   | 1:95:A:ALA:H   | 10       | 0.15          |
| (1,20)   | 1:89:A:ALA:H   | 1:95:A:ALA:H   | 19       | 0.15          |
| (1,14)   | 1:46:A:HIS:H   | 1:48:A:HIS:H   | 13       | 0.15          |
| (3,371)  | 1:132:A:GLU:N  | 2:201:A:CU:CU  | 12       | 0.14          |
| (3,319)  | 1:41:A:GLY:N   | 2:201:A:CU:CU  | 9        | 0.14          |
| (3,319)  | 1:41:A:GLY:N   | 2:201:A:CU:CU  | 18       | 0.14          |
| (3,310)  | 1:31:A:VAL:N   | 2:201:A:CU:CU  | 11       | 0.14          |
| (3,295)  | 1:9:A:LYS:N    | 2:201:A:CU:CU  | 1        | 0.14          |
| (3,295)  | 1:9:A:LYS:N    | 2:201:A:CU:CU  | 8        | 0.14          |
| (3,295)  | 1:9:A:LYS:N    | 2:201:A:CU:CU  | 9        | 0.14          |
| (3,282)  | 1:142:A:SER:C  | 2:201:A:CU:CU  | 6        | 0.14          |
| (3,281)  | 1:135:A:THR:C  | 2:201:A:CU:CU  | 6        | 0.14          |
| (3,274)  | 1:120:A:HIS:C  | 2:201:A:CU:CU  | 16       | 0.14          |
| (3,213)  | 1:10:A:GLY:C   | 2:201:A:CU:CU  | 1        | 0.14          |
| (3,213)  | 1:10:A:GLY:C   | 2:201:A:CU:CU  | 19       | 0.14          |
| (3,196)  | 1:139:A:ASN:C  | 2:201:A:CU:CU  | 1        | 0.14          |
| (3,195)  | 1:138:A:GLY:C  | 2:201:A:CU:CU  | 6        | 0.14          |
| (3,1)    | 1:2:A:THR:C    | 2:201:A:CU:CU  | 17       | 0.14          |
| (2,6884) | 1:31:A:VAL:CB  | 1:35:A:ILE:CD1 | 18       | 0.14          |
| (2,158)  | 1:107:A:SER:N  | 1:109:A:ASP:N  | 7        | 0.14          |
| (1,4533) | 1:40:A:GLU:O   | 1:91:A:LYS:H   | 3        | 0.14          |
| (1,4504) | 1:76:A:ASP:O   | 1:103:A:VAL:H  | 1        | 0.14          |
| (1,4486) | 1:57:A:CYS:N   | 1:145:A:ALA:O  | 5        | 0.14          |
| (1,4455) | 1:47:A:VAL:O   | 1:117:A:LEU:N  | 17       | 0.14          |
| (1,4442) | 1:42:A:LEU:N   | 1:121:A:GLU:O  | 18       | 0.14          |
| (1,4406) | 1:17:A:ILE:O   | 1:32:A:TRP:N   | 15       | 0.14          |
| (1,4404) | 1:18:A:ILE:H   | 1:32:A:TRP:O   | 19       | 0.14          |
| (1,4385) | 1:2:A:THR:O    | 1:21:A:GLU:H   | 12       | 0.14          |
| (1,4324) | 1:2:A:THR:O    | 1:21:A:GLU:H   | 12       | 0.14          |
| (1,3697) | 1:132:A:GLU:CB | 1:136:A:LYS:N  | 15       | 0.14          |
| (1,3480) | 1:126:A:LEU:CA | 1:128:A:LYS:C  | 11       | 0.14          |
| (1,3292) | 1:118:A:VAL:CB | 1:120:A:HIS:CA | 4        | 0.14          |
| (1,2972) | 1:105:A:SER:C  | 1:108:A:GLY:CA | 1        | 0.14          |

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| Key      | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|----------|---------------|---------------|----------|---------------|
| (1,2042) | 1:67:A:LEU:C  | 1:70:A:LYS:CB | 12       | 0.14          |
| (1,2034) | 1:67:A:LEU:C  | 1:69:A:ARG:N  | 15       | 0.14          |
| (1,2005) | 1:66:A:PRO:C  | 1:70:A:LYS:CA | 19       | 0.14          |
| (1,2004) | 1:66:A:PRO:C  | 1:70:A:LYS:N  | 19       | 0.14          |
| (1,1689) | 1:57:A:CYS:CB | 1:59:A:SER:CA | 3        | 0.14          |
| (1,1296) | 1:40:A:GLU:C  | 1:42:A:LEU:CB | 3        | 0.14          |
| (1,1286) | 1:40:A:GLU:CB | 1:42:A:LEU:CB | 11       | 0.14          |
| (1,1267) | 1:39:A:THR:C  | 1:41:A:GLY:N  | 3        | 0.14          |
| (1,1151) | 1:34:A:SER:CA | 1:36:A:LYS:CB | 15       | 0.14          |
| (1,1062) | 1:30:A:LYS:CB | 1:32:A:TRP:CB | 12       | 0.14          |
| (1,976)  | 1:27:A:GLY:CA | 1:30:A:LYS:CA | 6        | 0.14          |
| (1,292)  | 1:37:A:GLY:H  | 1:39:A:THR:H  | 5        | 0.14          |
| (1,271)  | 1:33:A:GLY:H  | 1:99:A:ILE:H  | 7        | 0.14          |
| (1,262)  | 1:17:A:ILE:H  | 1:33:A:GLY:H  | 2        | 0.14          |
| (1,252)  | 1:50:A:PHE:H  | 1:52:A:ASP:H  | 11       | 0.14          |
| (1,252)  | 1:50:A:PHE:H  | 1:52:A:ASP:H  | 16       | 0.14          |
| (1,249)  | 1:50:A:PHE:H  | 1:109:A:ASP:H | 5        | 0.14          |
| (1,247)  | 1:37:A:GLY:H  | 1:39:A:THR:H  | 5        | 0.14          |
| (1,232)  | 1:116:A:THR:H | 1:148:A:VAL:H | 16       | 0.14          |
| (1,228)  | 1:114:A:GLY:H | 1:116:A:THR:H | 5        | 0.14          |
| (1,217)  | 1:87:A:VAL:H  | 1:122:A:LYS:H | 12       | 0.14          |
| (1,211)  | 1:41:A:GLY:H  | 1:89:A:ALA:H  | 1        | 0.14          |
| (1,198)  | 1:52:A:ASP:H  | 1:56:A:GLY:H  | 8        | 0.14          |
| (1,198)  | 1:52:A:ASP:H  | 1:56:A:GLY:H  | 16       | 0.14          |
| (1,198)  | 1:52:A:ASP:H  | 1:56:A:GLY:H  | 17       | 0.14          |
| (1,191)  | 1:52:A:ASP:H  | 1:114:A:GLY:H | 9        | 0.14          |
| (1,191)  | 1:52:A:ASP:H  | 1:114:A:GLY:H | 13       | 0.14          |
| (1,187)  | 1:46:A:HIS:H  | 1:48:A:HIS:H  | 18       | 0.14          |
| (1,178)  | 1:112:A:ILE:H | 1:115:A:ARG:H | 6        | 0.14          |
| (1,177)  | 1:124:A:ASP:H | 1:126:A:LEU:H | 2        | 0.14          |
| (1,173)  | 1:73:A:GLY:H  | 1:126:A:LEU:H | 2        | 0.14          |
| (1,173)  | 1:73:A:GLY:H  | 1:126:A:LEU:H | 10       | 0.14          |
| (1,168)  | 1:88:A:THR:H  | 1:94:A:VAL:H  | 13       | 0.14          |
| (1,168)  | 1:88:A:THR:H  | 1:94:A:VAL:H  | 17       | 0.14          |
| (1,159)  | 1:49:A:GLU:H  | 1:118:A:VAL:H | 8        | 0.14          |
| (1,143)  | 1:36:A:LYS:H  | 1:94:A:VAL:H  | 10       | 0.14          |
| (1,141)  | 1:88:A:THR:H  | 1:94:A:VAL:H  | 13       | 0.14          |
| (1,141)  | 1:88:A:THR:H  | 1:94:A:VAL:H  | 17       | 0.14          |
| (1,139)  | 1:69:A:ARG:H  | 1:78:A:GLU:H  | 8        | 0.14          |
| (1,123)  | 1:22:A:GLN:H  | 1:106:A:LEU:H | 1        | 0.14          |
| (1,123)  | 1:22:A:GLN:H  | 1:106:A:LEU:H | 15       | 0.14          |
| (1,122)  | 1:42:A:LEU:H  | 1:124:A:ASP:H | 12       | 0.14          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,122)  | 1:42:A:LEU:H   | 1:124:A:ASP:H  | 13       | 0.14          |
| (1,120)  | 1:3:A:LYS:H    | 1:151:A:ILE:H  | 16       | 0.14          |
| (1,119)  | 1:45:A:PHE:H   | 1:84:A:LEU:H   | 9        | 0.14          |
| (1,119)  | 1:46:A:HIS:H   | 1:84:A:LEU:H   | 19       | 0.14          |
| (1,112)  | 1:14:A:VAL:H   | 1:36:A:LYS:H   | 4        | 0.14          |
| (1,101)  | 1:45:A:PHE:H   | 1:47:A:VAL:H   | 17       | 0.14          |
| (1,95)   | 1:9:A:LYS:H    | 1:145:A:ALA:H  | 3        | 0.14          |
| (1,47)   | 1:6:A:ALA:H    | 1:20:A:PHE:H   | 16       | 0.14          |
| (1,38)   | 1:6:A:ALA:H    | 1:152:A:ALA:H  | 6        | 0.14          |
| (1,38)   | 1:6:A:ALA:H    | 1:152:A:ALA:H  | 16       | 0.14          |
| (1,23)   | 1:23:A:LYS:H   | 1:106:A:LEU:H  | 2        | 0.14          |
| (1,14)   | 1:46:A:HIS:H   | 1:48:A:HIS:H   | 18       | 0.14          |
| (3,310)  | 1:31:A:VAL:N   | 2:201:A:CU:CU  | 4        | 0.13          |
| (3,253)  | 1:83:A:ASP:C   | 2:201:A:CU:CU  | 8        | 0.13          |
| (3,241)  | 1:59:A:SER:C   | 2:201:A:CU:CU  | 5        | 0.13          |
| (3,213)  | 1:10:A:GLY:C   | 2:201:A:CU:CU  | 4        | 0.13          |
| (3,202)  | 1:48:A:HIS:H   | 2:201:A:CU:CU  | 16       | 0.13          |
| (3,187)  | 1:118:A:VAL:C  | 2:201:A:CU:CU  | 19       | 0.13          |
| (3,183)  | 1:81:A:VAL:C   | 2:201:A:CU:CU  | 6        | 0.13          |
| (3,160)  | 1:113:A:ILE:N  | 2:201:A:CU:CU  | 5        | 0.13          |
| (3,155)  | 1:105:A:SER:N  | 2:201:A:CU:CU  | 8        | 0.13          |
| (3,134)  | 1:77:A:GLU:N   | 2:201:A:CU:CU  | 9        | 0.13          |
| (3,84)   | 1:150:A:GLY:C  | 2:201:A:CU:CU  | 19       | 0.13          |
| (3,1)    | 1:2:A:THR:C    | 2:201:A:CU:CU  | 2        | 0.13          |
| (3,1)    | 1:2:A:THR:C    | 2:201:A:CU:CU  | 12       | 0.13          |
| (2,8807) | 1:41:A:GLY:CA  | 1:44:A:GLY:CA  | 13       | 0.13          |
| (2,6957) | 1:31:A:VAL:CG2 | 1:35:A:ILE:CG1 | 1        | 0.13          |
| (2,156)  | 1:106:A:LEU:N  | 1:108:A:GLY:N  | 4        | 0.13          |
| (1,4586) | 1:22:A:GLN:O   | 1:105:A:SER:N  | 17       | 0.13          |
| (1,4571) | 1:77:A:GLU:N   | 1:102:A:SER:O  | 13       | 0.13          |
| (1,4551) | 1:33:A:GLY:N   | 1:97:A:VAL:O   | 7        | 0.13          |
| (1,4512) | 1:68:A:SER:H   | 1:78:A:GLU:O   | 8        | 0.13          |
| (1,4511) | 1:78:A:GLU:O   | 1:105:A:SER:N  | 4        | 0.13          |
| (1,4493) | 1:68:A:SER:H   | 1:78:A:GLU:O   | 8        | 0.13          |
| (1,4440) | 1:42:A:LEU:O   | 1:44:A:GLY:H   | 12       | 0.13          |
| (1,4427) | 1:39:A:THR:O   | 1:91:A:LYS:N   | 1        | 0.13          |
| (1,4405) | 1:32:A:TRP:H   | 1:97:A:VAL:O   | 3        | 0.13          |
| (1,4404) | 1:18:A:ILE:H   | 1:32:A:TRP:O   | 7        | 0.13          |
| (1,4402) | 1:31:A:VAL:N   | 1:100:A:GLU:O  | 18       | 0.13          |
| (1,4107) | 1:142:A:SER:C  | 1:145:A:ALA:CB | 4        | 0.13          |
| (1,4107) | 1:142:A:SER:C  | 1:145:A:ALA:CB | 8        | 0.13          |
| (1,4104) | 1:142:A:SER:C  | 1:144:A:LEU:C  | 10       | 0.13          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,3900) | 1:135:A:THR:CB | 1:137:A:THR:CB | 11       | 0.13          |
| (1,2975) | 1:106:A:LEU:N  | 1:108:A:GLY:CA | 10       | 0.13          |
| (1,2887) | 1:103:A:VAL:N  | 1:105:A:SER:CA | 4        | 0.13          |
| (1,2332) | 1:79:A:ARG:C   | 1:81:A:VAL:N   | 18       | 0.13          |
| (1,2054) | 1:68:A:SER:CA  | 1:70:A:LYS:CB  | 5        | 0.13          |
| (1,1958) | 1:65:A:ASN:C   | 1:69:A:ARG:CB  | 11       | 0.13          |
| (1,1702) | 1:57:A:CYS:C   | 1:60:A:ALA:N   | 8        | 0.13          |
| (1,1286) | 1:40:A:GLU:CB  | 1:42:A:LEU:CB  | 8        | 0.13          |
| (1,1099) | 1:31:A:VAL:C   | 1:34:A:SER:CB  | 15       | 0.13          |
| (1,356)  | 1:3:A:LYS:CA   | 1:5:A:VAL:CB   | 8        | 0.13          |
| (1,300)  | 1:72:A:GLY:H   | 1:127:A:GLY:H  | 1        | 0.13          |
| (1,300)  | 1:72:A:GLY:H   | 1:127:A:GLY:H  | 11       | 0.13          |
| (1,297)  | 1:73:A:GLY:H   | 1:77:A:GLU:H   | 18       | 0.13          |
| (1,292)  | 1:37:A:GLY:H   | 1:39:A:THR:H   | 1        | 0.13          |
| (1,280)  | 1:108:A:GLY:H  | 1:112:A:ILE:H  | 16       | 0.13          |
| (1,273)  | 1:27:A:GLY:H   | 1:105:A:SER:H  | 5        | 0.13          |
| (1,273)  | 1:27:A:GLY:H   | 1:105:A:SER:H  | 10       | 0.13          |
| (1,271)  | 1:33:A:GLY:H   | 1:99:A:ILE:H   | 15       | 0.13          |
| (1,267)  | 1:33:A:GLY:H   | 1:35:A:ILE:H   | 13       | 0.13          |
| (1,252)  | 1:50:A:PHE:H   | 1:52:A:ASP:H   | 18       | 0.13          |
| (1,251)  | 1:111:A:SER:H  | 1:115:A:ARG:H  | 3        | 0.13          |
| (1,247)  | 1:37:A:GLY:H   | 1:39:A:THR:H   | 1        | 0.13          |
| (1,235)  | 1:116:A:THR:H  | 1:118:A:VAL:H  | 16       | 0.13          |
| (1,232)  | 1:116:A:THR:H  | 1:148:A:VAL:H  | 2        | 0.13          |
| (1,232)  | 1:116:A:THR:H  | 1:148:A:VAL:H  | 18       | 0.13          |
| (1,222)  | 1:72:A:GLY:H   | 1:127:A:GLY:H  | 1        | 0.13          |
| (1,222)  | 1:72:A:GLY:H   | 1:127:A:GLY:H  | 11       | 0.13          |
| (1,218)  | 1:72:A:GLY:H   | 1:79:A:ARG:H   | 1        | 0.13          |
| (1,217)  | 1:87:A:VAL:H   | 1:122:A:LYS:H  | 2        | 0.13          |
| (1,217)  | 1:87:A:VAL:H   | 1:122:A:LYS:H  | 4        | 0.13          |
| (1,205)  | 1:11:A:ASP:H   | 1:145:A:ALA:H  | 14       | 0.13          |
| (1,201)  | 1:16:A:GLY:H   | 1:34:A:SER:H   | 17       | 0.13          |
| (1,201)  | 1:16:A:GLY:H   | 1:34:A:SER:H   | 19       | 0.13          |
| (1,198)  | 1:52:A:ASP:H   | 1:56:A:GLY:H   | 6        | 0.13          |
| (1,195)  | 1:40:A:GLU:H   | 1:91:A:LYS:H   | 13       | 0.13          |
| (1,195)  | 1:40:A:GLU:H   | 1:91:A:LYS:H   | 17       | 0.13          |
| (1,189)  | 1:89:A:ALA:H   | 1:122:A:LYS:H  | 12       | 0.13          |
| (1,187)  | 1:46:A:HIS:H   | 1:48:A:HIS:H   | 1        | 0.13          |
| (1,168)  | 1:88:A:THR:H   | 1:94:A:VAL:H   | 1        | 0.13          |
| (1,159)  | 1:49:A:GLU:H   | 1:118:A:VAL:H  | 5        | 0.13          |
| (1,141)  | 1:88:A:THR:H   | 1:94:A:VAL:H   | 1        | 0.13          |
| (1,138)  | 1:72:A:GLY:H   | 1:79:A:ARG:H   | 1        | 0.13          |

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| Key       | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|-----------|---------------|---------------|----------|---------------|
| (1,134)   | 1:68:A:SER:H  | 1:79:A:ARG:H  | 17       | 0.13          |
| (1,133)   | 1:70:A:LYS:H  | 1:78:A:GLU:H  | 17       | 0.13          |
| (1,131)   | 1:50:A:PHE:H  | 1:60:A:ALA:H  | 15       | 0.13          |
| (1,131)   | 1:50:A:PHE:H  | 1:60:A:ALA:H  | 19       | 0.13          |
| (1,128)   | 1:68:A:SER:H  | 1:79:A:ARG:H  | 17       | 0.13          |
| (1,127)   | 1:70:A:LYS:H  | 1:78:A:GLU:H  | 17       | 0.13          |
| (1,123)   | 1:22:A:GLN:H  | 1:106:A:LEU:H | 12       | 0.13          |
| (1,116)   | 1:42:A:LEU:H  | 1:123:A:ALA:H | 13       | 0.13          |
| (1,115)   | 1:20:A:PHE:H  | 1:151:A:ILE:H | 1        | 0.13          |
| (1,115)   | 1:20:A:PHE:H  | 1:151:A:ILE:H | 2        | 0.13          |
| (1,115)   | 1:20:A:PHE:H  | 1:151:A:ILE:H | 7        | 0.13          |
| (1,112)   | 1:14:A:VAL:H  | 1:36:A:LYS:H  | 5        | 0.13          |
| (1,96)    | 1:15:A:GLN:H  | 1:38:A:LEU:H  | 19       | 0.13          |
| (1,92)    | 1:3:A:LYS:H   | 1:21:A:GLU:H  | 8        | 0.13          |
| (1,73)    | 1:4:A:ALA:H   | 1:19:A:ASN:H  | 15       | 0.13          |
| (1,73)    | 1:4:A:ALA:H   | 1:19:A:ASN:H  | 17       | 0.13          |
| (1,67)    | 1:7:A:VAL:H   | 1:149:A:ILE:H | 13       | 0.13          |
| (1,64)    | 1:90:A:ASP:H  | 1:95:A:ALA:H  | 7        | 0.13          |
| (1,42)    | 1:19:A:ASN:H  | 1:31:A:VAL:H  | 10       | 0.13          |
| (1,38)    | 1:6:A:ALA:H   | 1:152:A:ALA:H | 11       | 0.13          |
| (1,14)    | 1:46:A:HIS:H  | 1:48:A:HIS:H  | 1        | 0.13          |
| (1,11)    | 1:48:A:HIS:H  | 1:83:A:ASP:H  | 8        | 0.13          |
| (3,367)   | 1:121:A:GLU:N | 2:201:A:CU:CU | 19       | 0.12          |
| (3,295)   | 1:9:A:LYS:N   | 2:201:A:CU:CU | 15       | 0.12          |
| (3,213)   | 1:10:A:GLY:C  | 2:201:A:CU:CU | 3        | 0.12          |
| (3,187)   | 1:118:A:VAL:C | 2:201:A:CU:CU | 18       | 0.12          |
| (3,178)   | 1:45:A:PHE:C  | 2:201:A:CU:CU | 3        | 0.12          |
| (3,134)   | 1:77:A:GLU:N  | 2:201:A:CU:CU | 18       | 0.12          |
| (3,84)    | 1:150:A:GLY:C | 2:201:A:CU:CU | 3        | 0.12          |
| (2,10616) | 1:86:A:ASN:CB | 1:89:A:ALA:C  | 13       | 0.12          |
| (2,10545) | 1:86:A:ASN:N  | 1:89:A:ALA:C  | 12       | 0.12          |
| (2,8659)  | 1:40:A:GLU:CB | 1:42:A:LEU:C  | 19       | 0.12          |
| (2,1684)  | 1:6:A:ALA:CB  | 1:9:A:LYS:C   | 18       | 0.12          |
| (2,1237)  | 1:4:A:ALA:CB  | 1:8:A:LEU:CA  | 3        | 0.12          |
| (2,156)   | 1:106:A:LEU:N | 1:108:A:GLY:N | 16       | 0.12          |
| (1,4660)  | 1:5:A:VAL:H   | 1:151:A:ILE:O | 4        | 0.12          |
| (1,4632)  | 1:119:A:VAL:H | 1:144:A:LEU:O | 5        | 0.12          |
| (1,4625)  | 1:41:A:GLY:O  | 1:121:A:GLU:H | 1        | 0.12          |
| (1,4624)  | 1:42:A:LEU:H  | 1:121:A:GLU:O | 6        | 0.12          |
| (1,4620)  | 1:45:A:PHE:H  | 1:120:A:HIS:O | 18       | 0.12          |
| (1,4596)  | 1:114:A:GLY:O | 1:149:A:ILE:H | 13       | 0.12          |
| (1,4565)  | 1:29:A:VAL:O  | 1:100:A:GLU:H | 5        | 0.12          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,4552) | 1:33:A:GLY:H   | 1:97:A:VAL:O   | 18       | 0.12          |
| (1,4547) | 1:33:A:GLY:N   | 1:96:A:ASP:O   | 4        | 0.12          |
| (1,4530) | 1:86:A:ASN:N   | 1:96:A:ASP:O   | 8        | 0.12          |
| (1,4515) | 1:68:A:SER:N   | 1:79:A:ARG:O   | 8        | 0.12          |
| (1,4514) | 1:67:A:LEU:O   | 1:78:A:GLU:N   | 13       | 0.12          |
| (1,4449) | 1:45:A:PHE:H   | 1:120:A:HIS:O  | 18       | 0.12          |
| (1,4441) | 1:42:A:LEU:H   | 1:121:A:GLU:O  | 6        | 0.12          |
| (1,4436) | 1:41:A:GLY:O   | 1:121:A:GLU:H  | 1        | 0.12          |
| (1,4424) | 1:38:A:LEU:O   | 1:93:A:GLY:H   | 12       | 0.12          |
| (1,4417) | 1:15:A:GLN:O   | 1:35:A:ILE:H   | 6        | 0.12          |
| (1,4404) | 1:18:A:ILE:H   | 1:32:A:TRP:O   | 17       | 0.12          |
| (1,4387) | 1:2:A:THR:N    | 1:22:A:GLN:O   | 10       | 0.12          |
| (1,4355) | 1:10:A:GLY:O   | 1:14:A:VAL:N   | 6        | 0.12          |
| (1,4108) | 1:142:A:SER:C  | 1:145:A:ALA:C  | 4        | 0.12          |
| (1,4107) | 1:142:A:SER:C  | 1:145:A:ALA:CB | 10       | 0.12          |
| (1,4106) | 1:142:A:SER:C  | 1:145:A:ALA:CA | 13       | 0.12          |
| (1,4104) | 1:142:A:SER:C  | 1:144:A:LEU:C  | 6        | 0.12          |
| (1,4104) | 1:142:A:SER:C  | 1:144:A:LEU:C  | 16       | 0.12          |
| (1,3940) | 1:136:A:LYS:CG | 1:138:A:GLY:C  | 3        | 0.12          |
| (1,3921) | 1:135:A:THR:C  | 1:138:A:GLY:C  | 14       | 0.12          |
| (1,3516) | 1:126:A:LEU:C  | 1:129:A:GLY:C  | 9        | 0.12          |
| (1,3292) | 1:118:A:VAL:CB | 1:120:A:HIS:CA | 2        | 0.12          |
| (1,2974) | 1:105:A:SER:C  | 1:109:A:ASP:N  | 18       | 0.12          |
| (1,2872) | 1:102:A:SER:CB | 1:105:A:SER:CA | 4        | 0.12          |
| (1,2760) | 1:98:A:SER:CB  | 1:100:A:GLU:CB | 12       | 0.12          |
| (1,2155) | 1:72:A:GLY:C   | 1:74:A:PRO:C   | 5        | 0.12          |
| (1,2064) | 1:68:A:SER:CB  | 1:70:A:LYS:C   | 10       | 0.12          |
| (1,2044) | 1:67:A:LEU:C   | 1:70:A:LYS:C   | 10       | 0.12          |
| (1,2034) | 1:67:A:LEU:C   | 1:69:A:ARG:N   | 4        | 0.12          |
| (1,2034) | 1:67:A:LEU:C   | 1:69:A:ARG:N   | 14       | 0.12          |
| (1,1824) | 1:62:A:PRO:CD  | 1:64:A:PHE:CA  | 18       | 0.12          |
| (1,1308) | 1:41:A:GLY:CA  | 1:43:A:HIS:CB  | 19       | 0.12          |
| (1,1296) | 1:40:A:GLU:C   | 1:42:A:LEU:CB  | 2        | 0.12          |
| (1,1099) | 1:31:A:VAL:C   | 1:34:A:SER:CB  | 5        | 0.12          |
| (1,977)  | 1:27:A:GLY:CA  | 1:30:A:LYS:CB  | 14       | 0.12          |
| (1,976)  | 1:27:A:GLY:CA  | 1:30:A:LYS:CA  | 7        | 0.12          |
| (1,604)  | 1:13:A:PRO:CD  | 1:15:A:GLN:CA  | 15       | 0.12          |
| (1,603)  | 1:13:A:PRO:CD  | 1:15:A:GLN:N   | 4        | 0.12          |
| (1,603)  | 1:13:A:PRO:CD  | 1:15:A:GLN:N   | 14       | 0.12          |
| (1,303)  | 1:69:A:ARG:H   | 1:82:A:GLY:H   | 2        | 0.12          |
| (1,276)  | 1:47:A:VAL:H   | 1:85:A:GLY:H   | 1        | 0.12          |
| (1,273)  | 1:27:A:GLY:H   | 1:105:A:SER:H  | 3        | 0.12          |

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| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,273) | 1:27:A:GLY:H  | 1:105:A:SER:H | 13       | 0.12          |
| (1,273) | 1:27:A:GLY:H  | 1:105:A:SER:H | 19       | 0.12          |
| (1,266) | 1:33:A:GLY:H  | 1:97:A:VAL:H  | 8        | 0.12          |
| (1,261) | 1:129:A:GLY:H | 1:136:A:LYS:H | 9        | 0.12          |
| (1,261) | 1:129:A:GLY:H | 1:136:A:LYS:H | 16       | 0.12          |
| (1,256) | 1:42:A:LEU:H  | 1:44:A:GLY:H  | 8        | 0.12          |
| (1,255) | 1:42:A:LEU:H  | 1:44:A:GLY:H  | 8        | 0.12          |
| (1,251) | 1:111:A:SER:H | 1:115:A:ARG:H | 11       | 0.12          |
| (1,248) | 1:40:A:GLU:H  | 1:93:A:GLY:H  | 16       | 0.12          |
| (1,239) | 1:68:A:SER:H  | 1:71:A:HIS:H  | 9        | 0.12          |
| (1,236) | 1:60:A:ALA:H  | 1:116:A:THR:H | 6        | 0.12          |
| (1,236) | 1:60:A:ALA:H  | 1:116:A:THR:H | 7        | 0.12          |
| (1,219) | 1:72:A:GLY:H  | 1:80:A:HIS:H  | 19       | 0.12          |
| (1,216) | 1:87:A:VAL:H  | 1:89:A:ALA:H  | 13       | 0.12          |
| (1,211) | 1:41:A:GLY:H  | 1:89:A:ALA:H  | 14       | 0.12          |
| (1,208) | 1:34:A:SER:H  | 1:95:A:ALA:H  | 11       | 0.12          |
| (1,208) | 1:34:A:SER:H  | 1:95:A:ALA:H  | 13       | 0.12          |
| (1,207) | 1:17:A:ILE:H  | 1:34:A:SER:H  | 11       | 0.12          |
| (1,201) | 1:16:A:GLY:H  | 1:34:A:SER:H  | 7        | 0.12          |
| (1,201) | 1:16:A:GLY:H  | 1:34:A:SER:H  | 10       | 0.12          |
| (1,195) | 1:40:A:GLU:H  | 1:91:A:LYS:H  | 2        | 0.12          |
| (1,195) | 1:40:A:GLU:H  | 1:91:A:LYS:H  | 14       | 0.12          |
| (1,191) | 1:52:A:ASP:H  | 1:114:A:GLY:H | 10       | 0.12          |
| (1,191) | 1:52:A:ASP:H  | 1:114:A:GLY:H | 16       | 0.12          |
| (1,187) | 1:46:A:HIS:H  | 1:48:A:HIS:H  | 2        | 0.12          |
| (1,177) | 1:124:A:ASP:H | 1:126:A:LEU:H | 14       | 0.12          |
| (1,174) | 1:53:A:ASN:H  | 1:57:A:CYS:H  | 8        | 0.12          |
| (1,162) | 1:67:A:LEU:H  | 1:70:A:LYS:H  | 19       | 0.12          |
| (1,161) | 1:72:A:GLY:H  | 1:80:A:HIS:H  | 19       | 0.12          |
| (1,151) | 1:89:A:ALA:H  | 1:94:A:VAL:H  | 19       | 0.12          |
| (1,143) | 1:36:A:LYS:H  | 1:94:A:VAL:H  | 17       | 0.12          |
| (1,137) | 1:51:A:GLY:H  | 1:111:A:SER:H | 15       | 0.12          |
| (1,135) | 1:79:A:ARG:H  | 1:82:A:GLY:H  | 7        | 0.12          |
| (1,131) | 1:50:A:PHE:H  | 1:60:A:ALA:H  | 16       | 0.12          |
| (1,129) | 1:60:A:ALA:H  | 1:63:A:HIS:H  | 6        | 0.12          |
| (1,129) | 1:60:A:ALA:H  | 1:63:A:HIS:H  | 18       | 0.12          |
| (1,123) | 1:22:A:GLN:H  | 1:106:A:LEU:H | 14       | 0.12          |
| (1,115) | 1:20:A:PHE:H  | 1:151:A:ILE:H | 4        | 0.12          |
| (1,112) | 1:14:A:VAL:H  | 1:36:A:LYS:H  | 9        | 0.12          |
| (1,112) | 1:14:A:VAL:H  | 1:36:A:LYS:H  | 15       | 0.12          |
| (1,95)  | 1:9:A:LYS:H   | 1:145:A:ALA:H | 1        | 0.12          |
| (1,95)  | 1:9:A:LYS:H   | 1:145:A:ALA:H | 10       | 0.12          |

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| Key       | Atom-1         | Atom-2        | Model ID | Violation (Å) |
|-----------|----------------|---------------|----------|---------------|
| (1,95)    | 1:9:A:LYS:H    | 1:145:A:ALA:H | 14       | 0.12          |
| (1,73)    | 1:4:A:ALA:H    | 1:19:A:ASN:H  | 4        | 0.12          |
| (1,73)    | 1:4:A:ALA:H    | 1:19:A:ASN:H  | 8        | 0.12          |
| (1,64)    | 1:90:A:ASP:H   | 1:95:A:ALA:H  | 12       | 0.12          |
| (1,48)    | 1:6:A:ALA:H    | 1:8:A:LEU:H   | 12       | 0.12          |
| (1,43)    | 1:8:A:LEU:H    | 1:18:A:ILE:H  | 5        | 0.12          |
| (1,42)    | 1:19:A:ASN:H   | 1:31:A:VAL:H  | 1        | 0.12          |
| (1,38)    | 1:6:A:ALA:H    | 1:152:A:ALA:H | 1        | 0.12          |
| (1,38)    | 1:6:A:ALA:H    | 1:152:A:ALA:H | 4        | 0.12          |
| (1,32)    | 1:52:A:ASP:H   | 1:149:A:ILE:H | 17       | 0.12          |
| (1,23)    | 1:23:A:LYS:H   | 1:106:A:LEU:H | 9        | 0.12          |
| (1,14)    | 1:46:A:HIS:H   | 1:48:A:HIS:H  | 2        | 0.12          |
| (3,333)   | 1:72:A:GLY:N   | 2:201:A:CU:CU | 11       | 0.11          |
| (3,310)   | 1:31:A:VAL:N   | 2:201:A:CU:CU | 5        | 0.11          |
| (3,310)   | 1:31:A:VAL:N   | 2:201:A:CU:CU | 13       | 0.11          |
| (3,310)   | 1:31:A:VAL:N   | 2:201:A:CU:CU | 17       | 0.11          |
| (3,295)   | 1:9:A:LYS:N    | 2:201:A:CU:CU | 2        | 0.11          |
| (3,279)   | 1:133:A:GLU:C  | 2:201:A:CU:CU | 18       | 0.11          |
| (3,265)   | 1:100:A:GLU:C  | 2:201:A:CU:CU | 8        | 0.11          |
| (3,253)   | 1:83:A:ASP:C   | 2:201:A:CU:CU | 10       | 0.11          |
| (3,241)   | 1:59:A:SER:C   | 2:201:A:CU:CU | 11       | 0.11          |
| (3,196)   | 1:139:A:ASN:C  | 2:201:A:CU:CU | 14       | 0.11          |
| (3,187)   | 1:118:A:VAL:C  | 2:201:A:CU:CU | 14       | 0.11          |
| (3,157)   | 1:109:A:ASP:N  | 2:201:A:CU:CU | 8        | 0.11          |
| (3,95)    | 1:12:A:GLY:N   | 2:201:A:CU:CU | 16       | 0.11          |
| (3,84)    | 1:150:A:GLY:C  | 2:201:A:CU:CU | 9        | 0.11          |
| (2,10792) | 1:87:A:VAL:CG1 | 1:89:A:ALA:CA | 10       | 0.11          |
| (2,10700) | 1:86:A:ASN:C   | 1:89:A:ALA:C  | 14       | 0.11          |
| (2,8661)  | 1:40:A:GLU:CB  | 1:43:A:HIS:CA | 19       | 0.11          |
| (2,4104)  | 1:18:A:ILE:CB  | 1:21:A:GLU:C  | 7        | 0.11          |
| (2,902)   | 1:3:A:LYS:CA   | 1:19:A:ASN:CA | 11       | 0.11          |
| (2,156)   | 1:106:A:LEU:N  | 1:108:A:GLY:N | 3        | 0.11          |
| (1,4660)  | 1:5:A:VAL:H    | 1:151:A:ILE:O | 8        | 0.11          |
| (1,4596)  | 1:114:A:GLY:O  | 1:149:A:ILE:H | 11       | 0.11          |
| (1,4581)  | 1:21:A:GLU:O   | 1:104:A:ILE:H | 11       | 0.11          |
| (1,4580)  | 1:22:A:GLN:H   | 1:104:A:ILE:O | 7        | 0.11          |
| (1,4578)  | 1:76:A:ASP:O   | 1:103:A:VAL:N | 11       | 0.11          |
| (1,4557)  | 1:86:A:ASN:O   | 1:98:A:SER:H  | 5        | 0.11          |
| (1,4495)  | 1:69:A:ARG:O   | 1:79:A:ARG:N  | 13       | 0.11          |
| (1,4486)  | 1:57:A:CYS:N   | 1:116:A:THR:O | 8        | 0.11          |
| (1,4461)  | 1:48:A:HIS:H   | 1:116:A:THR:O | 18       | 0.11          |
| (1,4445)  | 1:42:A:LEU:O   | 1:44:A:GLY:H  | 6        | 0.11          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,4440) | 1:42:A:LEU:O    | 1:44:A:GLY:H   | 6        | 0.11          |
| (1,4417) | 1:15:A:GLN:O    | 1:35:A:ILE:H   | 12       | 0.11          |
| (1,4389) | 1:22:A:GLN:H    | 1:104:A:ILE:O  | 7        | 0.11          |
| (1,4384) | 1:21:A:GLU:O    | 1:104:A:ILE:H  | 11       | 0.11          |
| (1,4355) | 1:10:A:GLY:O    | 1:14:A:VAL:N   | 8        | 0.11          |
| (1,4104) | 1:142:A:SER:C   | 1:144:A:LEU:C  | 18       | 0.11          |
| (1,3918) | 1:135:A:THR:C   | 1:137:A:THR:C  | 15       | 0.11          |
| (1,3831) | 1:134:A:SER:N   | 1:137:A:THR:CB | 19       | 0.11          |
| (1,3298) | 1:118:A:VAL:CG2 | 1:120:A:HIS:CA | 2        | 0.11          |
| (1,3003) | 1:107:A:SER:N   | 1:109:A:ASP:C  | 6        | 0.11          |
| (1,2892) | 1:103:A:VAL:CA  | 1:105:A:SER:CA | 6        | 0.11          |
| (1,2583) | 1:90:A:ASP:C    | 1:92:A:ASP:N   | 13       | 0.11          |
| (1,2576) | 1:90:A:ASP:CB   | 1:92:A:ASP:CG  | 6        | 0.11          |
| (1,2052) | 1:68:A:SER:CA   | 1:70:A:LYS:N   | 5        | 0.11          |
| (1,2046) | 1:68:A:SER:N    | 1:70:A:LYS:CA  | 15       | 0.11          |
| (1,2034) | 1:67:A:LEU:C    | 1:69:A:ARG:N   | 19       | 0.11          |
| (1,2013) | 1:67:A:LEU:CA   | 1:69:A:ARG:N   | 12       | 0.11          |
| (1,2008) | 1:67:A:LEU:N    | 1:69:A:ARG:CG  | 1        | 0.11          |
| (1,1717) | 1:58:A:THR:CA   | 1:60:A:ALA:C   | 9        | 0.11          |
| (1,1689) | 1:57:A:CYS:CB   | 1:59:A:SER:CA  | 4        | 0.11          |
| (1,1689) | 1:57:A:CYS:CB   | 1:59:A:SER:CA  | 5        | 0.11          |
| (1,1314) | 1:41:A:GLY:C    | 1:43:A:HIS:CB  | 3        | 0.11          |
| (1,1286) | 1:40:A:GLU:CB   | 1:42:A:LEU:CB  | 6        | 0.11          |
| (1,1267) | 1:39:A:THR:C    | 1:41:A:GLY:N   | 1        | 0.11          |
| (1,1267) | 1:39:A:THR:C    | 1:41:A:GLY:N   | 2        | 0.11          |
| (1,1267) | 1:39:A:THR:C    | 1:41:A:GLY:N   | 14       | 0.11          |
| (1,1267) | 1:39:A:THR:C    | 1:41:A:GLY:N   | 16       | 0.11          |
| (1,977)  | 1:27:A:GLY:CA   | 1:30:A:LYS:CB  | 5        | 0.11          |
| (1,976)  | 1:27:A:GLY:CA   | 1:30:A:LYS:CA  | 3        | 0.11          |
| (1,976)  | 1:27:A:GLY:CA   | 1:30:A:LYS:CA  | 10       | 0.11          |
| (1,766)  | 1:19:A:ASN:CA   | 1:21:A:GLU:CB  | 18       | 0.11          |
| (1,303)  | 1:69:A:ARG:H    | 1:82:A:GLY:H   | 11       | 0.11          |
| (1,301)  | 1:73:A:GLY:H    | 1:127:A:GLY:H  | 19       | 0.11          |
| (1,280)  | 1:108:A:GLY:H   | 1:112:A:ILE:H  | 1        | 0.11          |
| (1,280)  | 1:108:A:GLY:H   | 1:112:A:ILE:H  | 12       | 0.11          |
| (1,276)  | 1:47:A:VAL:H    | 1:85:A:GLY:H   | 3        | 0.11          |
| (1,266)  | 1:33:A:GLY:H    | 1:97:A:VAL:H   | 13       | 0.11          |
| (1,262)  | 1:17:A:ILE:H    | 1:33:A:GLY:H   | 9        | 0.11          |
| (1,255)  | 1:42:A:LEU:H    | 1:44:A:GLY:H   | 9        | 0.11          |
| (1,249)  | 1:50:A:PHE:H    | 1:109:A:ASP:H  | 6        | 0.11          |
| (1,246)  | 1:9:A:LYS:H     | 1:146:A:CYS:H  | 4        | 0.11          |
| (1,223)  | 1:51:A:GLY:H    | 1:114:A:GLY:H  | 11       | 0.11          |

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| Key      | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|----------|---------------|---------------|----------|---------------|
| (1,223)  | 1:51:A:GLY:H  | 1:114:A:GLY:H | 19       | 0.11          |
| (1,217)  | 1:87:A:VAL:H  | 1:122:A:LYS:H | 3        | 0.11          |
| (1,211)  | 1:41:A:GLY:H  | 1:89:A:ALA:H  | 16       | 0.11          |
| (1,195)  | 1:40:A:GLU:H  | 1:91:A:LYS:H  | 12       | 0.11          |
| (1,187)  | 1:46:A:HIS:H  | 1:48:A:HIS:H  | 7        | 0.11          |
| (1,183)  | 1:51:A:GLY:H  | 1:110:A:HIS:H | 1        | 0.11          |
| (1,177)  | 1:124:A:ASP:H | 1:126:A:LEU:H | 9        | 0.11          |
| (1,173)  | 1:73:A:GLY:H  | 1:126:A:LEU:H | 12       | 0.11          |
| (1,168)  | 1:88:A:THR:H  | 1:94:A:VAL:H  | 10       | 0.11          |
| (1,161)  | 1:72:A:GLY:H  | 1:80:A:HIS:H  | 11       | 0.11          |
| (1,151)  | 1:89:A:ALA:H  | 1:94:A:VAL:H  | 4        | 0.11          |
| (1,141)  | 1:88:A:THR:H  | 1:94:A:VAL:H  | 10       | 0.11          |
| (1,129)  | 1:60:A:ALA:H  | 1:63:A:HIS:H  | 19       | 0.11          |
| (1,122)  | 1:42:A:LEU:H  | 1:124:A:ASP:H | 19       | 0.11          |
| (1,118)  | 1:47:A:VAL:H  | 1:84:A:LEU:H  | 6        | 0.11          |
| (1,116)  | 1:42:A:LEU:H  | 1:123:A:ALA:H | 1        | 0.11          |
| (1,111)  | 1:17:A:ILE:H  | 1:33:A:GLY:H  | 9        | 0.11          |
| (1,98)   | 1:44:A:GLY:H  | 1:123:A:ALA:H | 11       | 0.11          |
| (1,95)   | 1:9:A:LYS:H   | 1:145:A:ALA:H | 8        | 0.11          |
| (1,64)   | 1:90:A:ASP:H  | 1:95:A:ALA:H  | 18       | 0.11          |
| (1,63)   | 1:88:A:THR:H  | 1:90:A:ASP:H  | 1        | 0.11          |
| (1,52)   | 1:21:A:GLU:H  | 1:32:A:TRP:H  | 13       | 0.11          |
| (1,49)   | 1:47:A:VAL:H  | 1:118:A:VAL:H | 17       | 0.11          |
| (1,49)   | 1:47:A:VAL:H  | 1:118:A:VAL:H | 19       | 0.11          |
| (1,43)   | 1:8:A:LEU:H   | 1:18:A:ILE:H  | 14       | 0.11          |
| (1,42)   | 1:19:A:ASN:H  | 1:31:A:VAL:H  | 17       | 0.11          |
| (1,38)   | 1:6:A:ALA:H   | 1:152:A:ALA:H | 5        | 0.11          |
| (1,32)   | 1:52:A:ASP:H  | 1:149:A:ILE:H | 2        | 0.11          |
| (1,14)   | 1:46:A:HIS:H  | 1:48:A:HIS:H  | 7        | 0.11          |
| (3,295)  | 1:9:A:LYS:N   | 2:201:A:CU:CU | 7        | 0.1           |
| (3,281)  | 1:135:A:THR:C | 2:201:A:CU:CU | 19       | 0.1           |
| (3,253)  | 1:83:A:ASP:C  | 2:201:A:CU:CU | 2        | 0.1           |
| (3,234)  | 1:42:A:LEU:C  | 2:201:A:CU:CU | 19       | 0.1           |
| (3,213)  | 1:10:A:GLY:C  | 2:201:A:CU:CU | 12       | 0.1           |
| (3,143)  | 1:90:A:ASP:N  | 2:201:A:CU:CU | 10       | 0.1           |
| (3,133)  | 1:76:A:ASP:N  | 2:201:A:CU:CU | 17       | 0.1           |
| (2,1237) | 1:4:A:ALA:CB  | 1:8:A:LEU:CA  | 15       | 0.1           |
| (2,101)  | 1:67:A:LEU:N  | 1:70:A:LYS:N  | 14       | 0.1           |
| (1,4568) | 1:29:A:VAL:H  | 1:101:A:ASP:O | 2        | 0.1           |
| (1,4515) | 1:68:A:SER:N  | 1:79:A:ARG:O  | 3        | 0.1           |
| (1,4513) | 1:68:A:SER:O  | 1:78:A:GLU:H  | 8        | 0.1           |
| (1,4481) | 1:56:A:GLY:H  | 1:146:A:CYS:O | 11       | 0.1           |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,4464) | 1:49:A:GLU:O   | 1:116:A:THR:H  | 13       | 0.1           |
| (1,4456) | 1:47:A:VAL:O   | 1:118:A:VAL:H  | 9        | 0.1           |
| (1,4440) | 1:42:A:LEU:O   | 1:44:A:GLY:H   | 2        | 0.1           |
| (1,4360) | 1:10:A:GLY:H   | 1:14:A:VAL:O   | 7        | 0.1           |
| (1,3940) | 1:136:A:LYS:CG | 1:138:A:GLY:C  | 2        | 0.1           |
| (1,2976) | 1:106:A:LEU:N  | 1:108:A:GLY:C  | 13       | 0.1           |
| (1,2975) | 1:106:A:LEU:N  | 1:108:A:GLY:CA | 5        | 0.1           |
| (1,1967) | 1:66:A:PRO:CD  | 1:68:A:SER:N   | 9        | 0.1           |
| (1,1314) | 1:41:A:GLY:C   | 1:43:A:HIS:CB  | 10       | 0.1           |
| (1,1267) | 1:39:A:THR:C   | 1:41:A:GLY:N   | 9        | 0.1           |
| (1,273)  | 1:27:A:GLY:H   | 1:105:A:SER:H  | 9        | 0.1           |
| (1,273)  | 1:27:A:GLY:H   | 1:105:A:SER:H  | 12       | 0.1           |
| (1,263)  | 1:27:A:GLY:H   | 1:102:A:SER:H  | 7        | 0.1           |
| (1,262)  | 1:17:A:ILE:H   | 1:33:A:GLY:H   | 6        | 0.1           |
| (1,261)  | 1:129:A:GLY:H  | 1:136:A:LYS:H  | 1        | 0.1           |
| (1,261)  | 1:129:A:GLY:H  | 1:136:A:LYS:H  | 7        | 0.1           |
| (1,252)  | 1:50:A:PHE:H   | 1:52:A:ASP:H   | 14       | 0.1           |
| (1,249)  | 1:50:A:PHE:H   | 1:109:A:ASP:H  | 8        | 0.1           |
| (1,232)  | 1:116:A:THR:H  | 1:148:A:VAL:H  | 3        | 0.1           |
| (1,232)  | 1:116:A:THR:H  | 1:148:A:VAL:H  | 9        | 0.1           |
| (1,219)  | 1:72:A:GLY:H   | 1:80:A:HIS:H   | 17       | 0.1           |
| (1,211)  | 1:41:A:GLY:H   | 1:89:A:ALA:H   | 11       | 0.1           |
| (1,201)  | 1:16:A:GLY:H   | 1:34:A:SER:H   | 1        | 0.1           |
| (1,201)  | 1:16:A:GLY:H   | 1:34:A:SER:H   | 3        | 0.1           |
| (1,199)  | 1:52:A:ASP:H   | 1:149:A:ILE:H  | 11       | 0.1           |
| (1,197)  | 1:52:A:ASP:H   | 1:148:A:VAL:H  | 1        | 0.1           |
| (1,187)  | 1:46:A:HIS:H   | 1:48:A:HIS:H   | 19       | 0.1           |
| (1,185)  | 1:20:A:PHE:H   | 1:150:A:GLY:H  | 3        | 0.1           |
| (1,168)  | 1:88:A:THR:H   | 1:94:A:VAL:H   | 3        | 0.1           |
| (1,161)  | 1:72:A:GLY:H   | 1:80:A:HIS:H   | 17       | 0.1           |
| (1,159)  | 1:49:A:GLU:H   | 1:118:A:VAL:H  | 12       | 0.1           |
| (1,159)  | 1:49:A:GLU:H   | 1:118:A:VAL:H  | 16       | 0.1           |
| (1,146)  | 1:67:A:LEU:H   | 1:109:A:ASP:H  | 14       | 0.1           |
| (1,143)  | 1:36:A:LYS:H   | 1:94:A:VAL:H   | 2        | 0.1           |
| (1,141)  | 1:88:A:THR:H   | 1:94:A:VAL:H   | 3        | 0.1           |
| (1,135)  | 1:79:A:ARG:H   | 1:82:A:GLY:H   | 17       | 0.1           |
| (1,130)  | 1:53:A:ASN:H   | 1:60:A:ALA:H   | 5        | 0.1           |
| (1,122)  | 1:42:A:LEU:H   | 1:124:A:ASP:H  | 8        | 0.1           |
| (1,115)  | 1:20:A:PHE:H   | 1:151:A:ILE:H  | 11       | 0.1           |
| (1,112)  | 1:14:A:VAL:H   | 1:36:A:LYS:H   | 6        | 0.1           |
| (1,111)  | 1:17:A:ILE:H   | 1:33:A:GLY:H   | 6        | 0.1           |
| (1,100)  | 1:46:A:HIS:H   | 1:83:A:ASP:H   | 12       | 0.1           |

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| Key    | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|--------|---------------|---------------|----------|---------------|
| (1,55) | 1:96:A:ASP:H  | 1:98:A:SER:H  | 9        | 0.1           |
| (1,42) | 1:19:A:ASN:H  | 1:31:A:VAL:H  | 19       | 0.1           |
| (1,32) | 1:52:A:ASP:H  | 1:149:A:ILE:H | 11       | 0.1           |
| (1,20) | 1:89:A:ALA:H  | 1:95:A:ALA:H  | 1        | 0.1           |
| (1,14) | 1:46:A:HIS:H  | 1:48:A:HIS:H  | 19       | 0.1           |
| (1,6)  | 1:125:A:ASP:H | 1:127:A:GLY:H | 6        | 0.1           |

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

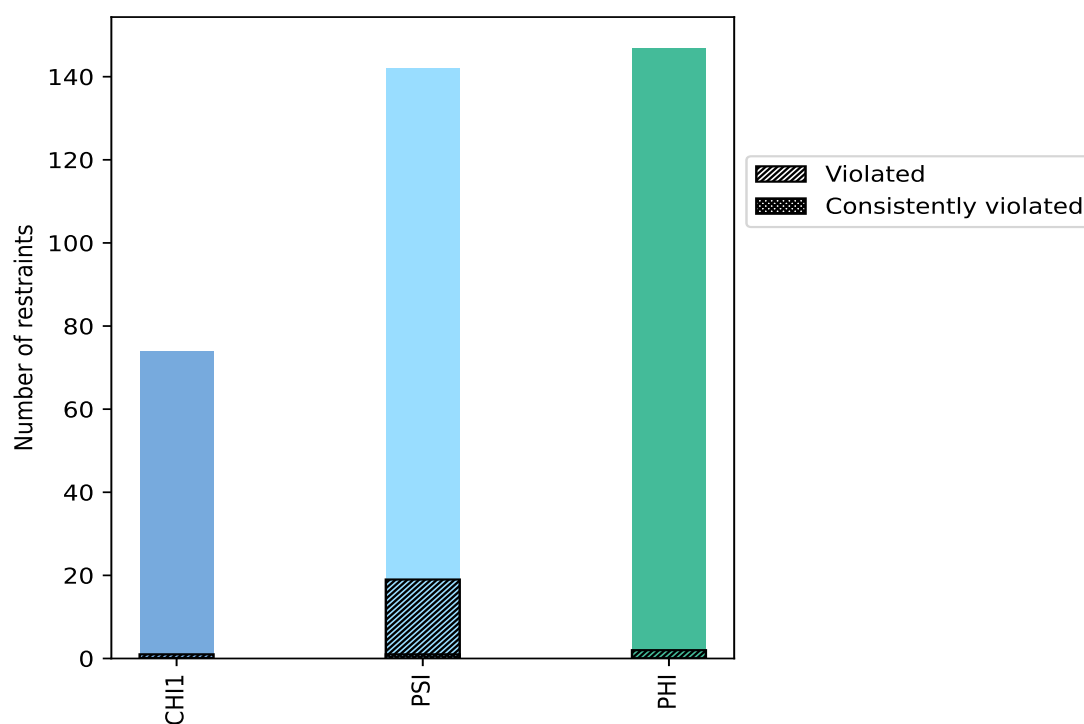
### 10.1 Summary of dihedral-angle violations [i](#)

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> |
| CHI1       | 74    | 20.4           | 1                     | 1.4            | 0.3            | 0                                  | 0.0            | 0.0            |
| PSI        | 142   | 39.1           | 19                    | 13.4           | 5.2            | 1                                  | 0.7            | 0.3            |
| PHI        | 147   | 40.5           | 2                     | 1.4            | 0.6            | 0                                  | 0.0            | 0.0            |
| Total      | 363   | 100.0          | 22                    | 6.1            | 6.1            | 1                                  | 0.3            | 0.3            |

<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](#)



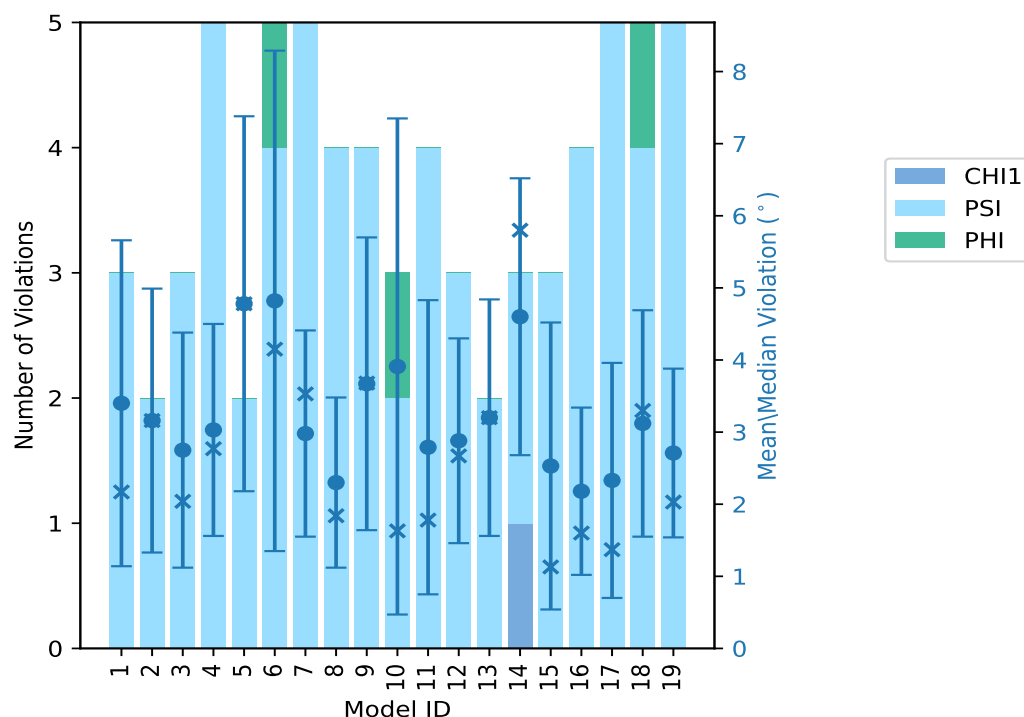
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

## 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 (°) |
|----------|----------------------|-----|-----|-------|----------|---------|--------|------------|
|          | CHI1                 | PSI | PHI | Total |          |         |        |            |
| 1        | 0                    | 3   | 0   | 3     | 3.4      | 6.56    | 2.26   | 2.17       |
| 2        | 0                    | 2   | 0   | 2     | 3.16     | 4.98    | 1.83   | 3.16       |
| 3        | 0                    | 3   | 0   | 3     | 2.75     | 5.01    | 1.63   | 2.04       |
| 4        | 0                    | 5   | 0   | 5     | 3.03     | 5.2     | 1.47   | 2.77       |
| 5        | 0                    | 2   | 0   | 2     | 4.78     | 7.39    | 2.6    | 4.78       |
| 6        | 0                    | 4   | 1   | 5     | 4.82     | 11.34   | 3.47   | 4.15       |
| 7        | 0                    | 5   | 0   | 5     | 2.98     | 4.97    | 1.43   | 3.53       |
| 8        | 0                    | 4   | 0   | 4     | 2.3      | 4.3     | 1.18   | 1.84       |
| 9        | 0                    | 4   | 0   | 4     | 3.67     | 5.79    | 2.03   | 3.68       |
| 10       | 0                    | 2   | 1   | 3     | 3.91     | 8.78    | 3.44   | 1.63       |
| 11       | 0                    | 4   | 0   | 4     | 2.79     | 6.29    | 2.04   | 1.78       |
| 12       | 0                    | 3   | 0   | 3     | 2.88     | 4.72    | 1.42   | 2.67       |
| 13       | 0                    | 2   | 0   | 2     | 3.2      | 4.84    | 1.64   | 3.2        |
| 14       | 1                    | 2   | 0   | 3     | 4.6      | 6.1     | 1.92   | 5.8        |
| 15       | 0                    | 3   | 0   | 3     | 2.53     | 5.35    | 1.99   | 1.13       |
| 16       | 0                    | 4   | 0   | 4     | 2.18     | 4.17    | 1.16   | 1.6        |
| 17       | 0                    | 5   | 0   | 5     | 2.33     | 5.47    | 1.63   | 1.37       |
| 18       | 0                    | 4   | 1   | 5     | 3.12     | 5.81    | 1.57   | 3.3        |
| 19       | 0                    | 5   | 0   | 5     | 2.71     | 4.37    | 1.17   | 2.03       |

### 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 |      |
|-------------------------------|-----|-----|-------|--------------------------|------|
| CHI1                          | PSI | PHI | Total | Count <sup>1</sup>       | %    |
| 1                             | 8   | 1   | 10    | 1                        | 5.3  |
| 0                             | 2   | 1   | 3     | 2                        | 10.5 |
| 0                             | 4   | 0   | 4     | 3                        | 15.8 |
| 0                             | 1   | 0   | 1     | 4                        | 21.1 |
| 0                             | 2   | 0   | 2     | 5                        | 26.3 |
| 0                             | 0   | 0   | 0     | 6                        | 31.6 |
| 0                             | 0   | 0   | 0     | 7                        | 36.8 |
| 0                             | 0   | 0   | 0     | 8                        | 42.1 |
| 0                             | 1   | 0   | 1     | 9                        | 47.4 |
| 0                             | 0   | 0   | 0     | 10                       | 52.6 |
| 0                             | 0   | 0   | 0     | 11                       | 57.9 |

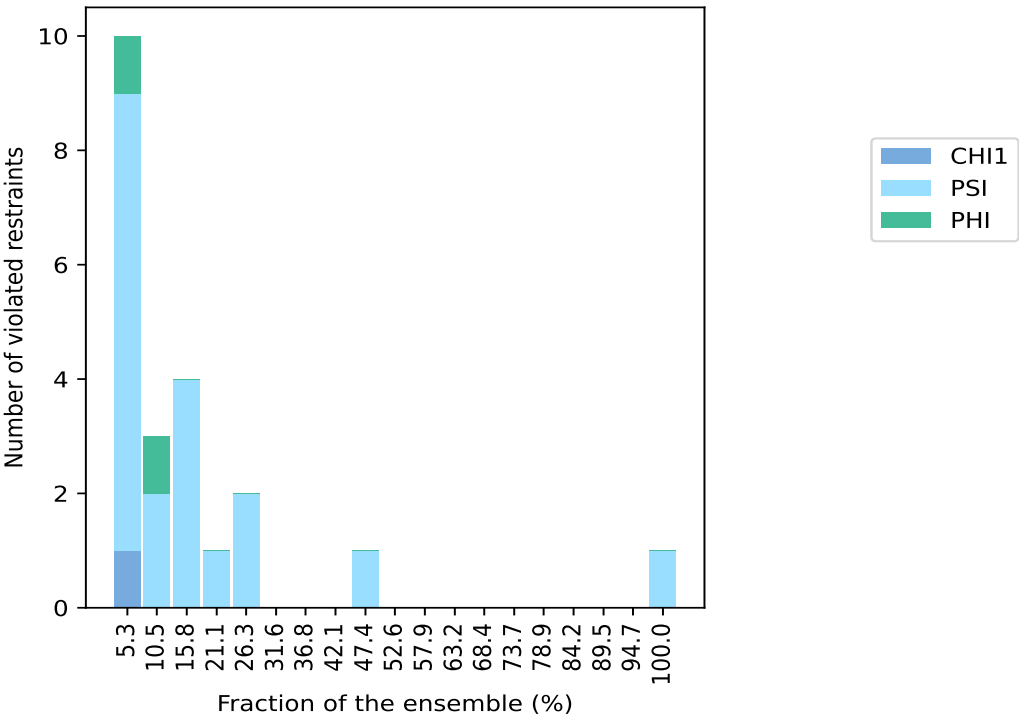
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| Number of violated restraints |     |     |       | Fraction of the ensemble |       |
|-------------------------------|-----|-----|-------|--------------------------|-------|
| CHI1                          | PSI | PHI | Total | Count <sup>1</sup>       | %     |
| 0                             | 0   | 0   | 0     | 12                       | 63.2  |
| 0                             | 0   | 0   | 0     | 13                       | 68.4  |
| 0                             | 0   | 0   | 0     | 14                       | 73.7  |
| 0                             | 0   | 0   | 0     | 15                       | 78.9  |
| 0                             | 0   | 0   | 0     | 16                       | 84.2  |
| 0                             | 0   | 0   | 0     | 17                       | 89.5  |
| 0                             | 0   | 0   | 0     | 18                       | 94.7  |
| 0                             | 1   | 0   | 1     | 19                       | 100.0 |

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

10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)

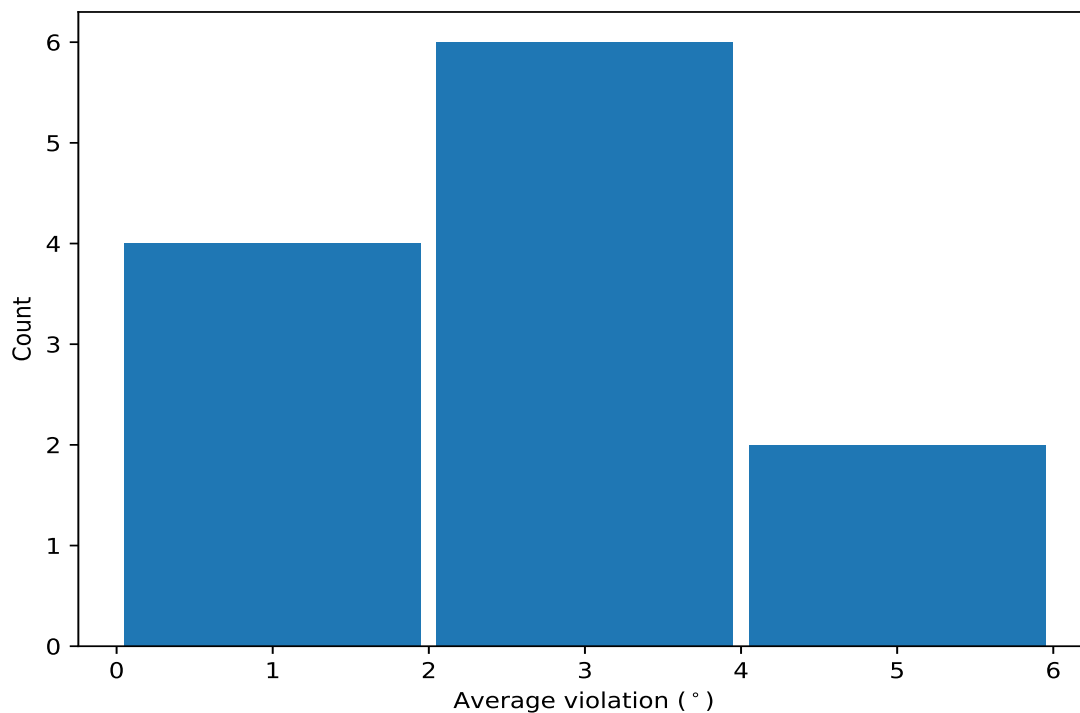


10.4 Most violated dihedral-angle restraints in the ensemble [i](#)

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

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

in the ensemble



#### 10.4.2 Table: Most violated dihedral-angle restraints ⓘ

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.

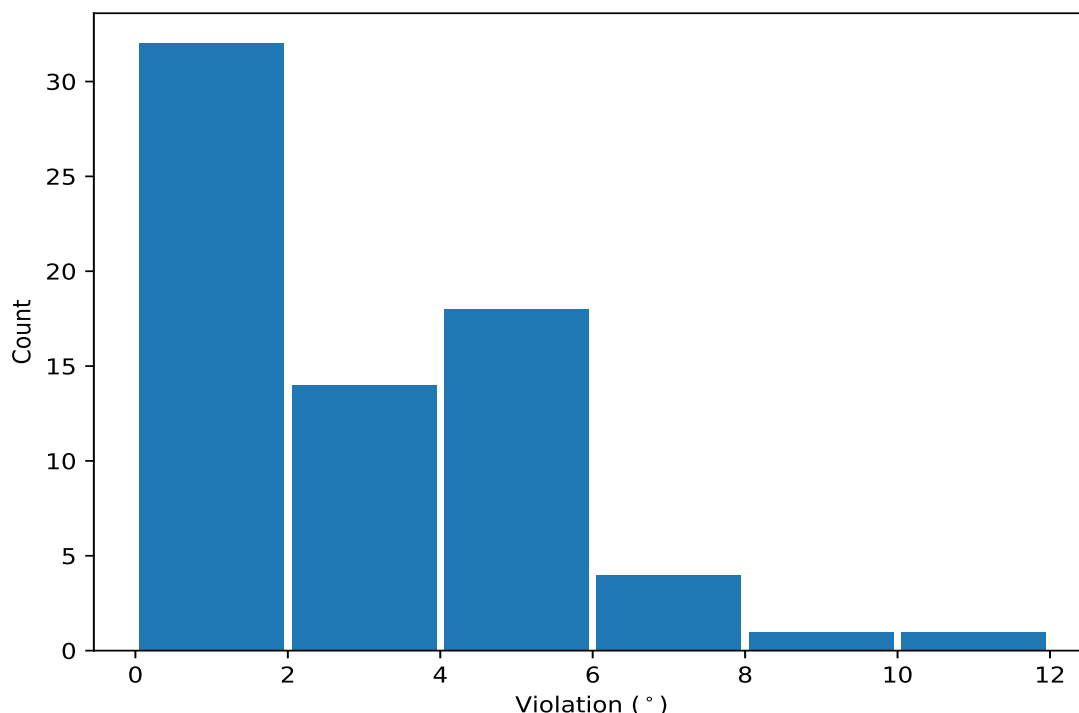
| Key     | Atom-1        | Atom-2         | Atom-3        | Atom-4        | Models <sup>1</sup> | Mean | SD <sup>2</sup> | Median |
|---------|---------------|----------------|---------------|---------------|---------------------|------|-----------------|--------|
| (1,355) | 1:37:A:GLY:N  | 1:37:A:GLY:CA  | 1:37:A:GLY:C  | 1:38:A:LEU:N  | 19                  | 5.47 | 1.14            | 5.2    |
| (1,361) | 1:108:A:GLY:N | 1:108:A:GLY:CA | 1:108:A:GLY:C | 1:109:A:ASP:N | 9                   | 2.13 | 0.83            | 1.75   |
| (1,358) | 1:41:A:GLY:N  | 1:41:A:GLY:CA  | 1:41:A:GLY:C  | 1:42:A:LEU:N  | 5                   | 2.11 | 0.95            | 1.91   |
| (1,98)  | 1:42:A:LEU:N  | 1:42:A:LEU:CA  | 1:42:A:LEU:C  | 1:43:A:HIS:N  | 5                   | 1.47 | 0.26            | 1.33   |
| (1,157) | 1:68:A:SER:N  | 1:68:A:SER:CA  | 1:68:A:SER:C  | 1:69:A:ARG:N  | 4                   | 4.88 | 4.13            | 3.46   |
| (1,251) | 1:109:A:ASP:N | 1:109:A:ASP:CA | 1:109:A:ASP:C | 1:110:A:HIS:N | 3                   | 2.03 | 1.06            | 1.33   |
| (1,357) | 1:10:A:GLY:N  | 1:10:A:GLY:CA  | 1:10:A:GLY:C  | 1:11:A:ASP:N  | 3                   | 2.01 | 0.54            | 2.03   |
| (1,359) | 1:56:A:GLY:N  | 1:56:A:GLY:CA  | 1:56:A:GLY:C  | 1:57:A:CYS:N  | 3                   | 1.72 | 0.23            | 1.65   |
| (1,163) | 1:70:A:LYS:N  | 1:70:A:LYS:CA  | 1:70:A:LYS:C  | 1:71:A:HIS:N  | 3                   | 1.64 | 0.54            | 1.53   |
| (1,142) | 1:60:A:ALA:C  | 1:61:A:GLY:N   | 1:61:A:GLY:CA | 1:61:A:GLY:C  | 2                   | 3.88 | 0.5             | 3.88   |
| (1,290) | 1:124:A:ASP:N | 1:124:A:ASP:CA | 1:124:A:ASP:C | 1:125:A:ASP:N | 2                   | 2.28 | 1.02            | 2.28   |
| (1,363) | 1:150:A:GLY:N | 1:150:A:GLY:CA | 1:150:A:GLY:C | 1:151:A:ILE:N | 2                   | 1.2  | 0.17            | 1.2    |

<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 (°) |
|---------|--------------|---------------|---------------|---------------|----------|---------------|
| (1,157) | 1:68:A:SER:N | 1:68:A:SER:CA | 1:68:A:SER:C  | 1:69:A:ARG:N  | 6        | 11.34         |
| (1,355) | 1:37:A:GLY:N | 1:37:A:GLY:CA | 1:37:A:GLY:C  | 1:38:A:LEU:N  | 10       | 8.78          |
| (1,355) | 1:37:A:GLY:N | 1:37:A:GLY:CA | 1:37:A:GLY:C  | 1:38:A:LEU:N  | 5        | 7.39          |
| (1,355) | 1:37:A:GLY:N | 1:37:A:GLY:CA | 1:37:A:GLY:C  | 1:38:A:LEU:N  | 1        | 6.56          |
| (1,355) | 1:37:A:GLY:N | 1:37:A:GLY:CA | 1:37:A:GLY:C  | 1:38:A:LEU:N  | 11       | 6.29          |
| (1,113) | 1:48:A:HIS:N | 1:48:A:HIS:CA | 1:48:A:HIS:CB | 1:48:A:HIS:CG | 14       | 6.1           |
| (1,355) | 1:37:A:GLY:N | 1:37:A:GLY:CA | 1:37:A:GLY:C  | 1:38:A:LEU:N  | 18       | 5.81          |
| (1,355) | 1:37:A:GLY:N | 1:37:A:GLY:CA | 1:37:A:GLY:C  | 1:38:A:LEU:N  | 14       | 5.8           |
| (1,355) | 1:37:A:GLY:N | 1:37:A:GLY:CA | 1:37:A:GLY:C  | 1:38:A:LEU:N  | 9        | 5.79          |
| (1,157) | 1:68:A:SER:N | 1:68:A:SER:CA | 1:68:A:SER:C  | 1:69:A:ARG:N  | 9        | 5.62          |
| (1,355) | 1:37:A:GLY:N | 1:37:A:GLY:CA | 1:37:A:GLY:C  | 1:38:A:LEU:N  | 17       | 5.47          |
| (1,355) | 1:37:A:GLY:N | 1:37:A:GLY:CA | 1:37:A:GLY:C  | 1:38:A:LEU:N  | 15       | 5.35          |
| (1,355) | 1:37:A:GLY:N | 1:37:A:GLY:CA | 1:37:A:GLY:C  | 1:38:A:LEU:N  | 4        | 5.2           |
| (1,355) | 1:37:A:GLY:N | 1:37:A:GLY:CA | 1:37:A:GLY:C  | 1:38:A:LEU:N  | 3        | 5.01          |

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| Key     | Atom-1        | Atom-2         | Atom-3        | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|---------------|---------------|----------|---------------|
| (1,355) | 1:37:A:GLY:N  | 1:37:A:GLY:CA  | 1:37:A:GLY:C  | 1:38:A:LEU:N  | 2        | 4.98          |
| (1,355) | 1:37:A:GLY:N  | 1:37:A:GLY:CA  | 1:37:A:GLY:C  | 1:38:A:LEU:N  | 7        | 4.97          |
| (1,355) | 1:37:A:GLY:N  | 1:37:A:GLY:CA  | 1:37:A:GLY:C  | 1:38:A:LEU:N  | 13       | 4.84          |
| (1,355) | 1:37:A:GLY:N  | 1:37:A:GLY:CA  | 1:37:A:GLY:C  | 1:38:A:LEU:N  | 12       | 4.72          |
| (1,142) | 1:60:A:ALA:C  | 1:61:A:GLY:N   | 1:61:A:GLY:CA | 1:61:A:GLY:C  | 6        | 4.38          |
| (1,355) | 1:37:A:GLY:N  | 1:37:A:GLY:CA  | 1:37:A:GLY:C  | 1:38:A:LEU:N  | 19       | 4.37          |
| (1,355) | 1:37:A:GLY:N  | 1:37:A:GLY:CA  | 1:37:A:GLY:C  | 1:38:A:LEU:N  | 8        | 4.3           |
| (1,355) | 1:37:A:GLY:N  | 1:37:A:GLY:CA  | 1:37:A:GLY:C  | 1:38:A:LEU:N  | 16       | 4.17          |
| (1,187) | 1:80:A:HIS:N  | 1:80:A:HIS:CA  | 1:80:A:HIS:C  | 1:81:A:VAL:N  | 4        | 4.17          |
| (1,355) | 1:37:A:GLY:N  | 1:37:A:GLY:CA  | 1:37:A:GLY:C  | 1:38:A:LEU:N  | 6        | 4.15          |
| (1,358) | 1:41:A:GLY:N  | 1:41:A:GLY:CA  | 1:41:A:GLY:C  | 1:42:A:LEU:N  | 19       | 3.87          |
| (1,361) | 1:108:A:GLY:N | 1:108:A:GLY:CA | 1:108:A:GLY:C | 1:109:A:ASP:N | 7        | 3.68          |
| (1,251) | 1:109:A:ASP:N | 1:109:A:ASP:CA | 1:109:A:ASP:C | 1:110:A:HIS:N | 7        | 3.53          |
| (1,142) | 1:60:A:ALA:C  | 1:61:A:GLY:N   | 1:61:A:GLY:CA | 1:61:A:GLY:C  | 18       | 3.38          |
| (1,290) | 1:124:A:ASP:N | 1:124:A:ASP:CA | 1:124:A:ASP:C | 1:125:A:ASP:N | 18       | 3.3           |
| (1,361) | 1:108:A:GLY:N | 1:108:A:GLY:CA | 1:108:A:GLY:C | 1:109:A:ASP:N | 6        | 3.22          |
| (1,361) | 1:108:A:GLY:N | 1:108:A:GLY:CA | 1:108:A:GLY:C | 1:109:A:ASP:N | 4        | 2.77          |
| (1,357) | 1:10:A:GLY:N  | 1:10:A:GLY:CA  | 1:10:A:GLY:C  | 1:11:A:ASP:N  | 12       | 2.67          |
| (1,163) | 1:70:A:LYS:N  | 1:70:A:LYS:CA  | 1:70:A:LYS:C  | 1:71:A:HIS:N  | 17       | 2.35          |
| (1,360) | 1:85:A:GLY:N  | 1:85:A:GLY:CA  | 1:85:A:GLY:C  | 1:86:A:ASN:N  | 5        | 2.18          |
| (1,358) | 1:41:A:GLY:N  | 1:41:A:GLY:CA  | 1:41:A:GLY:C  | 1:42:A:LEU:N  | 1        | 2.17          |
| (1,123) | 1:52:A:ASP:N  | 1:52:A:ASP:CA  | 1:52:A:ASP:C  | 1:53:A:ASN:N  | 11       | 2.09          |
| (1,359) | 1:56:A:GLY:N  | 1:56:A:GLY:CA  | 1:56:A:GLY:C  | 1:57:A:CYS:N  | 3        | 2.04          |
| (1,357) | 1:10:A:GLY:N  | 1:10:A:GLY:CA  | 1:10:A:GLY:C  | 1:11:A:ASP:N  | 19       | 2.03          |
| (1,358) | 1:41:A:GLY:N  | 1:41:A:GLY:CA  | 1:41:A:GLY:C  | 1:42:A:LEU:N  | 8        | 1.91          |
| (1,98)  | 1:42:A:LEU:N  | 1:42:A:LEU:CA  | 1:42:A:LEU:C  | 1:43:A:HIS:N  | 14       | 1.89          |
| (1,361) | 1:108:A:GLY:N | 1:108:A:GLY:CA | 1:108:A:GLY:C | 1:109:A:ASP:N | 8        | 1.77          |
| (1,178) | 1:77:A:GLU:N  | 1:77:A:GLU:CA  | 1:77:A:GLU:C  | 1:78:A:GLU:N  | 18       | 1.76          |
| (1,361) | 1:108:A:GLY:N | 1:108:A:GLY:CA | 1:108:A:GLY:C | 1:109:A:ASP:N | 9        | 1.75          |
| (1,361) | 1:108:A:GLY:N | 1:108:A:GLY:CA | 1:108:A:GLY:C | 1:109:A:ASP:N | 16       | 1.73          |
| (1,256) | 1:111:A:SER:N | 1:111:A:SER:CA | 1:111:A:SER:C | 1:112:A:ILE:N | 7        | 1.69          |
| (1,55)  | 1:23:A:LYS:N  | 1:23:A:LYS:CA  | 1:23:A:LYS:C  | 1:24:A:GLU:N  | 4        | 1.69          |
| (1,359) | 1:56:A:GLY:N  | 1:56:A:GLY:CA  | 1:56:A:GLY:C  | 1:57:A:CYS:N  | 19       | 1.65          |
| (1,361) | 1:108:A:GLY:N | 1:108:A:GLY:CA | 1:108:A:GLY:C | 1:109:A:ASP:N | 19       | 1.63          |
| (1,98)  | 1:42:A:LEU:N  | 1:42:A:LEU:CA  | 1:42:A:LEU:C  | 1:43:A:HIS:N  | 10       | 1.63          |
| (1,208) | 1:90:A:ASP:N  | 1:90:A:ASP:CA  | 1:90:A:ASP:C  | 1:91:A:LYS:N  | 13       | 1.55          |
| (1,163) | 1:70:A:LYS:N  | 1:70:A:LYS:CA  | 1:70:A:LYS:C  | 1:71:A:HIS:N  | 9        | 1.53          |
| (1,359) | 1:56:A:GLY:N  | 1:56:A:GLY:CA  | 1:56:A:GLY:C  | 1:57:A:CYS:N  | 16       | 1.48          |
| (1,358) | 1:41:A:GLY:N  | 1:41:A:GLY:CA  | 1:41:A:GLY:C  | 1:42:A:LEU:N  | 11       | 1.47          |
| (1,361) | 1:108:A:GLY:N | 1:108:A:GLY:CA | 1:108:A:GLY:C | 1:109:A:ASP:N | 1        | 1.46          |
| (1,363) | 1:150:A:GLY:N | 1:150:A:GLY:CA | 1:150:A:GLY:C | 1:151:A:ILE:N | 17       | 1.37          |
| (1,357) | 1:10:A:GLY:N  | 1:10:A:GLY:CA  | 1:10:A:GLY:C  | 1:11:A:ASP:N  | 16       | 1.34          |
| (1,251) | 1:109:A:ASP:N | 1:109:A:ASP:CA | 1:109:A:ASP:C | 1:110:A:HIS:N | 18       | 1.33          |
| (1,121) | 1:50:A:PHE:C  | 1:51:A:GLY:N   | 1:51:A:GLY:CA | 1:51:A:GLY:C  | 10       | 1.33          |
| (1,98)  | 1:42:A:LEU:N  | 1:42:A:LEU:CA  | 1:42:A:LEU:C  | 1:43:A:HIS:N  | 2        | 1.33          |
| (1,98)  | 1:42:A:LEU:N  | 1:42:A:LEU:CA  | 1:42:A:LEU:C  | 1:43:A:HIS:N  | 4        | 1.33          |
| (1,157) | 1:68:A:SER:N  | 1:68:A:SER:CA  | 1:68:A:SER:C  | 1:69:A:ARG:N  | 11       | 1.3           |
| (1,290) | 1:124:A:ASP:N | 1:124:A:ASP:CA | 1:124:A:ASP:C | 1:125:A:ASP:N | 17       | 1.26          |
| (1,157) | 1:68:A:SER:N  | 1:68:A:SER:CA  | 1:68:A:SER:C  | 1:69:A:ARG:N  | 12       | 1.26          |
| (1,251) | 1:109:A:ASP:N | 1:109:A:ASP:CA | 1:109:A:ASP:C | 1:110:A:HIS:N | 8        | 1.22          |
| (1,175) | 1:76:A:ASP:N  | 1:76:A:ASP:CA  | 1:76:A:ASP:C  | 1:77:A:GLU:N  | 3        | 1.2           |

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| Key     | Atom-1        | Atom-2         | Atom-3        | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|---------------|---------------|----------|---------------|
| (1,98)  | 1:42:A:LEU:N  | 1:42:A:LEU:CA  | 1:42:A:LEU:C  | 1:43:A:HIS:N  | 17       | 1.18          |
| (1,358) | 1:41:A:GLY:N  | 1:41:A:GLY:CA  | 1:41:A:GLY:C  | 1:42:A:LEU:N  | 15       | 1.13          |
| (1,361) | 1:108:A:GLY:N | 1:108:A:GLY:CA | 1:108:A:GLY:C | 1:109:A:ASP:N | 15       | 1.12          |
| (1,163) | 1:70:A:LYS:N  | 1:70:A:LYS:CA  | 1:70:A:LYS:C  | 1:71:A:HIS:N  | 7        | 1.04          |
| (1,363) | 1:150:A:GLY:N | 1:150:A:GLY:CA | 1:150:A:GLY:C | 1:151:A:ILE:N | 6        | 1.03          |