



# Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2026 – 02:09 AM UTC

PDB ID : 2MPX / pdb\_00002mpx  
BMRB ID : 25005  
Title : Three-dimensional structure of CAP-GLY DOMAIN ASSEMBLED ON MICROTUBULES DETERMINED BY MAS NMR SPECTROSCOPY  
Authors : Yan, S.; Hou, G.; Zhang, H.; Polenova, T.; Williams, J.C.  
Deposited on : 2014-06-08

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

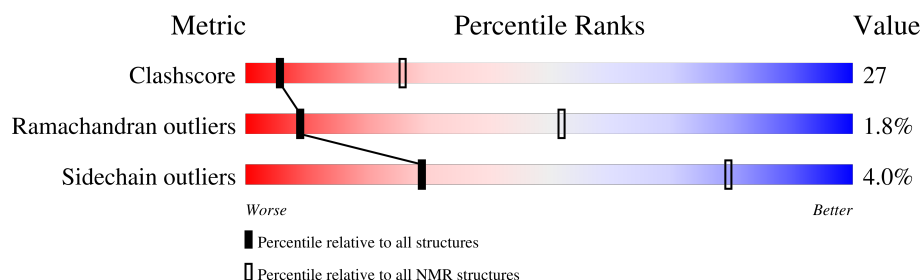
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLID-STATE NMR*

The overall completeness of chemical shifts assignment is 33%.

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



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

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

| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 1   | C     | 70     |  |

## 2 Ensemble composition and analysis

This entry contains 10 models. Model 1 is the overall representative, medoid model (most similar to other models).

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

| Well-defined (core) protein residues |                       |                   |              |
|--------------------------------------|-----------------------|-------------------|--------------|
| Well-defined core                    | Residue range (total) | Backbone RMSD (Å) | Medoid model |
| 1                                    | C:28-C:95 (68)        | 0.44              | 1            |

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

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

The models can be grouped into 2 clusters and 6 single-model clusters were found.

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

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

There is only 1 type of molecule in this entry. The entry contains 1074 atoms, of which 540 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Dynactin subunit 1.

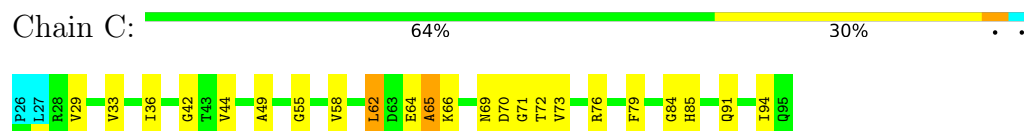
| Mol | Chain | Residues | Atoms |     |     |     |    |   | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---|-------|
| 1   | C     | 70       | Total | C   | H   | N   | O  | S | 0     |
|     |       |          | 1074  | 336 | 540 | 100 | 97 | 1 |       |

## 4 Residue-property plots

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

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

- Molecule 1: Dynactin subunit 1

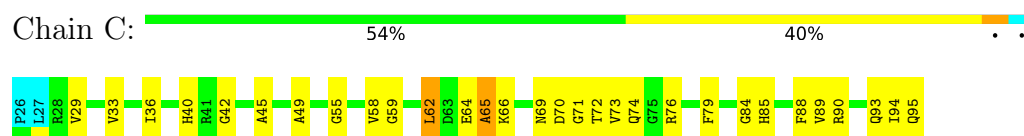


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

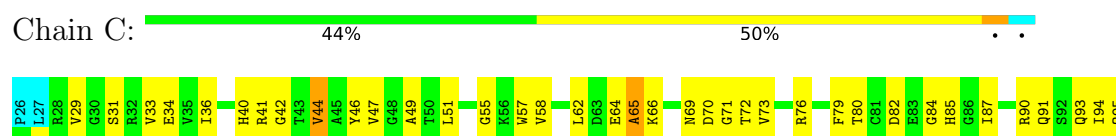
#### 4.2.1 Score per residue for model 1 (medoid)

- Molecule 1: Dynactin subunit 1



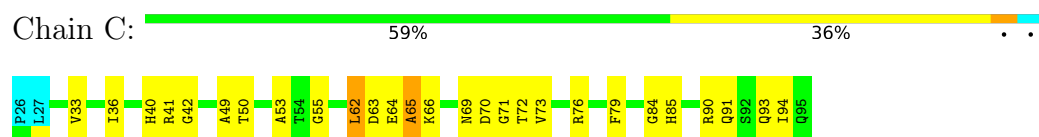
#### 4.2.2 Score per residue for model 2

- Molecule 1: Dynactin subunit 1



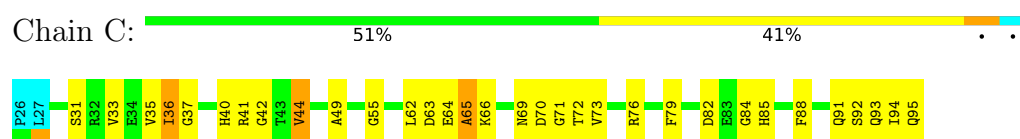
### 4.2.3 Score per residue for model 3

- Molecule 1: Dynactin subunit 1



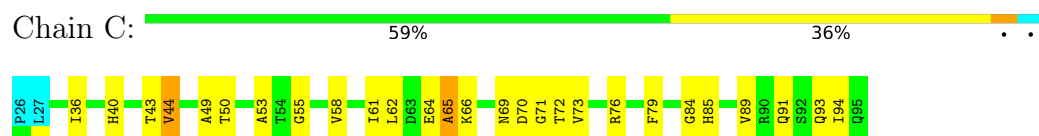
### 4.2.4 Score per residue for model 4

- Molecule 1: Dynactin subunit 1



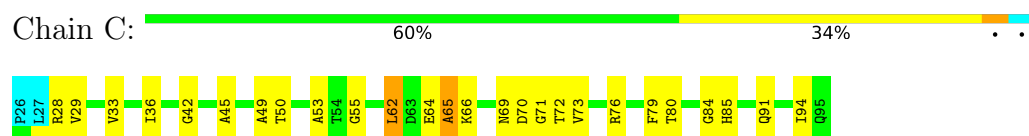
### 4.2.5 Score per residue for model 5

- Molecule 1: Dynactin subunit 1



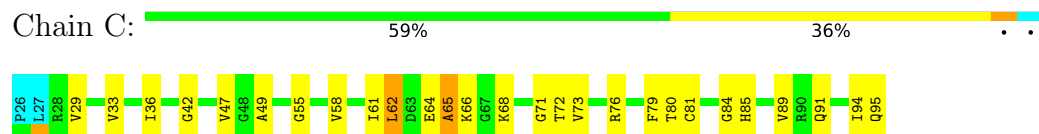
### 4.2.6 Score per residue for model 6

- Molecule 1: Dynactin subunit 1



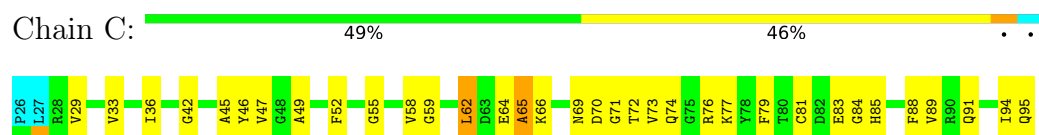
### 4.2.7 Score per residue for model 7

- Molecule 1: Dynactin subunit 1



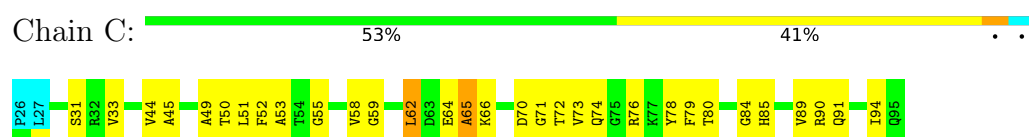
### 4.2.8 Score per residue for model 8

- Molecule 1: Dynactin subunit 1



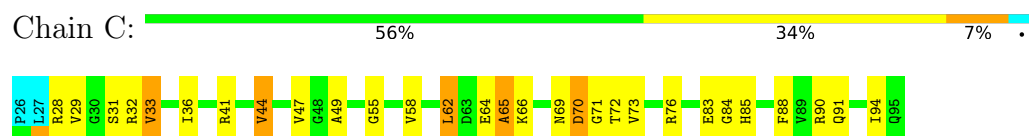
### 4.2.9 Score per residue for model 9

- Molecule 1: Dynactin subunit 1



### 4.2.10 Score per residue for model 10

- Molecule 1: Dynactin subunit 1



## 5 Refinement protocol and experimental data overview

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

Of the 500 calculated structures, 10 were deposited, based on the following criterion: *structures with the lowest energy*.

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

| Software name | Classification     | Version |
|---------------|--------------------|---------|
| X-PLOR NIH    | structure solution | 2.35    |
| X-PLOR NIH    | refinement         | 2.35    |

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                       | 312            |
| Number of shifts mapped to atoms             | 312            |
| Number of unparsed shifts                    | 0              |
| Number of shifts with mapping errors         | 0              |
| Number of shifts with mapping warnings       | 0              |
| Assignment completeness (well-defined parts) | 33%            |

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 [i](#)

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

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes |
|-----|-------|-------|----------|----------|---------|
| 1   | C     | 519   | 520      | 520      | 28±4    |
| All | All   | 5190  | 5200     | 5200     | 285     |

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 27.

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

| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:C:49:ALA:HB2  | 1:C:55:GLY:O    | 0.71     | 1.84        | 2      | 9     |
| 1:C:31:SER:O    | 1:C:44:VAL:HG12 | 0.67     | 1.89        | 10     | 2     |
| 1:C:33:VAL:HG12 | 1:C:42:GLY:C    | 0.67     | 2.14        | 8      | 5     |
| 1:C:31:SER:O    | 1:C:44:VAL:HG23 | 0.65     | 1.91        | 9      | 1     |
| 1:C:62:LEU:O    | 1:C:85:HIS:ND1  | 0.63     | 2.31        | 6      | 6     |
| 1:C:33:VAL:HG12 | 1:C:44:VAL:HG13 | 0.62     | 1.69        | 4      | 1     |
| 1:C:73:VAL:O    | 1:C:76:ARG:N    | 0.62     | 2.32        | 9      | 8     |
| 1:C:71:GLY:O    | 1:C:72:THR:HG23 | 0.62     | 1.94        | 10     | 10    |
| 1:C:91:GLN:CD   | 1:C:91:GLN:H    | 0.61     | 2.04        | 2      | 2     |
| 1:C:64:GLU:O    | 1:C:65:ALA:HB3  | 0.61     | 1.96        | 1      | 10    |
| 1:C:85:HIS:N    | 1:C:85:HIS:ND1  | 0.59     | 2.49        | 7      | 4     |
| 1:C:88:PHE:CD2  | 1:C:88:PHE:O    | 0.57     | 2.58        | 1      | 3     |
| 1:C:66:LYS:N    | 1:C:84:GLY:O    | 0.57     | 2.37        | 7      | 10    |
| 1:C:32:ARG:NE   | 1:C:41:ARG:HH21 | 0.56     | 1.98        | 10     | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:C:70:ASP:OD1  | 1:C:79:PHE:N    | 0.56     | 2.39        | 2      | 2     |
| 1:C:36:ILE:HG22 | 1:C:36:ILE:O    | 0.55     | 2.02        | 4      | 4     |
| 1:C:40:HIS:CE1  | 1:C:41:ARG:O    | 0.54     | 2.61        | 3      | 2     |
| 1:C:69:ASN:ND2  | 1:C:72:THR:O    | 0.54     | 2.40        | 3      | 4     |
| 1:C:45:ALA:HB3  | 1:C:59:GLY:O    | 0.54     | 2.03        | 8      | 3     |
| 1:C:40:HIS:ND1  | 1:C:62:LEU:HD11 | 0.53     | 2.18        | 1      | 1     |
| 1:C:47:VAL:CG2  | 1:C:91:GLN:HE21 | 0.53     | 2.16        | 7      | 1     |
| 1:C:52:PHE:N    | 1:C:74:GLN:OE1  | 0.53     | 2.41        | 9      | 1     |
| 1:C:49:ALA:CB   | 1:C:55:GLY:O    | 0.53     | 2.55        | 2      | 6     |
| 1:C:90:ARG:NH1  | 1:C:93:GLN:OE1  | 0.53     | 2.42        | 1      | 1     |
| 1:C:62:LEU:O    | 1:C:85:HIS:CD2  | 0.53     | 2.62        | 2      | 3     |
| 1:C:91:GLN:NE2  | 1:C:92:SER:OG   | 0.53     | 2.42        | 4      | 1     |
| 1:C:70:ASP:OD1  | 1:C:70:ASP:N    | 0.52     | 2.41        | 5      | 2     |
| 1:C:40:HIS:CD2  | 1:C:41:ARG:O    | 0.52     | 2.62        | 4      | 1     |
| 1:C:90:ARG:N    | 1:C:90:ARG:CD   | 0.52     | 2.73        | 2      | 1     |
| 1:C:34:GLU:N    | 1:C:95:GLN:OXT  | 0.51     | 2.43        | 2      | 1     |
| 1:C:33:VAL:N    | 1:C:42:GLY:O    | 0.51     | 2.44        | 2      | 1     |
| 1:C:91:GLN:CD   | 1:C:91:GLN:N    | 0.51     | 2.69        | 10     | 1     |
| 1:C:64:GLU:O    | 1:C:65:ALA:CB   | 0.51     | 2.58        | 10     | 10    |
| 1:C:69:ASN:N    | 1:C:69:ASN:OD1  | 0.50     | 2.44        | 2      | 1     |
| 1:C:61:ILE:HD11 | 1:C:79:PHE:CD1  | 0.50     | 2.41        | 5      | 1     |
| 1:C:84:GLY:C    | 1:C:85:HIS:CD2  | 0.50     | 2.89        | 3      | 3     |
| 1:C:43:THR:CG2  | 1:C:61:ILE:HD12 | 0.50     | 2.37        | 5      | 1     |
| 1:C:50:THR:HG21 | 1:C:78:TYR:OH   | 0.50     | 2.06        | 9      | 1     |
| 1:C:36:ILE:CG1  | 1:C:93:GLN:O    | 0.49     | 2.60        | 4      | 5     |
| 1:C:52:PHE:CD2  | 1:C:88:PHE:CZ   | 0.49     | 3.00        | 8      | 1     |
| 1:C:71:GLY:O    | 1:C:72:THR:CG2  | 0.49     | 2.61        | 10     | 10    |
| 1:C:73:VAL:N    | 1:C:76:ARG:O    | 0.49     | 2.41        | 8      | 6     |
| 1:C:33:VAL:CG1  | 1:C:44:VAL:HG13 | 0.49     | 2.37        | 4      | 1     |
| 1:C:76:ARG:NH1  | 1:C:77:LYS:O    | 0.49     | 2.44        | 8      | 1     |
| 1:C:91:GLN:O    | 1:C:94:ILE:O    | 0.49     | 2.30        | 5      | 9     |
| 1:C:58:VAL:N    | 1:C:89:VAL:O    | 0.49     | 2.42        | 1      | 5     |
| 1:C:49:ALA:CA   | 1:C:55:GLY:O    | 0.49     | 2.61        | 4      | 10    |
| 1:C:91:GLN:CD   | 1:C:92:SER:N    | 0.49     | 2.71        | 4      | 1     |
| 1:C:51:LEU:CD2  | 1:C:51:LEU:N    | 0.48     | 2.76        | 2      | 1     |
| 1:C:40:HIS:HE2  | 1:C:63:ASP:H    | 0.48     | 1.51        | 4      | 1     |
| 1:C:85:HIS:CD2  | 1:C:85:HIS:N    | 0.48     | 2.81        | 3      | 3     |
| 1:C:51:LEU:HD12 | 1:C:51:LEU:N    | 0.48     | 2.24        | 9      | 1     |
| 1:C:84:GLY:C    | 1:C:85:HIS:ND1  | 0.47     | 2.72        | 2      | 4     |
| 1:C:47:VAL:HG12 | 1:C:58:VAL:HG22 | 0.47     | 1.86        | 10     | 1     |
| 1:C:51:LEU:N    | 1:C:51:LEU:HD22 | 0.47     | 2.23        | 2      | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:C:52:PHE:CE2  | 1:C:88:PHE:CE2  | 0.47     | 3.02        | 8      | 1     |
| 1:C:50:THR:CG2  | 1:C:78:TYR:OH   | 0.47     | 2.62        | 9      | 1     |
| 1:C:88:PHE:O    | 1:C:88:PHE:CG   | 0.46     | 2.67        | 1      | 2     |
| 1:C:90:ARG:HD2  | 1:C:90:ARG:H    | 0.46     | 1.71        | 10     | 2     |
| 1:C:81:CYS:SG   | 1:C:85:HIS:CG   | 0.46     | 3.09        | 7      | 1     |
| 1:C:69:ASN:O    | 1:C:73:VAL:CG2  | 0.46     | 2.64        | 1      | 4     |
| 1:C:47:VAL:HG23 | 1:C:58:VAL:HG22 | 0.45     | 1.88        | 7      | 1     |
| 1:C:50:THR:O    | 1:C:53:ALA:O    | 0.45     | 2.35        | 3      | 4     |
| 1:C:62:LEU:HD22 | 1:C:87:ILE:CD1  | 0.45     | 2.41        | 2      | 1     |
| 1:C:79:PHE:CD1  | 1:C:80:THR:N    | 0.45     | 2.85        | 7      | 1     |
| 1:C:73:VAL:O    | 1:C:76:ARG:O    | 0.45     | 2.34        | 1      | 5     |
| 1:C:32:ARG:CZ   | 1:C:41:ARG:HH21 | 0.45     | 2.25        | 10     | 1     |
| 1:C:29:VAL:HG23 | 1:C:45:ALA:O    | 0.45     | 2.11        | 6      | 2     |
| 1:C:69:ASN:O    | 1:C:69:ASN:CG   | 0.45     | 2.60        | 10     | 4     |
| 1:C:94:ILE:O    | 1:C:95:GLN:OXT  | 0.45     | 2.35        | 4      | 1     |
| 1:C:57:TRP:HE1  | 1:C:90:ARG:NE   | 0.45     | 2.10        | 2      | 1     |
| 1:C:69:ASN:O    | 1:C:69:ASN:OD1  | 0.45     | 2.35        | 3      | 2     |
| 1:C:90:ARG:N    | 1:C:90:ARG:HD2  | 0.44     | 2.27        | 2      | 1     |
| 1:C:44:VAL:HG23 | 1:C:58:VAL:CG1  | 0.44     | 2.43        | 5      | 3     |
| 1:C:70:ASP:C    | 1:C:79:PHE:O    | 0.43     | 2.61        | 1      | 6     |
| 1:C:35:VAL:O    | 1:C:37:GLY:N    | 0.43     | 2.51        | 4      | 1     |
| 1:C:63:ASP:C    | 1:C:63:ASP:OD1  | 0.43     | 2.60        | 3      | 1     |
| 1:C:52:PHE:CE2  | 1:C:88:PHE:CD2  | 0.43     | 3.07        | 8      | 1     |
| 1:C:40:HIS:CG   | 1:C:62:LEU:HD11 | 0.43     | 2.47        | 1      | 1     |
| 1:C:33:VAL:CG1  | 1:C:44:VAL:N    | 0.43     | 2.82        | 2      | 2     |
| 1:C:61:ILE:HD11 | 1:C:79:PHE:CG   | 0.43     | 2.49        | 5      | 2     |
| 1:C:71:GLY:C    | 1:C:72:THR:HG23 | 0.43     | 2.39        | 2      | 10    |
| 1:C:74:GLN:C    | 1:C:76:ARG:H    | 0.43     | 2.22        | 1      | 1     |
| 1:C:70:ASP:OD1  | 1:C:85:HIS:O    | 0.43     | 2.37        | 5      | 2     |
| 1:C:80:THR:O    | 1:C:80:THR:OG1  | 0.43     | 2.36        | 6      | 1     |
| 1:C:68:LYS:O    | 1:C:85:HIS:O    | 0.43     | 2.36        | 7      | 1     |
| 1:C:51:LEU:N    | 1:C:51:LEU:CD1  | 0.43     | 2.82        | 9      | 1     |
| 1:C:94:ILE:O    | 1:C:95:GLN:C    | 0.43     | 2.61        | 7      | 3     |
| 1:C:33:VAL:HG22 | 1:C:42:GLY:C    | 0.43     | 2.38        | 4      | 1     |
| 1:C:46:TYR:CE2  | 1:C:47:VAL:O    | 0.43     | 2.71        | 8      | 2     |
| 1:C:89:VAL:HG21 | 1:C:94:ILE:CG2  | 0.42     | 2.44        | 7      | 3     |
| 1:C:89:VAL:HG21 | 1:C:94:ILE:HG21 | 0.42     | 1.89        | 5      | 1     |
| 1:C:69:ASN:CG   | 1:C:72:THR:O    | 0.42     | 2.62        | 3      | 1     |
| 1:C:82:ASP:OD1  | 1:C:82:ASP:C    | 0.42     | 2.62        | 4      | 2     |
| 1:C:31:SER:O    | 1:C:44:VAL:HG22 | 0.42     | 2.15        | 4      | 1     |
| 1:C:45:ALA:CB   | 1:C:59:GLY:O    | 0.42     | 2.67        | 8      | 2     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:C:74:GLN:C    | 1:C:76:ARG:N    | 0.42     | 2.78        | 8      | 2     |
| 1:C:40:HIS:CE1  | 1:C:64:GLU:CG   | 0.42     | 3.03        | 5      | 1     |
| 1:C:71:GLY:N    | 1:C:81:CYS:O    | 0.41     | 2.53        | 8      | 1     |
| 1:C:91:GLN:CD   | 1:C:91:GLN:C    | 0.41     | 2.88        | 4      | 1     |
| 1:C:73:VAL:O    | 1:C:74:GLN:C    | 0.41     | 2.64        | 9      | 1     |
| 1:C:32:ARG:NE   | 1:C:41:ARG:NH2  | 0.41     | 2.68        | 10     | 1     |
| 1:C:79:PHE:CG   | 1:C:80:THR:N    | 0.41     | 2.89        | 9      | 1     |
| 1:C:36:ILE:O    | 1:C:36:ILE:HG22 | 0.41     | 2.15        | 10     | 1     |
| 1:C:29:VAL:CG2  | 1:C:47:VAL:HG12 | 0.41     | 2.46        | 7      | 1     |
| 1:C:91:GLN:H    | 1:C:91:GLN:CD   | 0.41     | 2.24        | 7      | 1     |
| 1:C:69:ASN:O    | 1:C:73:VAL:HG23 | 0.41     | 2.16        | 8      | 2     |
| 1:C:63:ASP:OD1  | 1:C:64:GLU:N    | 0.40     | 2.54        | 3      | 1     |
| 1:C:50:THR:HG23 | 1:C:53:ALA:H    | 0.40     | 1.76        | 9      | 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   | C     | 67/70 (96%)   | 57±1 (85±2%) | 9±1 (13±2%) | 1±0 (2±1%) | 9           | 52 |
| All | All   | 670/700 (96%) | 571 (85%)    | 87 (13%)    | 12 (2%)    | 9           | 52 |

All 3 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | C     | 65  | ALA  | 10             |
| 1   | C     | 36  | ILE  | 1              |
| 1   | C     | 83  | GLU  | 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   | C     | 52/54 (96%)   | 50±1 (96±2%) | 2±1 (4±2%) | 29          | 79 |
| All | All   | 520/540 (96%) | 499 (96%)    | 21 (4%)    | 29          | 79 |

All 8 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | C     | 62  | LEU  | 8              |
| 1   | C     | 44  | VAL  | 4              |
| 1   | C     | 29  | VAL  | 3              |
| 1   | C     | 33  | VAL  | 2              |
| 1   | C     | 80  | THR  | 1              |
| 1   | C     | 90  | ARG  | 1              |
| 1   | C     | 83  | GLU  | 1              |
| 1   | C     | 70  | ASP  | 1              |

### 6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

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

There are no ligands in this entry.

### 6.7 Other polymers [i](#)

There are no such molecules in this entry.

## 6.8 Polymer linkage issues

There are no chain breaks in this entry.

## 7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 33% for the well-defined parts and 33% 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                  | 312 |
| Number of shifts mapped to atoms        | 312 |
| Number of unparsed shifts               | 0   |
| Number of shifts with mapping errors    | 0   |
| Number of shifts with mapping warnings  | 0   |
| Number of shift outliers (ShiftChecker) | 2   |

#### 7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

| Nucleus                | # values | Correction $\pm$ precision, ppm | Suggested action           |
|------------------------|----------|---------------------------------|----------------------------|
| $^{13}\text{C}_\alpha$ | 68       | $-0.17 \pm 0.21$                | None needed ( $< 0.5$ ppm) |
| $^{13}\text{C}_\beta$  | 55       | $-0.30 \pm 0.32$                | None needed ( $< 0.5$ ppm) |
| $^{13}\text{C}'$       | 64       | $-0.17 \pm 0.22$                | None needed ( $< 0.5$ ppm) |
| $^{15}\text{N}$        | 69       | $0.04 \pm 0.73$                 | None needed ( $< 0.5$ ppm) |

#### 7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 33%, i.e. 302 atoms were assigned a chemical shift out of a possible 908. 0 out of 11 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total         | $^1\text{H}$ | $^{13}\text{C}$ | $^{15}\text{N}$ |
|-----------|---------------|--------------|-----------------|-----------------|
| Backbone  | 198/352 (56%) | 0/148 (0%)   | 130/136 (96%)   | 68/68 (100%)    |
| Sidechain | 104/482 (22%) | 0/312 (0%)   | 104/145 (72%)   | 0/25 (0%)       |

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|          | Total         | <sup>1</sup> H | <sup>13</sup> C | <sup>15</sup> N |
|----------|---------------|----------------|-----------------|-----------------|
| Aromatic | 0/74 (0%)     | 0/37 (0%)      | 0/34 (0%)       | 0/3 (0%)        |
| Overall  | 302/908 (33%) | 0/497 (0%)     | 234/315 (74%)   | 68/96 (71%)     |

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 33%, i.e. 310 atoms were assigned a chemical shift out of a possible 938. 0 out of 12 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total         | <sup>1</sup> H | <sup>13</sup> C | <sup>15</sup> N |
|-----------|---------------|----------------|-----------------|-----------------|
| Backbone  | 201/360 (56%) | 0/151 (0%)     | 132/140 (94%)   | 69/69 (100%)    |
| Sidechain | 109/504 (22%) | 0/327 (0%)     | 109/152 (72%)   | 0/25 (0%)       |
| Aromatic  | 0/74 (0%)     | 0/37 (0%)      | 0/34 (0%)       | 0/3 (0%)        |
| Overall   | 310/938 (33%) | 0/515 (0%)     | 241/326 (74%)   | 69/97 (71%)     |

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 ⓘ

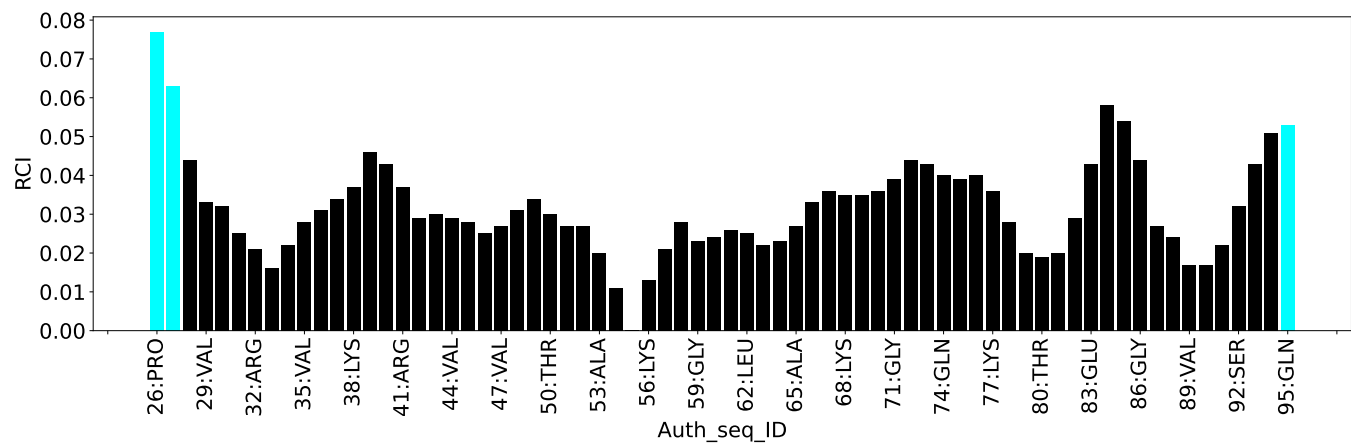
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

| List Id | Chain | Res | Type | Atom | Shift, ppm | Expected range, ppm | Z-score |
|---------|-------|-----|------|------|------------|---------------------|---------|
| 1       | C     | 55  | GLY  | CA   | 172.82     | 38.93 – 51.79       | 99.1    |
| 1       | C     | 55  | GLY  | C    | 45.92      | 164.92 – 182.89     | -71.2   |

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

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

Random coil index (RCI) for chain C:



## 8 NMR restraints analysis

### 8.1 Conformationally restricting restraints

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

| Description                                              | Value |
|----------------------------------------------------------|-------|
| Total distance restraints                                | 1578  |
| Intra-residue ( $ i-j =0$ )                              | 327   |
| Sequential ( $ i-j =1$ )                                 | 290   |
| Medium range ( $ i-j >1$ and $ i-j <5$ )                 | 328   |
| Long range ( $ i-j \geq 5$ )                             | 557   |
| Inter-chain                                              | 0     |
| Hydrogen bond restraints                                 | 76    |
| Disulfide bond restraints                                | 0     |
| Total dihedral-angle restraints                          | 112   |
| Number of unmapped restraints                            | 0     |
| Number of restraints per residue                         | 24.1  |
| Number of long range restraints per residue <sup>1</sup> | 8.7   |

<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)  | 26.1                                   | 0.2     |
| 0.2-0.5 (Medium) | 33.0                                   | 0.5     |
| >0.5 (Large)     | 153.1                                  | 9.18    |

### 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)   | 8.9                                    | 9.69    |
| 10.0-20.0 (Medium) | 4.8                                    | 19.95   |
| >20.0 (Large)      | 5.3                                    | 42.89   |

## 9 Distance violation analysis ⓘ

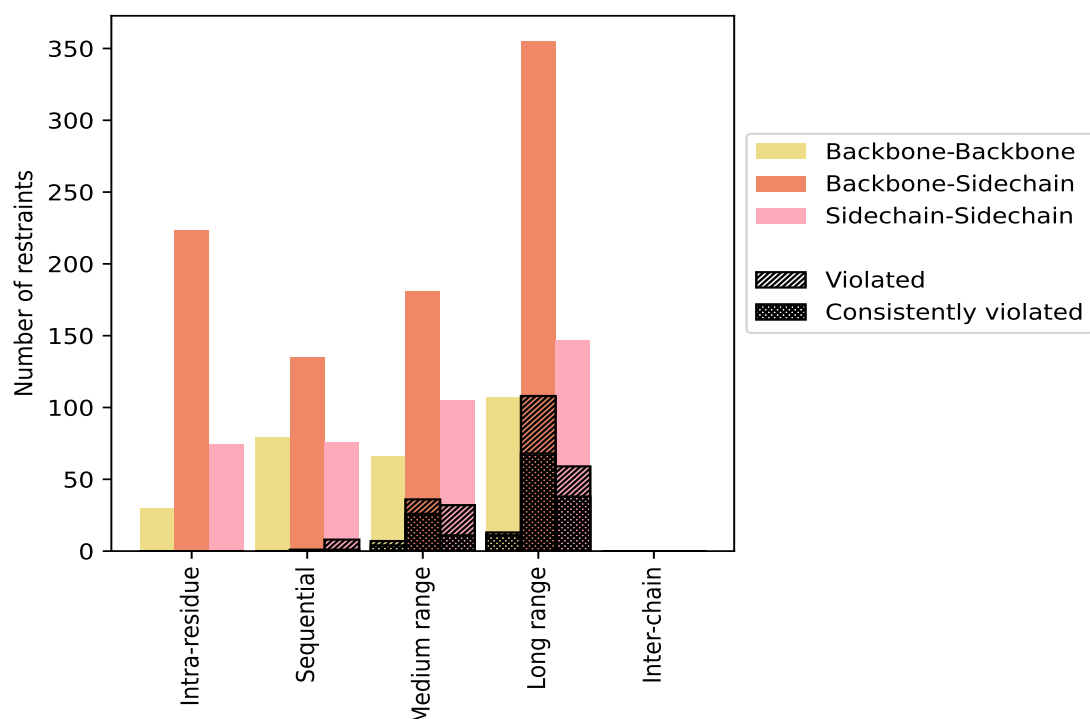
### 9.1 Summary of distance violations ⓘ

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

| Restrains type                                                              | Count       | % <sup>1</sup> | Violated <sup>3</sup> |                |                | Consistently Violated <sup>4</sup> |                |                |
|-----------------------------------------------------------------------------|-------------|----------------|-----------------------|----------------|----------------|------------------------------------|----------------|----------------|
|                                                                             |             |                | Count                 | % <sup>2</sup> | % <sup>1</sup> | Count                              | % <sup>2</sup> | % <sup>1</sup> |
| <b>Intra-residue (<math> i-j =0</math>)</b>                                 | <b>327</b>  | <b>20.7</b>    | <b>0</b>              | <b>0.0</b>     | <b>0.0</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| Backbone-Backbone                                                           | 30          | 1.9            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 223         | 14.1           | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Sidechain-Sidechain                                                         | 74          | 4.7            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| <b>Sequential (<math> i-j =1</math>)</b>                                    | <b>290</b>  | <b>18.4</b>    | <b>9</b>              | <b>3.1</b>     | <b>0.6</b>     | <b>1</b>                           | <b>0.3</b>     | <b>0.1</b>     |
| Backbone-Backbone                                                           | 79          | 5.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 135         | 8.6            | 1                     | 0.7            | 0.1            | 0                                  | 0.0            | 0.0            |
| Sidechain-Sidechain                                                         | 76          | 4.8            | 8                     | 10.5           | 0.5            | 1                                  | 1.3            | 0.1            |
| <b>Medium range (<math> i-j &gt;1</math> &amp; <math> i-j &lt;5</math>)</b> | <b>328</b>  | <b>20.8</b>    | <b>72</b>             | <b>22.0</b>    | <b>4.6</b>     | <b>40</b>                          | <b>12.2</b>    | <b>2.5</b>     |
| Backbone-Backbone                                                           | 66          | 4.2            | 7                     | 10.6           | 0.4            | 4                                  | 6.1            | 0.3            |
| Backbone-Sidechain                                                          | 157         | 9.9            | 33                    | 21.0           | 2.1            | 25                                 | 15.9           | 1.6            |
| Sidechain-Sidechain                                                         | 105         | 6.7            | 32                    | 30.5           | 2.0            | 11                                 | 10.5           | 0.7            |
| <b>Long range (<math> i-j \geq 5</math>)</b>                                | <b>557</b>  | <b>35.3</b>    | <b>171</b>            | <b>30.7</b>    | <b>10.8</b>    | <b>114</b>                         | <b>20.5</b>    | <b>7.2</b>     |
| Backbone-Backbone                                                           | 107         | 6.8            | 13                    | 12.1           | 0.8            | 11                                 | 10.3           | 0.7            |
| Backbone-Sidechain                                                          | 303         | 19.2           | 99                    | 32.7           | 6.3            | 65                                 | 21.5           | 4.1            |
| Sidechain-Sidechain                                                         | 147         | 9.3            | 59                    | 40.1           | 3.7            | 38                                 | 25.9           | 2.4            |
| <b>Inter-chain</b>                                                          | <b>0</b>    | <b>0.0</b>     | <b>0</b>              | <b>0.0</b>     | <b>0.0</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| Backbone-Backbone                                                           | 0           | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 0           | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Sidechain-Sidechain                                                         | 0           | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| <b>Hydrogen bond</b>                                                        | <b>76</b>   | <b>4.8</b>     | <b>12</b>             | <b>15.8</b>    | <b>0.8</b>     | <b>4</b>                           | <b>5.3</b>     | <b>0.3</b>     |
| <b>Disulfide bond</b>                                                       | <b>0</b>    | <b>0.0</b>     | <b>0</b>              | <b>0.0</b>     | <b>0.0</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| <b>Total</b>                                                                | <b>1578</b> | <b>100.0</b>   | <b>264</b>            | <b>16.7</b>    | <b>16.7</b>    | <b>159</b>                         | <b>10.1</b>    | <b>10.1</b>    |
| Backbone-Backbone                                                           | 282         | 17.9           | 20                    | 7.1            | 1.3            | 15                                 | 5.3            | 1.0            |
| Backbone-Sidechain                                                          | 894         | 56.7           | 145                   | 16.2           | 9.2            | 94                                 | 10.5           | 6.0            |
| Sidechain-Sidechain                                                         | 402         | 25.5           | 99                    | 24.6           | 6.3            | 50                                 | 12.4           | 3.2            |

<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

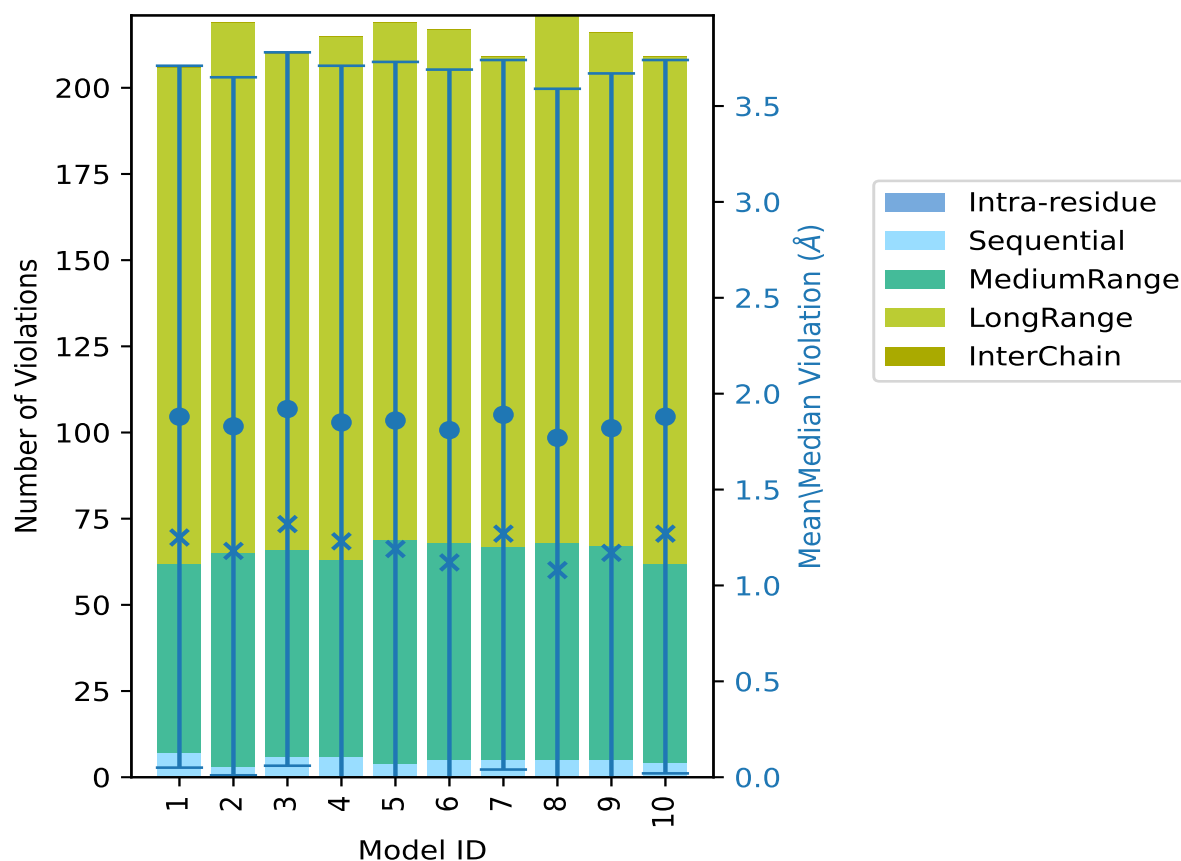
## 9.2 Distance violation statistics for each model [i](#)

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                    | 7               | 55              | 144             | 0               | 206   | 1.88     | 9.04    | 1.83                | 1.25       |
| 2        | 0                    | 3               | 62              | 154             | 0               | 219   | 1.83     | 8.84    | 1.82                | 1.18       |
| 3        | 0                    | 6               | 60              | 144             | 0               | 210   | 1.92     | 8.96    | 1.86                | 1.32       |
| 4        | 0                    | 6               | 57              | 152             | 0               | 215   | 1.85     | 9.07    | 1.86                | 1.23       |
| 5        | 0                    | 4               | 65              | 150             | 0               | 219   | 1.86     | 9.11    | 1.87                | 1.19       |
| 6        | 0                    | 5               | 63              | 149             | 0               | 217   | 1.81     | 9.18    | 1.88                | 1.12       |
| 7        | 0                    | 5               | 62              | 142             | 0               | 209   | 1.89     | 9.15    | 1.85                | 1.27       |
| 8        | 0                    | 5               | 63              | 153             | 0               | 221   | 1.77     | 9.09    | 1.82                | 1.08       |
| 9        | 0                    | 5               | 62              | 149             | 0               | 216   | 1.82     | 9.01    | 1.85                | 1.17       |
| 10       | 0                    | 4               | 58              | 147             | 0               | 209   | 1.88     | 8.97    | 1.86                | 1.27       |

<sup>1</sup>Intra-residue restraints, <sup>2</sup>Sequential restraints, <sup>3</sup>Medium range restraints, <sup>4</sup>Long range restraints, <sup>5</sup>Inter-chain restraints, <sup>6</sup>Standard deviation

### 9.2.1 Bar graph : Distance Violation statistics for each model [i](#)



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

### 9.3 Distance violation statistics for the ensemble [i](#)

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1250(IR:327, SQ:281, MR:256, LR:386, 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                             | 1               | 5               | 8               | 0               | 14    | 1                        | 10.0 |
| 0                             | 4               | 2               | 4               | 0               | 10    | 2                        | 20.0 |
| 0                             | 0               | 5               | 6               | 0               | 11    | 3                        | 30.0 |

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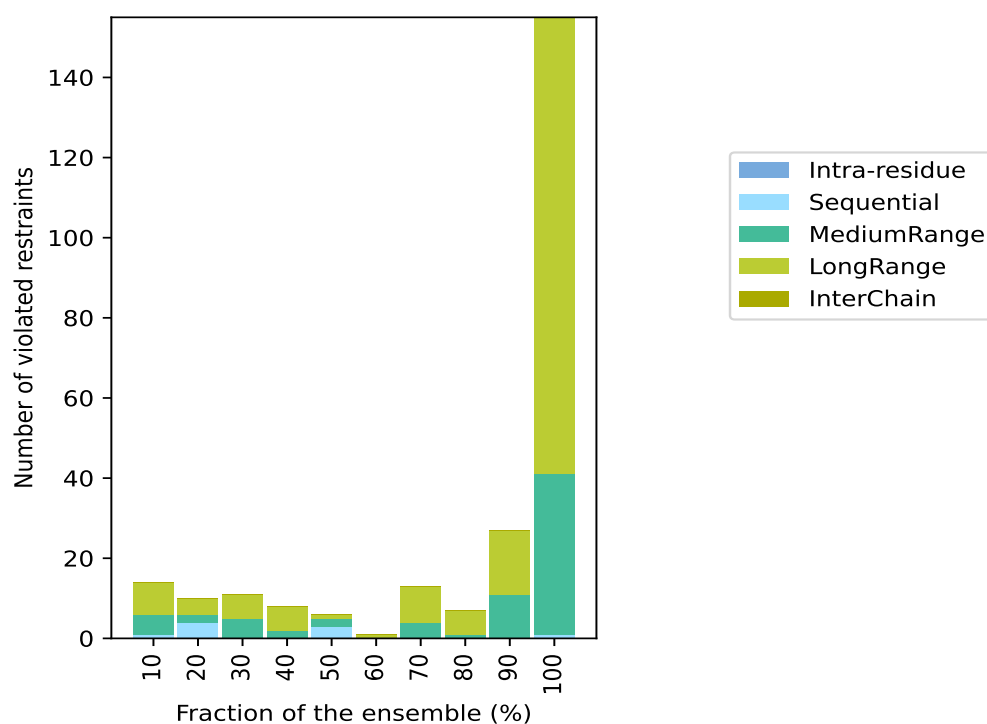
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| Number of violated restraints |                 |                 |                 |                 |       | Fraction of the ensemble |       |
|-------------------------------|-----------------|-----------------|-----------------|-----------------|-------|--------------------------|-------|
| IR <sup>1</sup>               | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total | Count <sup>6</sup>       | %     |
| 0                             | 0               | 2               | 6               | 0               | 8     | 4                        | 40.0  |
| 0                             | 3               | 2               | 1               | 0               | 6     | 5                        | 50.0  |
| 0                             | 0               | 0               | 1               | 0               | 1     | 6                        | 60.0  |
| 0                             | 0               | 4               | 9               | 0               | 13    | 7                        | 70.0  |
| 0                             | 0               | 1               | 6               | 0               | 7     | 8                        | 80.0  |
| 0                             | 0               | 11              | 16              | 0               | 27    | 9                        | 90.0  |
| 0                             | 1               | 40              | 114             | 0               | 155   | 10                       | 100.0 |

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

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

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

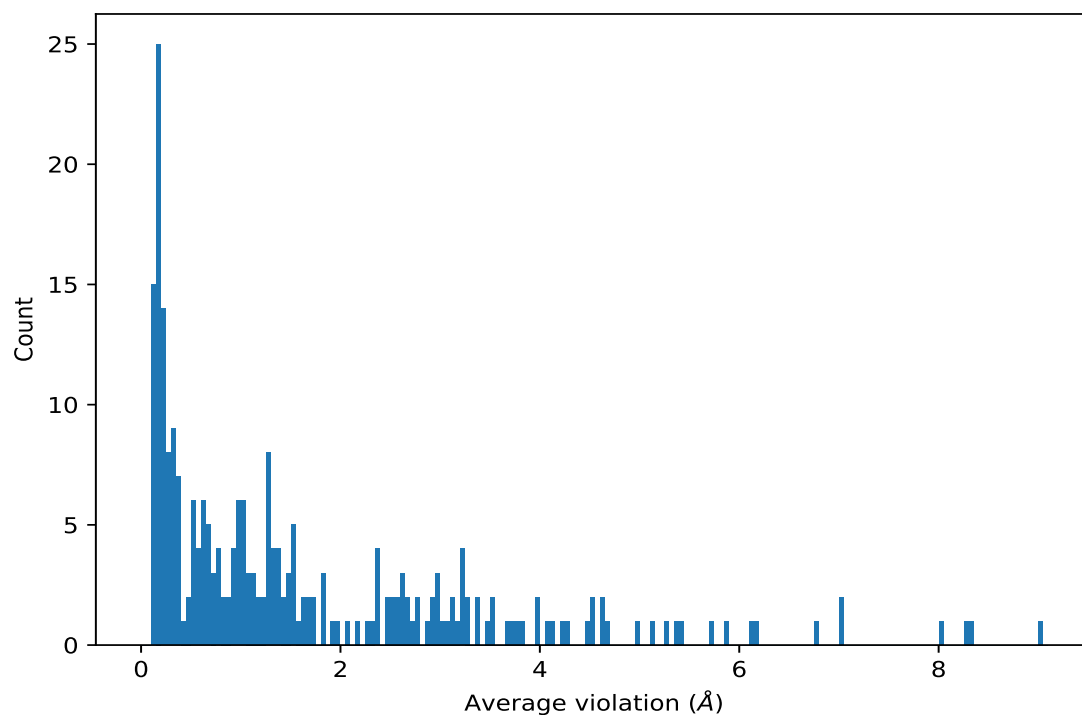


## 9.4 Most violated distance restraints in the ensemble [i](#)

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

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

in the ensemble



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

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

| Key      | Atom-1         | Atom-2        | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|----------------|---------------|---------------------|----------|---------------------|------------|
| (1,41)   | 1:89:C:VAL:CG1 | 1:81:C:CYS:CA | 10                  | 9.04     | 0.1                 | 9.06       |
| (1,362)  | 1:93:C:GLN:CA  | 1:32:C:ARG:CB | 10                  | 8.3      | 0.16                | 8.28       |
| (1,315)  | 1:35:C:VAL:CA  | 1:70:C:ASP:CA | 10                  | 8.27     | 0.24                | 8.24       |
| (1,249)  | 1:69:C:ASN:CB  | 1:63:C:ASP:CG | 10                  | 8.0      | 0.32                | 7.92       |
| (1,404)  | 1:70:C:ASP:CA  | 1:66:C:LYS:CG | 10                  | 7.01     | 0.3                 | 7.12       |
| (1,699)  | 1:66:C:LYS:CG  | 1:70:C:ASP:CA | 10                  | 7.01     | 0.3                 | 7.12       |
| (1,1323) | 1:66:C:LYS:CB  | 1:71:C:GLY:CA | 10                  | 6.79     | 0.11                | 6.8        |
| (1,609)  | 1:56:C:LYS:CB  | 1:52:C:PHE:CB | 10                  | 6.16     | 0.25                | 6.19       |
| (1,363)  | 1:93:C:GLN:CA  | 1:32:C:ARG:CG | 10                  | 6.12     | 0.89                | 5.73       |
| (1,1242) | 1:65:C:ALA:CA  | 1:79:C:PHE:CA | 10                  | 5.89     | 0.24                | 5.9        |
| (1,385)  | 1:51:C:LEU:CA  | 1:77:C:LYS:CB | 10                  | 5.73     | 0.23                | 5.66       |
| (1,66)   | 1:51:C:LEU:CG  | 1:77:C:LYS:CB | 10                  | 5.44     | 0.43                | 5.55       |
| (1,478)  | 1:33:C:VAL:CA  | 1:90:C:ARG:CD | 10                  | 5.38     | 0.15                | 5.42       |
| (1,121)  | 1:73:C:VAL:CG2 | 1:53:C:ALA:CB | 10                  | 5.28     | 0.1                 | 5.27       |
| (1,825)  | 1:70:C:ASP:CB  | 1:51:C:LEU:C  | 10                  | 5.14     | 0.3                 | 5.14       |

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| Key      | Atom-1         | Atom-2         | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|----------------|----------------|---------------------|----------|---------------------|------------|
| (1,421)  | 1:80:C:THR:CB  | 1:76:C:ARG:CB  | 10                  | 4.99     | 0.12                | 5.0        |
| (1,660)  | 1:52:C:PHE:CB  | 1:56:C:LYS:CA  | 10                  | 4.65     | 0.24                | 4.67       |
| (1,434)  | 1:35:C:VAL:CB  | 1:32:C:ARG:CG  | 10                  | 4.64     | 0.75                | 4.56       |
| (1,812)  | 1:71:C:GLY:CA  | 1:66:C:LYS:C   | 10                  | 4.6      | 0.16                | 4.6        |
| (1,393)  | 1:51:C:LEU:CA  | 1:57:C:TRP:CB  | 10                  | 4.53     | 0.24                | 4.59       |
| (1,499)  | 1:33:C:VAL:CB  | 1:91:C:GLN:CG  | 10                  | 4.5      | 0.62                | 4.46       |
| (1,1282) | 1:94:C:ILE:CB  | 1:38:C:LYS:CB  | 10                  | 4.48     | 0.35                | 4.42       |
| (1,1143) | 1:77:C:LYS:CA  | 1:83:C:GLU:CB  | 10                  | 4.26     | 0.16                | 4.21       |
| (1,1102) | 1:78:C:TYR:CA  | 1:82:C:ASP:CB  | 10                  | 4.23     | 0.24                | 4.19       |
| (1,651)  | 1:58:C:VAL:CG2 | 1:61:C:ILE:CB  | 10                  | 4.13     | 0.11                | 4.18       |
| (1,352)  | 1:31:C:SER:CB  | 1:46:C:TYR:CB  | 10                  | 4.05     | 0.09                | 4.08       |
| (1,147)  | 1:40:C:HIS:CA  | 1:36:C:ILE:CG1 | 10                  | 3.98     | 0.18                | 4.0        |
| (1,815)  | 1:51:C:LEU:CB  | 1:78:C:TYR:C   | 10                  | 3.95     | 0.21                | 3.92       |
| (1,46)   | 1:83:C:GLU:CA  | 1:73:C:VAL:CB  | 10                  | 3.8      | 0.17                | 3.79       |
| (1,556)  | 1:68:C:LYS:CD  | 1:77:C:LYS:CG  | 10                  | 3.77     | 0.31                | 3.86       |
| (1,1088) | 1:31:C:SER:CA  | 1:26:C:PRO:CG  | 10                  | 3.74     | 0.39                | 3.84       |
| (1,368)  | 1:79:C:PHE:CA  | 1:47:C:VAL:CB  | 10                  | 3.68     | 0.21                | 3.6        |
| (1,767)  | 1:83:C:GLU:CB  | 1:63:C:ASP:CA  | 10                  | 3.5      | 0.14                | 3.46       |
| (1,1373) | 1:62:C:LEU:CG  | 1:43:C:THR:CG2 | 10                  | 3.5      | 0.79                | 3.95       |
| (1,1286) | 1:46:C:TYR:CB  | 1:60:C:VAL:CG1 | 10                  | 3.49     | 0.15                | 3.46       |
| (1,1166) | 1:41:C:ARG:CA  | 1:87:C:ILE:CD1 | 10                  | 3.38     | 0.78                | 3.38       |
| (1,221)  | 1:74:C:GLN:CB  | 1:71:C:GLY:C   | 10                  | 3.35     | 0.06                | 3.34       |
| (1,692)  | 1:61:C:ILE:CG1 | 1:66:C:LYS:CA  | 10                  | 3.28     | 0.13                | 3.29       |
| (1,533)  | 1:73:C:VAL:CB  | 1:83:C:GLU:CB  | 10                  | 3.26     | 0.21                | 3.21       |
| (1,701)  | 1:77:C:LYS:CG  | 1:82:C:ASP:CA  | 10                  | 3.22     | 0.1                 | 3.2        |
| (1,701)  | 1:77:C:LYS:CG  | 1:51:C:LEU:CA  | 10                  | 3.22     | 0.1                 | 3.2        |
| (1,375)  | 1:62:C:LEU:CA  | 1:88:C:PHE:CB  | 10                  | 3.21     | 0.13                | 3.28       |
| (1,1074) | 1:83:C:GLU:CB  | 1:80:C:THR:CA  | 10                  | 3.21     | 0.05                | 3.22       |
| (1,216)  | 1:61:C:ILE:CG1 | 1:40:C:HIS:C   | 10                  | 3.17     | 0.71                | 3.33       |
| (1,496)  | 1:61:C:ILE:CB  | 1:83:C:GLU:CB  | 10                  | 3.14     | 0.34                | 3.22       |
| (1,1106) | 1:78:C:TYR:CA  | 1:74:C:GLN:CG  | 10                  | 3.13     | 0.7                 | 3.54       |
| (1,1275) | 1:48:C:GLY:CA  | 1:51:C:LEU:CB  | 10                  | 3.07     | 0.06                | 3.06       |
| (1,668)  | 1:60:C:VAL:CB  | 1:66:C:LYS:CA  | 10                  | 3.01     | 0.24                | 3.04       |
| (1,1228) | 1:89:C:VAL:CA  | 1:53:C:ALA:CA  | 10                  | 2.97     | 0.37                | 2.96       |
| (1,1440) | 1:33:C:VAL:CG2 | 1:91:C:GLN:CG  | 10                  | 2.96     | 1.0                 | 2.8        |
| (1,22)   | 1:56:C:LYS:CA  | 1:88:C:PHE:CB  | 10                  | 2.95     | 0.2                 | 2.98       |
| (1,961)  | 1:80:C:THR:CB  | 1:73:C:VAL:CG2 | 10                  | 2.93     | 0.07                | 2.96       |
| (1,635)  | 1:46:C:TYR:CB  | 1:61:C:ILE:CG2 | 10                  | 2.92     | 0.94                | 2.88       |
| (1,559)  | 1:76:C:ARG:CG  | 1:68:C:LYS:CG  | 10                  | 2.85     | 0.39                | 3.0        |
| (1,1353) | 1:76:C:ARG:CB  | 1:68:C:LYS:CB  | 10                  | 2.79     | 0.21                | 2.74       |
| (1,1165) | 1:41:C:ARG:CA  | 1:36:C:ILE:CG1 | 10                  | 2.76     | 0.39                | 2.82       |
| (1,1213) | 1:31:C:SER:CA  | 1:26:C:PRO:CA  | 10                  | 2.74     | 0.31                | 2.72       |

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| Key      | Atom-1         | Atom-2         | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|----------------|----------------|---------------------|----------|---------------------|------------|
| (1,132)  | 1:36:C:ILE:CG1 | 1:40:C:HIS:CA  | 10                  | 2.68     | 0.18                | 2.7        |
| (1,1219) | 1:78:C:TYR:CA  | 1:51:C:LEU:CA  | 10                  | 2.68     | 0.19                | 2.69       |
| (1,142)  | 1:51:C:LEU:CA  | 1:73:C:VAL:CB  | 10                  | 2.63     | 0.29                | 2.71       |
| (1,557)  | 1:68:C:LYS:CD  | 1:66:C:LYS:CG  | 10                  | 2.62     | 0.33                | 2.65       |
| (1,557)  | 1:36:C:ILE:CG1 | 1:38:C:LYS:CG  | 10                  | 2.62     | 0.33                | 2.65       |
| (1,1478) | 1:58:C:VAL:CB  | 1:43:C:THR:CB  | 10                  | 2.59     | 0.16                | 2.62       |
| (1,814)  | 1:90:C:ARG:CD  | 1:59:C:GLY:C   | 10                  | 2.57     | 0.28                | 2.61       |
| (1,792)  | 1:51:C:LEU:CA  | 1:73:C:VAL:CB  | 10                  | 2.53     | 0.29                | 2.61       |
| (1,359)  | 1:93:C:GLN:CA  | 1:27:C:LEU:CG  | 10                  | 2.51     | 0.17                | 2.48       |
| (1,707)  | 1:80:C:THR:CG2 | 1:69:C:ASN:CA  | 10                  | 2.49     | 0.1                 | 2.48       |
| (1,79)   | 1:85:C:HIS:CB  | 1:66:C:LYS:CB  | 10                  | 2.46     | 0.05                | 2.48       |
| (1,1301) | 1:82:C:ASP:CB  | 1:68:C:LYS:CG  | 10                  | 2.37     | 0.24                | 2.33       |
| (1,77)   | 1:60:C:VAL:CB  | 1:85:C:HIS:CB  | 10                  | 2.36     | 0.16                | 2.3        |
| (1,326)  | 1:63:C:ASP:CA  | 1:82:C:ASP:CA  | 10                  | 2.36     | 0.24                | 2.27       |
| (1,326)  | 1:56:C:LYS:CA  | 1:51:C:LEU:CA  | 10                  | 2.36     | 0.24                | 2.27       |
| (1,535)  | 1:91:C:GLN:CG  | 1:36:C:ILE:CG1 | 10                  | 2.34     | 0.47                | 2.16       |
| (1,1205) | 1:65:C:ALA:CA  | 1:40:C:HIS:CB  | 10                  | 2.26     | 0.29                | 2.24       |
| (1,593)  | 1:94:C:ILE:CG1 | 1:32:C:ARG:CG  | 10                  | 2.16     | 0.76                | 2.02       |
| (1,1049) | 1:45:C:ALA:CB  | 1:28:C:ARG:CA  | 10                  | 2.05     | 0.13                | 2.05       |
| (1,1351) | 1:29:C:VAL:CB  | 1:26:C:PRO:CG  | 10                  | 1.99     | 0.47                | 2.04       |
| (1,634)  | 1:33:C:VAL:CG2 | 1:41:C:ARG:CD  | 10                  | 1.91     | 0.77                | 1.98       |
| (1,109)  | 1:40:C:HIS:CB  | 1:64:C:GLU:CA  | 10                  | 1.82     | 0.23                | 1.85       |
| (1,112)  | 1:84:C:GLY:CA  | 1:81:C:CYS:C   | 10                  | 1.8      | 0.05                | 1.8        |
| (1,682)  | 1:76:C:ARG:CB  | 1:53:C:ALA:CA  | 10                  | 1.8      | 0.35                | 1.89       |
| (1,1178) | 1:66:C:LYS:CA  | 1:69:C:ASN:CB  | 10                  | 1.74     | 0.07                | 1.72       |
| (1,1178) | 1:76:C:ARG:CA  | 1:69:C:ASN:CB  | 10                  | 1.74     | 0.07                | 1.72       |
| (1,384)  | 1:51:C:LEU:CA  | 1:73:C:VAL:CB  | 10                  | 1.68     | 0.29                | 1.76       |
| (1,1039) | 1:77:C:LYS:CG  | 1:69:C:ASN:CA  | 10                  | 1.67     | 0.08                | 1.65       |
| (1,465)  | 1:87:C:ILE:CA  | 1:94:C:ILE:CD1 | 10                  | 1.61     | 0.29                | 1.7        |
| (1,1023) | 1:61:C:ILE:CG1 | 1:82:C:ASP:CA  | 10                  | 1.6      | 0.39                | 1.56       |
| (1,427)  | 1:92:C:SER:CB  | 1:26:C:PRO:CB  | 10                  | 1.56     | 0.12                | 1.6        |
| (1,218)  | 1:27:C:LEU:CG  | 1:92:C:SER:C   | 10                  | 1.54     | 0.19                | 1.51       |
| (1,173)  | 1:82:C:ASP:CB  | 1:72:C:THR:C   | 10                  | 1.54     | 0.19                | 1.6        |
| (1,1163) | 1:41:C:ARG:CA  | 1:38:C:LYS:CB  | 10                  | 1.53     | 0.22                | 1.59       |
| (1,791)  | 1:81:C:CYS:CA  | 1:83:C:GLU:CB  | 10                  | 1.49     | 0.02                | 1.5        |
| (1,988)  | 1:69:C:ASN:CB  | 1:74:C:GLN:CA  | 10                  | 1.46     | 0.24                | 1.5        |
| (1,425)  | 1:91:C:GLN:CA  | 1:57:C:TRP:CB  | 10                  | 1.45     | 0.13                | 1.48       |
| (1,846)  | 1:60:C:VAL:CB  | 1:84:C:GLY:C   | 10                  | 1.43     | 0.2                 | 1.39       |
| (1,1001) | 1:60:C:VAL:CB  | 1:46:C:TYR:CA  | 10                  | 1.4      | 0.14                | 1.4        |
| (1,1336) | 1:40:C:HIS:CB  | 1:61:C:ILE:CG1 | 10                  | 1.36     | 0.71                | 1.47       |
| (1,1336) | 1:41:C:ARG:CB  | 1:61:C:ILE:CG1 | 10                  | 1.36     | 0.71                | 1.47       |
| (1,428)  | 1:54:C:THR:CA  | 1:56:C:LYS:CB  | 10                  | 1.35     | 0.11                | 1.36       |

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| Key      | Atom-1         | Atom-2         | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|----------------|----------------|---------------------|----------|---------------------|------------|
| (1,199)  | 1:26:C:PRO:CB  | 1:28:C:ARG:C   | 10                  | 1.32     | 0.26                | 1.3        |
| (1,790)  | 1:36:C:ILE:CA  | 1:40:C:HIS:C   | 10                  | 1.3      | 0.25                | 1.36       |
| (1,80)   | 1:34:C:GLU:CB  | 1:32:C:ARG:CB  | 10                  | 1.27     | 0.2                 | 1.2        |
| (1,184)  | 1:33:C:VAL:CB  | 1:91:C:GLN:C   | 10                  | 1.26     | 0.43                | 1.34       |
| (1,836)  | 1:33:C:VAL:CB  | 1:91:C:GLN:C   | 10                  | 1.26     | 0.43                | 1.34       |
| (1,763)  | 1:36:C:ILE:CB  | 1:91:C:GLN:CA  | 10                  | 1.26     | 0.08                | 1.25       |
| (1,378)  | 1:41:C:ARG:CA  | 1:60:C:VAL:CB  | 10                  | 1.26     | 0.37                | 1.24       |
| (1,153)  | 1:46:C:TYR:CB  | 1:29:C:VAL:CA  | 10                  | 1.25     | 0.07                | 1.27       |
| (1,485)  | 1:90:C:ARG:CD  | 1:36:C:ILE:CG1 | 10                  | 1.23     | 0.16                | 1.31       |
| (1,1437) | 1:72:C:THR:CG2 | 1:81:C:CYS:CB  | 10                  | 1.23     | 0.13                | 1.23       |
| (1,1245) | 1:66:C:LYS:CA  | 1:61:C:ILE:CA  | 10                  | 1.15     | 0.16                | 1.18       |
| (1,789)  | 1:74:C:GLN:CG  | 1:52:C:PHE:C   | 10                  | 1.14     | 0.4                 | 1.09       |
| (1,149)  | 1:85:C:HIS:CA  | 1:83:C:GLU:CB  | 10                  | 1.13     | 0.04                | 1.12       |
| (1,631)  | 1:63:C:ASP:CB  | 1:41:C:ARG:CD  | 10                  | 1.1      | 0.45                | 1.03       |
| (1,355)  | 1:63:C:ASP:CA  | 1:60:C:VAL:CB  | 10                  | 1.08     | 0.19                | 1.02       |
| (1,310)  | 1:80:C:THR:CB  | 1:70:C:ASP:CA  | 10                  | 1.07     | 0.1                 | 1.04       |
| (1,1391) | 1:58:C:VAL:CG1 | 1:56:C:LYS:CB  | 10                  | 1.04     | 0.1                 | 1.05       |
| (1,422)  | 1:43:C:THR:CA  | 1:41:C:ARG:CB  | 10                  | 1.03     | 0.11                | 1.05       |
| (1,18)   | 1:51:C:LEU:CG  | 1:53:C:ALA:C   | 10                  | 1.02     | 0.12                | 1.06       |
| (1,271)  | 1:41:C:ARG:CA  | 1:43:C:THR:C   | 10                  | 1.01     | 0.28                | 0.91       |
| (1,258)  | 1:70:C:ASP:CA  | 1:83:C:GLU:C   | 10                  | 1.0      | 0.1                 | 1.02       |
| (1,43)   | 1:40:C:HIS:CA  | 1:34:C:GLU:CB  | 10                  | 0.98     | 0.1                 | 1.02       |
| (1,1121) | 1:43:C:THR:CA  | 1:94:C:ILE:CG2 | 10                  | 0.97     | 0.19                | 0.9        |
| (1,564)  | 1:87:C:ILE:CD1 | 1:61:C:ILE:CG2 | 10                  | 0.96     | 0.21                | 0.94       |
| (1,141)  | 1:28:C:ARG:CA  | 1:47:C:VAL:CB  | 10                  | 0.95     | 0.3                 | 0.95       |
| (1,1174) | 1:76:C:ARG:CA  | 1:46:C:TYR:CB  | 10                  | 0.95     | 0.16                | 0.94       |
| (1,1109) | 1:87:C:ILE:CA  | 1:57:C:TRP:CB  | 10                  | 0.94     | 0.19                | 0.91       |
| (1,435)  | 1:92:C:SER:CB  | 1:27:C:LEU:CG  | 10                  | 0.93     | 0.27                | 0.85       |
| (1,166)  | 1:29:C:VAL:CG2 | 1:31:C:SER:CB  | 10                  | 0.91     | 0.12                | 0.92       |
| (1,92)   | 1:33:C:VAL:C   | 1:40:C:HIS:CA  | 10                  | 0.9      | 0.17                | 0.88       |
| (1,823)  | 1:82:C:ASP:CB  | 1:79:C:PHE:C   | 10                  | 0.89     | 0.09                | 0.86       |
| (1,52)   | 1:29:C:VAL:CG2 | 1:43:C:THR:CB  | 10                  | 0.88     | 0.7                 | 0.53       |
| (1,733)  | 1:58:C:VAL:CG1 | 1:92:C:SER:CA  | 10                  | 0.81     | 0.22                | 0.87       |
| (1,733)  | 1:89:C:VAL:CG1 | 1:92:C:SER:CA  | 10                  | 0.81     | 0.22                | 0.87       |
| (1,379)  | 1:64:C:GLU:CA  | 1:85:C:HIS:CB  | 10                  | 0.79     | 0.11                | 0.83       |
| (1,1280) | 1:30:C:GLY:CA  | 1:27:C:LEU:CG  | 10                  | 0.79     | 0.35                | 0.96       |
| (1,156)  | 1:61:C:ILE:CB  | 1:45:C:ALA:CB  | 10                  | 0.77     | 0.12                | 0.74       |
| (1,797)  | 1:62:C:LEU:CG  | 1:66:C:LYS:CA  | 10                  | 0.73     | 0.25                | 0.84       |
| (1,1195) | 1:70:C:ASP:CA  | 1:76:C:ARG:CB  | 10                  | 0.7      | 0.2                 | 0.63       |
| (1,1270) | 1:86:C:GLY:CA  | 1:83:C:GLU:CB  | 10                  | 0.68     | 0.05                | 0.66       |
| (1,640)  | 1:45:C:ALA:CB  | 1:61:C:ILE:CB  | 10                  | 0.67     | 0.12                | 0.64       |
| (1,47)   | 1:88:C:PHE:CA  | 1:60:C:VAL:CB  | 10                  | 0.67     | 0.08                | 0.66       |

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| Key      | Atom-1         | Atom-2         | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|----------------|----------------|---------------------|----------|---------------------|------------|
| (1,852)  | 1:56:C:LYS:CB  | 1:53:C:ALA:C   | 10                  | 0.64     | 0.18                | 0.68       |
| (1,44)   | 1:57:C:TRP:CA  | 1:47:C:VAL:CB  | 10                  | 0.61     | 0.24                | 0.51       |
| (1,653)  | 1:61:C:ILE:CG1 | 1:87:C:ILE:CB  | 10                  | 0.6      | 0.12                | 0.6        |
| (1,106)  | 1:40:C:HIS:C   | 1:33:C:VAL:CB  | 10                  | 0.59     | 0.31                | 0.56       |
| (1,727)  | 1:51:C:LEU:CG  | 1:54:C:THR:CA  | 10                  | 0.57     | 0.08                | 0.58       |
| (1,473)  | 1:70:C:ASP:CA  | 1:72:C:THR:CG2 | 10                  | 0.56     | 0.02                | 0.57       |
| (1,662)  | 1:68:C:LYS:CB  | 1:82:C:ASP:CA  | 10                  | 0.5      | 0.12                | 0.5        |
| (1,974)  | 1:37:C:GLY:CA  | 1:93:C:GLN:CA  | 10                  | 0.46     | 0.27                | 0.33       |
| (1,105)  | 1:44:C:VAL:C   | 1:60:C:VAL:CB  | 10                  | 0.45     | 0.19                | 0.44       |
| (1,1431) | 1:49:C:ALA:CB  | 1:51:C:LEU:CB  | 10                  | 0.38     | 0.1                 | 0.4        |
| (1,78)   | 1:57:C:TRP:CB  | 1:90:C:ARG:CB  | 10                  | 0.37     | 0.07                | 0.37       |
| (1,245)  | 1:72:C:THR:CG2 | 1:78:C:TYR:C   | 10                  | 0.36     | 0.03                | 0.36       |
| (1,602)  | 1:90:C:ARG:CG  | 1:58:C:VAL:CB  | 10                  | 0.32     | 0.14                | 0.29       |
| (2,28)   | 1:49:C:ALA:H   | 1:55:C:GLY:O   | 10                  | 0.3      | 0.02                | 0.3        |
| (1,351)  | 1:29:C:VAL:CA  | 1:46:C:TYR:CB  | 10                  | 0.3      | 0.07                | 0.32       |
| (1,1393) | 1:89:C:VAL:CG1 | 1:62:C:LEU:CB  | 10                  | 0.3      | 0.09                | 0.32       |
| (2,62)   | 1:65:C:ALA:H   | 1:84:C:GLY:O   | 10                  | 0.28     | 0.06                | 0.28       |
| (2,58)   | 1:85:C:HIS:H   | 1:82:C:ASP:O   | 10                  | 0.26     | 0.05                | 0.26       |
| (1,493)  | 1:69:C:ASN:CB  | 1:77:C:LYS:CB  | 10                  | 0.23     | 0.04                | 0.23       |
| (1,35)   | 1:73:C:VAL:CA  | 1:71:C:GLY:CA  | 10                  | 0.21     | 0.04                | 0.21       |
| (1,1432) | 1:72:C:THR:CG2 | 1:70:C:ASP:CB  | 10                  | 0.19     | 0.02                | 0.19       |
| (1,1433) | 1:72:C:THR:CG2 | 1:73:C:VAL:CG1 | 10                  | 0.18     | 0.03                | 0.18       |
| (2,40)   | 1:84:C:GLY:H   | 1:67:C:GLY:O   | 10                  | 0.17     | 0.04                | 0.16       |
| (1,718)  | 1:72:C:THR:CG2 | 1:78:C:TYR:CA  | 10                  | 0.15     | 0.02                | 0.15       |
| (1,56)   | 1:74:C:GLN:CG  | 1:76:C:ARG:CG  | 9                   | 1.5      | 0.05                | 1.49       |
| (1,64)   | 1:76:C:ARG:CG  | 1:74:C:GLN:CG  | 9                   | 1.5      | 0.05                | 1.49       |
| (1,131)  | 1:68:C:LYS:CD  | 1:70:C:ASP:CA  | 9                   | 1.27     | 0.27                | 1.36       |
| (1,424)  | 1:91:C:GLN:CA  | 1:95:C:GLN:CB  | 9                   | 1.09     | 0.55                | 0.85       |
| (1,1426) | 1:29:C:VAL:CG2 | 1:27:C:LEU:CG  | 9                   | 0.68     | 0.37                | 0.8        |
| (1,870)  | 1:68:C:LYS:CD  | 1:84:C:GLY:C   | 9                   | 0.66     | 0.38                | 0.47       |
| (1,901)  | 1:94:C:ILE:CD1 | 1:87:C:ILE:C   | 9                   | 0.63     | 0.22                | 0.69       |
| (1,367)  | 1:52:C:PHE:CA  | 1:76:C:ARG:CB  | 9                   | 0.62     | 0.37                | 0.55       |
| (1,1399) | 1:29:C:VAL:CG1 | 1:27:C:LEU:CD1 | 9                   | 0.54     | 0.17                | 0.57       |
| (1,874)  | 1:62:C:LEU:CG  | 1:67:C:GLY:C   | 9                   | 0.54     | 0.15                | 0.55       |
| (1,405)  | 1:70:C:ASP:CA  | 1:76:C:ARG:CG  | 9                   | 0.5      | 0.26                | 0.43       |
| (1,689)  | 1:76:C:ARG:CG  | 1:70:C:ASP:CA  | 9                   | 0.5      | 0.26                | 0.43       |
| (1,1421) | 1:29:C:VAL:CG2 | 1:27:C:LEU:CD1 | 9                   | 0.33     | 0.07                | 0.33       |
| (1,1119) | 1:43:C:THR:CA  | 1:29:C:VAL:CB  | 9                   | 0.32     | 0.16                | 0.24       |
| (1,1144) | 1:93:C:GLN:CA  | 1:27:C:LEU:CD1 | 9                   | 0.31     | 0.09                | 0.31       |
| (1,508)  | 1:36:C:ILE:CB  | 1:89:C:VAL:CG2 | 9                   | 0.29     | 0.07                | 0.31       |
| (1,231)  | 1:29:C:VAL:CG1 | 1:47:C:VAL:C   | 9                   | 0.28     | 0.12                | 0.25       |
| (1,1104) | 1:87:C:ILE:CA  | 1:84:C:GLY:CA  | 9                   | 0.28     | 0.06                | 0.3        |

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| Key      | Atom-1         | Atom-2         | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|----------------|----------------|---------------------|----------|---------------------|------------|
| (1,1470) | 1:89:C:VAL:CG2 | 1:36:C:ILE:CA  | 9                   | 0.24     | 0.08                | 0.23       |
| (1,637)  | 1:73:C:VAL:CG1 | 1:69:C:ASN:CB  | 9                   | 0.22     | 0.06                | 0.21       |
| (1,290)  | 1:31:C:SER:CB  | 1:43:C:THR:C   | 9                   | 0.22     | 0.06                | 0.22       |
| (1,14)   | 1:46:C:TYR:CB  | 1:77:C:LYS:CB  | 9                   | 0.2      | 0.07                | 0.17       |
| (1,500)  | 1:79:C:PHE:CB  | 1:77:C:LYS:CB  | 9                   | 0.18     | 0.03                | 0.17       |
| (1,1185) | 1:69:C:ASN:CA  | 1:77:C:LYS:CB  | 9                   | 0.18     | 0.06                | 0.17       |
| (1,589)  | 1:58:C:VAL:CG1 | 1:57:C:TRP:CB  | 9                   | 0.17     | 0.04                | 0.18       |
| (1,480)  | 1:94:C:ILE:CB  | 1:90:C:ARG:CD  | 9                   | 0.14     | 0.03                | 0.14       |
| (1,1291) | 1:90:C:ARG:CD  | 1:94:C:ILE:CB  | 9                   | 0.14     | 0.03                | 0.14       |
| (1,58)   | 1:32:C:ARG:CG  | 1:41:C:ARG:CB  | 8                   | 1.32     | 0.47                | 1.46       |
| (1,65)   | 1:41:C:ARG:CB  | 1:32:C:ARG:CG  | 8                   | 1.32     | 0.47                | 1.46       |
| (1,555)  | 1:85:C:HIS:CB  | 1:68:C:LYS:CG  | 8                   | 1.0      | 0.09                | 0.98       |
| (1,616)  | 1:36:C:ILE:CG1 | 1:95:C:GLN:CG  | 8                   | 0.77     | 0.36                | 0.76       |
| (1,477)  | 1:71:C:GLY:CA  | 1:82:C:ASP:CB  | 8                   | 0.28     | 0.1                 | 0.26       |
| (1,1293) | 1:88:C:PHE:CB  | 1:90:C:ARG:CB  | 8                   | 0.19     | 0.05                | 0.18       |
| (1,1296) | 1:88:C:PHE:CB  | 1:58:C:VAL:CG2 | 8                   | 0.18     | 0.05                | 0.16       |
| (1,374)  | 1:41:C:ARG:CA  | 1:32:C:ARG:CG  | 7                   | 0.97     | 0.12                | 0.96       |
| (1,617)  | 1:76:C:ARG:CG  | 1:52:C:PHE:CB  | 7                   | 0.73     | 0.56                | 0.56       |
| (1,1466) | 1:61:C:ILE:CB  | 1:41:C:ARG:CA  | 7                   | 0.56     | 0.37                | 0.39       |
| (1,865)  | 1:76:C:ARG:CB  | 1:52:C:PHE:C   | 7                   | 0.51     | 0.28                | 0.41       |
| (1,794)  | 1:76:C:ARG:CG  | 1:51:C:LEU:CA  | 7                   | 0.41     | 0.22                | 0.37       |
| (1,1063) | 1:89:C:VAL:CG2 | 1:34:C:GLU:CA  | 7                   | 0.37     | 0.24                | 0.34       |
| (1,444)  | 1:36:C:ILE:CA  | 1:89:C:VAL:CG1 | 7                   | 0.23     | 0.17                | 0.19       |
| (1,913)  | 1:83:C:GLU:CA  | 1:86:C:GLY:C   | 7                   | 0.17     | 0.03                | 0.17       |
| (1,1240) | 1:52:C:PHE:CA  | 1:49:C:ALA:CA  | 7                   | 0.15     | 0.03                | 0.14       |
| (1,1241) | 1:52:C:PHE:CA  | 1:49:C:ALA:CA  | 7                   | 0.15     | 0.03                | 0.14       |
| (1,723)  | 1:72:C:THR:CG2 | 1:79:C:PHE:CA  | 7                   | 0.13     | 0.02                | 0.13       |
| (1,1158) | 1:79:C:PHE:CA  | 1:72:C:THR:CG2 | 7                   | 0.13     | 0.02                | 0.13       |
| (2,22)   | 1:53:C:ALA:H   | 1:50:C:THR:O   | 7                   | 0.13     | 0.02                | 0.13       |
| (1,702)  | 1:89:C:VAL:CG1 | 1:90:C:ARG:CA  | 7                   | 0.11     | 0.01                | 0.12       |
| (2,14)   | 1:61:C:ILE:H   | 1:43:C:THR:O   | 6                   | 0.21     | 0.03                | 0.22       |
| (1,531)  | 1:32:C:ARG:CB  | 1:27:C:LEU:CD1 | 6                   | 0.19     | 0.02                | 0.2        |
| (2,13)   | 1:61:C:ILE:N   | 1:43:C:THR:O   | 6                   | 0.19     | 0.04                | 0.2        |
| (1,137)  | 1:32:C:ARG:CG  | 1:31:C:SER:CB  | 5                   | 0.64     | 0.37                | 0.92       |
| (1,45)   | 1:62:C:LEU:CA  | 1:60:C:VAL:CB  | 5                   | 0.36     | 0.18                | 0.43       |
| (1,159)  | 1:62:C:LEU:CA  | 1:61:C:ILE:CG2 | 5                   | 0.3      | 0.05                | 0.28       |
| (1,110)  | 1:70:C:ASP:CA  | 1:68:C:LYS:CG  | 5                   | 0.18     | 0.02                | 0.19       |
| (1,72)   | 1:61:C:ILE:CG1 | 1:60:C:VAL:CB  | 5                   | 0.18     | 0.04                | 0.19       |
| (1,1355) | 1:85:C:HIS:CB  | 1:71:C:GLY:CA  | 5                   | 0.14     | 0.02                | 0.14       |
| (1,596)  | 1:32:C:ARG:CG  | 1:34:C:GLU:CB  | 4                   | 1.35     | 0.52                | 1.6        |
| (1,1190) | 1:32:C:ARG:CA  | 1:95:C:GLN:CG  | 4                   | 1.26     | 0.75                | 1.2        |
| (1,1284) | 1:41:C:ARG:CD  | 1:33:C:VAL:CG1 | 4                   | 1.15     | 0.43                | 1.24       |

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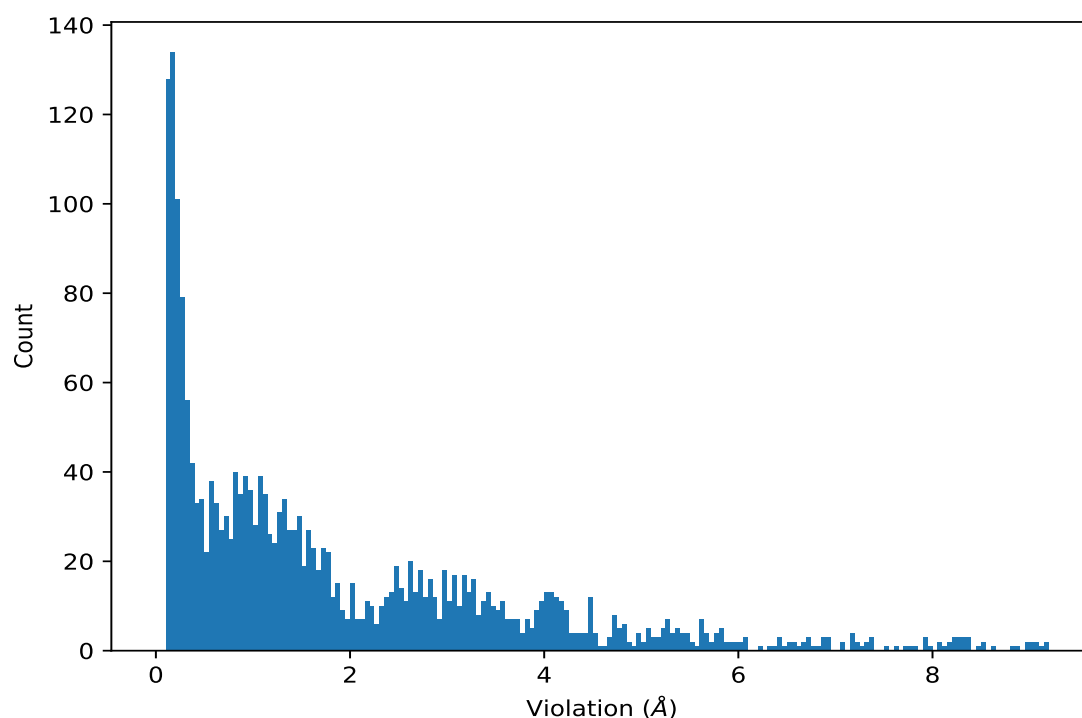
| Key      | Atom-1         | Atom-2         | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|----------------|----------------|---------------------|----------|---------------------|------------|
| (1,598)  | 1:91:C:GLN:CB  | 1:56:C:LYS:CB  | 4                   | 0.37     | 0.14                | 0.34       |
| (1,598)  | 1:27:C:LEU:CG  | 1:95:C:GLN:CB  | 4                   | 0.37     | 0.14                | 0.34       |
| (1,606)  | 1:38:C:LYS:CG  | 1:40:C:HIS:CB  | 4                   | 0.25     | 0.02                | 0.26       |
| (1,918)  | 1:85:C:HIS:CA  | 1:63:C:ASP:CG  | 4                   | 0.21     | 0.07                | 0.2        |
| (1,1314) | 1:60:C:VAL:CB  | 1:43:C:THR:CG2 | 4                   | 0.21     | 0.03                | 0.21       |
| (1,590)  | 1:62:C:LEU:CG  | 1:85:C:HIS:CB  | 4                   | 0.18     | 0.09                | 0.15       |
| (1,872)  | 1:27:C:LEU:CG  | 1:92:C:SER:C   | 3                   | 0.26     | 0.04                | 0.25       |
| (1,59)   | 1:32:C:ARG:CB  | 1:34:C:GLU:CB  | 3                   | 0.22     | 0.09                | 0.17       |
| (1,60)   | 1:32:C:ARG:CB  | 1:34:C:GLU:CB  | 3                   | 0.22     | 0.09                | 0.17       |
| (1,67)   | 1:68:C:LYS:CG  | 1:83:C:GLU:CB  | 3                   | 0.16     | 0.07                | 0.12       |
| (1,697)  | 1:74:C:GLN:CB  | 1:77:C:LYS:CA  | 3                   | 0.16     | 0.07                | 0.11       |
| (1,843)  | 1:73:C:VAL:CB  | 1:52:C:PHE:C   | 3                   | 0.15     | 0.03                | 0.16       |
| (1,1419) | 1:62:C:LEU:CD1 | 1:67:C:GLY:CA  | 3                   | 0.15     | 0.05                | 0.12       |
| (1,89)   | 1:55:C:GLY:C   | 1:50:C:THR:CA  | 3                   | 0.15     | 0.03                | 0.16       |
| (1,1)    | 1:26:C:PRO:CG  | 1:28:C:ARG:C   | 3                   | 0.13     | 0.03                | 0.13       |
| (1,672)  | 1:34:C:GLU:CB  | 1:40:C:HIS:CA  | 3                   | 0.12     | 0.02                | 0.12       |
| (1,144)  | 1:70:C:ASP:CA  | 1:68:C:LYS:CD  | 3                   | 0.12     | 0.01                | 0.12       |
| (2,20)   | 1:57:C:TRP:H   | 1:48:C:GLY:O   | 3                   | 0.11     | 0.01                | 0.11       |
| (1,1354) | 1:83:C:GLU:CB  | 1:68:C:LYS:CD  | 2                   | 0.3      | 0.12                | 0.3        |
| (1,61)   | 1:32:C:ARG:CB  | 1:41:C:ARG:CB  | 2                   | 0.22     | 0.01                | 0.22       |
| (1,54)   | 1:91:C:GLN:CG  | 1:90:C:ARG:CG  | 2                   | 0.2      | 0.02                | 0.2        |
| (1,1369) | 1:32:C:ARG:CG  | 1:34:C:GLU:CB  | 2                   | 0.18     | 0.01                | 0.18       |
| (1,1400) | 1:33:C:VAL:CG1 | 1:95:C:GLN:CB  | 2                   | 0.16     | 0.0                 | 0.16       |
| (1,1083) | 1:80:C:THR:CA  | 1:61:C:ILE:CB  | 2                   | 0.16     | 0.02                | 0.16       |
| (1,601)  | 1:62:C:LEU:CG  | 1:66:C:LYS:CB  | 2                   | 0.12     | 0.01                | 0.12       |
| (1,618)  | 1:61:C:ILE:CG1 | 1:60:C:VAL:CB  | 2                   | 0.12     | 0.02                | 0.12       |
| (1,1368) | 1:61:C:ILE:CG1 | 1:62:C:LEU:CG  | 2                   | 0.1      | 0.0                 | 0.1        |
| (1,1374) | 1:62:C:LEU:CG  | 1:61:C:ILE:CG1 | 2                   | 0.1      | 0.0                 | 0.1        |

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

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

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

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



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

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

| Key     | Atom-1         | Atom-2        | Model ID | Violation (Å) |
|---------|----------------|---------------|----------|---------------|
| (1,41)  | 1:89:C:VAL:CG1 | 1:81:C:CYS:CA | 6        | 9.18          |
| (1,41)  | 1:89:C:VAL:CG1 | 1:81:C:CYS:CA | 7        | 9.15          |
| (1,41)  | 1:89:C:VAL:CG1 | 1:81:C:CYS:CA | 5        | 9.11          |
| (1,41)  | 1:89:C:VAL:CG1 | 1:81:C:CYS:CA | 8        | 9.09          |
| (1,41)  | 1:89:C:VAL:CG1 | 1:81:C:CYS:CA | 4        | 9.07          |
| (1,41)  | 1:89:C:VAL:CG1 | 1:81:C:CYS:CA | 1        | 9.04          |
| (1,41)  | 1:89:C:VAL:CG1 | 1:81:C:CYS:CA | 9        | 9.01          |
| (1,41)  | 1:89:C:VAL:CG1 | 1:81:C:CYS:CA | 10       | 8.97          |
| (1,41)  | 1:89:C:VAL:CG1 | 1:81:C:CYS:CA | 3        | 8.96          |
| (1,315) | 1:35:C:VAL:CA  | 1:70:C:ASP:CA | 10       | 8.87          |
| (1,41)  | 1:89:C:VAL:CG1 | 1:81:C:CYS:CA | 2        | 8.84          |
| (1,362) | 1:93:C:GLN:CA  | 1:32:C:ARG:CB | 2        | 8.61          |
| (1,362) | 1:93:C:GLN:CA  | 1:32:C:ARG:CB | 5        | 8.53          |
| (1,249) | 1:69:C:ASN:CB  | 1:63:C:ASP:CG | 7        | 8.52          |
| (1,249) | 1:69:C:ASN:CB  | 1:63:C:ASP:CG | 3        | 8.46          |
| (1,315) | 1:35:C:VAL:CA  | 1:70:C:ASP:CA | 9        | 8.37          |

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| Key      | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|----------|---------------|---------------|----------|---------------|
| (1,249)  | 1:69:C:ASN:CB | 1:63:C:ASP:CG | 6        | 8.37          |
| (1,315)  | 1:35:C:VAL:CA | 1:70:C:ASP:CA | 4        | 8.36          |
| (1,362)  | 1:93:C:GLN:CA | 1:32:C:ARG:CB | 6        | 8.34          |
| (1,362)  | 1:93:C:GLN:CA | 1:32:C:ARG:CB | 4        | 8.32          |
| (1,315)  | 1:35:C:VAL:CA | 1:70:C:ASP:CA | 1        | 8.3           |
| (1,362)  | 1:93:C:GLN:CA | 1:32:C:ARG:CB | 3        | 8.28          |
| (1,362)  | 1:93:C:GLN:CA | 1:32:C:ARG:CB | 7        | 8.28          |
| (1,315)  | 1:35:C:VAL:CA | 1:70:C:ASP:CA | 5        | 8.28          |
| (1,362)  | 1:93:C:GLN:CA | 1:32:C:ARG:CB | 1        | 8.23          |
| (1,362)  | 1:93:C:GLN:CA | 1:32:C:ARG:CB | 10       | 8.21          |
| (1,315)  | 1:35:C:VAL:CA | 1:70:C:ASP:CA | 6        | 8.2           |
| (1,315)  | 1:35:C:VAL:CA | 1:70:C:ASP:CA | 8        | 8.18          |
| (1,362)  | 1:93:C:GLN:CA | 1:32:C:ARG:CB | 9        | 8.15          |
| (1,315)  | 1:35:C:VAL:CA | 1:70:C:ASP:CA | 7        | 8.14          |
| (1,315)  | 1:35:C:VAL:CA | 1:70:C:ASP:CA | 3        | 8.06          |
| (1,362)  | 1:93:C:GLN:CA | 1:32:C:ARG:CB | 8        | 8.05          |
| (1,249)  | 1:69:C:ASN:CB | 1:63:C:ASP:CG | 2        | 7.99          |
| (1,315)  | 1:35:C:VAL:CA | 1:70:C:ASP:CA | 2        | 7.92          |
| (1,249)  | 1:69:C:ASN:CB | 1:63:C:ASP:CG | 9        | 7.92          |
| (1,249)  | 1:69:C:ASN:CB | 1:63:C:ASP:CG | 5        | 7.91          |
| (1,249)  | 1:69:C:ASN:CB | 1:63:C:ASP:CG | 4        | 7.82          |
| (1,249)  | 1:69:C:ASN:CB | 1:63:C:ASP:CG | 10       | 7.75          |
| (1,249)  | 1:69:C:ASN:CB | 1:63:C:ASP:CG | 8        | 7.74          |
| (1,363)  | 1:93:C:GLN:CA | 1:32:C:ARG:CG | 5        | 7.6           |
| (1,249)  | 1:69:C:ASN:CB | 1:63:C:ASP:CG | 1        | 7.54          |
| (1,699)  | 1:66:C:LYS:CG | 1:70:C:ASP:CA | 4        | 7.39          |
| (1,404)  | 1:70:C:ASP:CA | 1:66:C:LYS:CG | 4        | 7.39          |
| (1,363)  | 1:93:C:GLN:CA | 1:32:C:ARG:CG | 3        | 7.39          |
| (1,699)  | 1:66:C:LYS:CG | 1:70:C:ASP:CA | 9        | 7.33          |
| (1,404)  | 1:70:C:ASP:CA | 1:66:C:LYS:CG | 9        | 7.33          |
| (1,363)  | 1:93:C:GLN:CA | 1:32:C:ARG:CG | 10       | 7.26          |
| (1,699)  | 1:66:C:LYS:CG | 1:70:C:ASP:CA | 7        | 7.24          |
| (1,404)  | 1:70:C:ASP:CA | 1:66:C:LYS:CG | 7        | 7.24          |
| (1,699)  | 1:66:C:LYS:CG | 1:70:C:ASP:CA | 6        | 7.19          |
| (1,404)  | 1:70:C:ASP:CA | 1:66:C:LYS:CG | 6        | 7.19          |
| (1,699)  | 1:66:C:LYS:CG | 1:70:C:ASP:CA | 1        | 7.17          |
| (1,404)  | 1:70:C:ASP:CA | 1:66:C:LYS:CG | 1        | 7.17          |
| (1,699)  | 1:66:C:LYS:CG | 1:70:C:ASP:CA | 5        | 7.08          |
| (1,404)  | 1:70:C:ASP:CA | 1:66:C:LYS:CG | 5        | 7.08          |
| (1,1323) | 1:66:C:LYS:CB | 1:71:C:GLY:CA | 4        | 6.94          |
| (1,1323) | 1:66:C:LYS:CB | 1:71:C:GLY:CA | 1        | 6.92          |
| (1,1323) | 1:66:C:LYS:CB | 1:71:C:GLY:CA | 6        | 6.9           |

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| Key      | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|----------|---------------|---------------|----------|---------------|
| (1,699)  | 1:66:C:LYS:CG | 1:70:C:ASP:CA | 8        | 6.89          |
| (1,404)  | 1:70:C:ASP:CA | 1:66:C:LYS:CG | 8        | 6.89          |
| (1,1323) | 1:66:C:LYS:CB | 1:71:C:GLY:CA | 9        | 6.88          |
| (1,1323) | 1:66:C:LYS:CB | 1:71:C:GLY:CA | 7        | 6.83          |
| (1,1323) | 1:66:C:LYS:CB | 1:71:C:GLY:CA | 8        | 6.76          |
| (1,1323) | 1:66:C:LYS:CB | 1:71:C:GLY:CA | 10       | 6.72          |
| (1,699)  | 1:66:C:LYS:CG | 1:70:C:ASP:CA | 10       | 6.7           |
| (1,404)  | 1:70:C:ASP:CA | 1:66:C:LYS:CG | 10       | 6.7           |
| (1,1323) | 1:66:C:LYS:CB | 1:71:C:GLY:CA | 5        | 6.68          |
| (1,1323) | 1:66:C:LYS:CB | 1:71:C:GLY:CA | 2        | 6.65          |
| (1,1323) | 1:66:C:LYS:CB | 1:71:C:GLY:CA | 3        | 6.63          |
| (1,699)  | 1:66:C:LYS:CG | 1:70:C:ASP:CA | 3        | 6.58          |
| (1,404)  | 1:70:C:ASP:CA | 1:66:C:LYS:CG | 3        | 6.58          |
| (1,699)  | 1:66:C:LYS:CG | 1:70:C:ASP:CA | 2        | 6.52          |
| (1,404)  | 1:70:C:ASP:CA | 1:66:C:LYS:CG | 2        | 6.52          |
| (1,609)  | 1:56:C:LYS:CB | 1:52:C:PHE:CB | 3        | 6.46          |
| (1,609)  | 1:56:C:LYS:CB | 1:52:C:PHE:CB | 5        | 6.42          |
| (1,1242) | 1:65:C:ALA:CA | 1:79:C:PHE:CA | 3        | 6.41          |
| (1,609)  | 1:56:C:LYS:CB | 1:52:C:PHE:CB | 6        | 6.4           |
| (1,609)  | 1:56:C:LYS:CB | 1:52:C:PHE:CB | 2        | 6.36          |
| (1,609)  | 1:56:C:LYS:CB | 1:52:C:PHE:CB | 9        | 6.33          |
| (1,385)  | 1:51:C:LEU:CA | 1:77:C:LYS:CB | 4        | 6.24          |
| (1,363)  | 1:93:C:GLN:CA | 1:32:C:ARG:CG | 2        | 6.06          |
| (1,1242) | 1:65:C:ALA:CA | 1:79:C:PHE:CA | 6        | 6.05          |
| (1,609)  | 1:56:C:LYS:CB | 1:52:C:PHE:CB | 4        | 6.05          |
| (1,609)  | 1:56:C:LYS:CB | 1:52:C:PHE:CB | 8        | 6.04          |
| (1,1242) | 1:65:C:ALA:CA | 1:79:C:PHE:CA | 8        | 6.03          |
| (1,1242) | 1:65:C:ALA:CA | 1:79:C:PHE:CA | 9        | 5.98          |
| (1,385)  | 1:51:C:LEU:CA | 1:77:C:LYS:CB | 9        | 5.97          |
| (1,609)  | 1:56:C:LYS:CB | 1:52:C:PHE:CB | 7        | 5.93          |
| (1,1242) | 1:65:C:ALA:CA | 1:79:C:PHE:CA | 2        | 5.92          |
| (1,1242) | 1:65:C:ALA:CA | 1:79:C:PHE:CA | 4        | 5.88          |
| (1,66)   | 1:51:C:LEU:CG | 1:77:C:LYS:CB | 10       | 5.88          |
| (1,609)  | 1:56:C:LYS:CB | 1:52:C:PHE:CB | 1        | 5.84          |
| (1,66)   | 1:51:C:LEU:CG | 1:77:C:LYS:CB | 5        | 5.84          |
| (1,385)  | 1:51:C:LEU:CA | 1:77:C:LYS:CB | 8        | 5.82          |
| (1,66)   | 1:51:C:LEU:CG | 1:77:C:LYS:CB | 4        | 5.81          |
| (1,66)   | 1:51:C:LEU:CG | 1:77:C:LYS:CB | 6        | 5.81          |
| (1,1242) | 1:65:C:ALA:CA | 1:79:C:PHE:CA | 1        | 5.79          |
| (1,609)  | 1:56:C:LYS:CB | 1:52:C:PHE:CB | 10       | 5.79          |
| (1,434)  | 1:35:C:VAL:CB | 1:32:C:ARG:CG | 3        | 5.79          |
| (1,363)  | 1:93:C:GLN:CA | 1:32:C:ARG:CG | 8        | 5.78          |

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| Key      | Atom-1         | Atom-2        | Model ID | Violation (Å) |
|----------|----------------|---------------|----------|---------------|
| (1,1242) | 1:65:C:ALA:CA  | 1:79:C:PHE:CA | 5        | 5.71          |
| (1,385)  | 1:51:C:LEU:CA  | 1:77:C:LYS:CB | 2        | 5.71          |
| (1,363)  | 1:93:C:GLN:CA  | 1:32:C:ARG:CG | 6        | 5.68          |
| (1,478)  | 1:33:C:VAL:CA  | 1:90:C:ARG:CD | 6        | 5.66          |
| (1,385)  | 1:51:C:LEU:CA  | 1:77:C:LYS:CB | 10       | 5.66          |
| (1,385)  | 1:51:C:LEU:CA  | 1:77:C:LYS:CB | 6        | 5.65          |
| (1,825)  | 1:70:C:ASP:CB  | 1:51:C:LEU:C  | 2        | 5.63          |
| (1,385)  | 1:51:C:LEU:CA  | 1:77:C:LYS:CB | 5        | 5.63          |
| (1,1242) | 1:65:C:ALA:CA  | 1:79:C:PHE:CA | 7        | 5.62          |
| (1,385)  | 1:51:C:LEU:CA  | 1:77:C:LYS:CB | 3        | 5.62          |
| (1,66)   | 1:51:C:LEU:CG  | 1:77:C:LYS:CB | 9        | 5.62          |
| (1,385)  | 1:51:C:LEU:CA  | 1:77:C:LYS:CB | 1        | 5.6           |
| (1,363)  | 1:93:C:GLN:CA  | 1:32:C:ARG:CG | 4        | 5.6           |
| (1,434)  | 1:35:C:VAL:CB  | 1:32:C:ARG:CG | 10       | 5.55          |
| (1,1242) | 1:65:C:ALA:CA  | 1:79:C:PHE:CA | 10       | 5.54          |
| (1,434)  | 1:35:C:VAL:CB  | 1:32:C:ARG:CG | 5        | 5.53          |
| (1,478)  | 1:33:C:VAL:CA  | 1:90:C:ARG:CD | 5        | 5.49          |
| (1,66)   | 1:51:C:LEU:CG  | 1:77:C:LYS:CB | 7        | 5.48          |
| (1,478)  | 1:33:C:VAL:CA  | 1:90:C:ARG:CD | 3        | 5.46          |
| (1,121)  | 1:73:C:VAL:CG2 | 1:53:C:ALA:CB | 10       | 5.45          |
| (1,499)  | 1:33:C:VAL:CB  | 1:91:C:GLN:CG | 6        | 5.44          |
| (1,478)  | 1:33:C:VAL:CA  | 1:90:C:ARG:CD | 8        | 5.44          |
| (1,478)  | 1:33:C:VAL:CA  | 1:90:C:ARG:CD | 2        | 5.43          |
| (1,478)  | 1:33:C:VAL:CA  | 1:90:C:ARG:CD | 1        | 5.41          |
| (1,121)  | 1:73:C:VAL:CG2 | 1:53:C:ALA:CB | 1        | 5.39          |
| (1,825)  | 1:70:C:ASP:CB  | 1:51:C:LEU:C  | 3        | 5.38          |
| (1,825)  | 1:70:C:ASP:CB  | 1:51:C:LEU:C  | 4        | 5.38          |
| (1,478)  | 1:33:C:VAL:CA  | 1:90:C:ARG:CD | 7        | 5.37          |
| (1,385)  | 1:51:C:LEU:CA  | 1:77:C:LYS:CB | 7        | 5.36          |
| (1,363)  | 1:93:C:GLN:CA  | 1:32:C:ARG:CG | 9        | 5.34          |
| (1,825)  | 1:70:C:ASP:CB  | 1:51:C:LEU:C  | 9        | 5.33          |
| (1,121)  | 1:73:C:VAL:CG2 | 1:53:C:ALA:CB | 8        | 5.33          |
| (1,121)  | 1:73:C:VAL:CG2 | 1:53:C:ALA:CB | 5        | 5.31          |
| (1,478)  | 1:33:C:VAL:CA  | 1:90:C:ARG:CD | 4        | 5.28          |
| (1,121)  | 1:73:C:VAL:CG2 | 1:53:C:ALA:CB | 4        | 5.27          |
| (1,121)  | 1:73:C:VAL:CG2 | 1:53:C:ALA:CB | 6        | 5.27          |
| (1,121)  | 1:73:C:VAL:CG2 | 1:53:C:ALA:CB | 2        | 5.26          |
| (1,499)  | 1:33:C:VAL:CB  | 1:91:C:GLN:CG | 8        | 5.25          |
| (1,363)  | 1:93:C:GLN:CA  | 1:32:C:ARG:CG | 7        | 5.25          |
| (1,121)  | 1:73:C:VAL:CG2 | 1:53:C:ALA:CB | 9        | 5.25          |
| (1,66)   | 1:51:C:LEU:CG  | 1:77:C:LYS:CB | 2        | 5.24          |
| (1,121)  | 1:73:C:VAL:CG2 | 1:53:C:ALA:CB | 3        | 5.22          |

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| Key      | Atom-1         | Atom-2        | Model ID | Violation (Å) |
|----------|----------------|---------------|----------|---------------|
| (1,66)   | 1:51:C:LEU:CG  | 1:77:C:LYS:CB | 8        | 5.22          |
| (1,1282) | 1:94:C:ILE:CB  | 1:38:C:LYS:CB | 9        | 5.21          |
| (1,363)  | 1:93:C:GLN:CA  | 1:32:C:ARG:CG | 1        | 5.21          |
| (1,825)  | 1:70:C:ASP:CB  | 1:51:C:LEU:C  | 7        | 5.19          |
| (1,421)  | 1:80:C:THR:CB  | 1:76:C:ARG:CB | 1        | 5.17          |
| (1,499)  | 1:33:C:VAL:CB  | 1:91:C:GLN:CG | 3        | 5.16          |
| (1,478)  | 1:33:C:VAL:CA  | 1:90:C:ARG:CD | 9        | 5.14          |
| (1,478)  | 1:33:C:VAL:CA  | 1:90:C:ARG:CD | 10       | 5.14          |
| (1,421)  | 1:80:C:THR:CB  | 1:76:C:ARG:CB | 9        | 5.11          |
| (1,421)  | 1:80:C:THR:CB  | 1:76:C:ARG:CB | 7        | 5.09          |
| (1,825)  | 1:70:C:ASP:CB  | 1:51:C:LEU:C  | 1        | 5.08          |
| (1,121)  | 1:73:C:VAL:CG2 | 1:53:C:ALA:CB | 7        | 5.07          |
| (1,421)  | 1:80:C:THR:CB  | 1:76:C:ARG:CB | 8        | 5.06          |
| (1,825)  | 1:70:C:ASP:CB  | 1:51:C:LEU:C  | 6        | 5.05          |
| (1,421)  | 1:80:C:THR:CB  | 1:76:C:ARG:CB | 3        | 5.02          |
| (1,66)   | 1:51:C:LEU:CG  | 1:77:C:LYS:CB | 1        | 5.0           |
| (1,421)  | 1:80:C:THR:CB  | 1:76:C:ARG:CB | 6        | 4.98          |
| (1,825)  | 1:70:C:ASP:CB  | 1:51:C:LEU:C  | 8        | 4.96          |
| (1,421)  | 1:80:C:THR:CB  | 1:76:C:ARG:CB | 10       | 4.96          |
| (1,825)  | 1:70:C:ASP:CB  | 1:51:C:LEU:C  | 10       | 4.95          |
| (1,660)  | 1:52:C:PHE:CB  | 1:56:C:LYS:CA | 3        | 4.94          |
| (1,660)  | 1:52:C:PHE:CB  | 1:56:C:LYS:CA | 5        | 4.89          |
| (1,660)  | 1:52:C:PHE:CB  | 1:56:C:LYS:CA | 6        | 4.87          |
| (1,660)  | 1:52:C:PHE:CB  | 1:56:C:LYS:CA | 2        | 4.84          |
| (1,421)  | 1:80:C:THR:CB  | 1:76:C:ARG:CB | 4        | 4.84          |
| (1,812)  | 1:71:C:GLY:CA  | 1:66:C:LYS:C  | 4        | 4.82          |
| (1,421)  | 1:80:C:THR:CB  | 1:76:C:ARG:CB | 2        | 4.81          |
| (1,421)  | 1:80:C:THR:CB  | 1:76:C:ARG:CB | 5        | 4.81          |
| (1,660)  | 1:52:C:PHE:CB  | 1:56:C:LYS:CA | 9        | 4.8           |
| (1,393)  | 1:51:C:LEU:CA  | 1:57:C:TRP:CB | 2        | 4.77          |
| (1,393)  | 1:51:C:LEU:CA  | 1:57:C:TRP:CB | 6        | 4.77          |
| (1,1282) | 1:94:C:ILE:CB  | 1:38:C:LYS:CB | 2        | 4.76          |
| (1,812)  | 1:71:C:GLY:CA  | 1:66:C:LYS:C  | 1        | 4.76          |
| (1,812)  | 1:71:C:GLY:CA  | 1:66:C:LYS:C  | 9        | 4.76          |
| (1,393)  | 1:51:C:LEU:CA  | 1:57:C:TRP:CB | 5        | 4.74          |
| (1,1282) | 1:94:C:ILE:CB  | 1:38:C:LYS:CB | 3        | 4.73          |
| (1,812)  | 1:71:C:GLY:CA  | 1:66:C:LYS:C  | 7        | 4.72          |
| (1,434)  | 1:35:C:VAL:CB  | 1:32:C:ARG:CG | 2        | 4.72          |
| (1,393)  | 1:51:C:LEU:CA  | 1:57:C:TRP:CB | 9        | 4.72          |
| (1,812)  | 1:71:C:GLY:CA  | 1:66:C:LYS:C  | 6        | 4.71          |
| (1,499)  | 1:33:C:VAL:CB  | 1:91:C:GLN:CG | 5        | 4.71          |
| (1,393)  | 1:51:C:LEU:CA  | 1:57:C:TRP:CB | 7        | 4.7           |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1282) | 1:94:C:ILE:CB  | 1:38:C:LYS:CB  | 4        | 4.67          |
| (1,1143) | 1:77:C:LYS:CA  | 1:83:C:GLU:CB  | 2        | 4.66          |
| (1,1102) | 1:78:C:TYR:CA  | 1:82:C:ASP:CB  | 2        | 4.66          |
| (1,434)  | 1:35:C:VAL:CB  | 1:32:C:ARG:CG  | 9        | 4.63          |
| (1,1166) | 1:41:C:ARG:CA  | 1:87:C:ILE:CD1 | 10       | 4.59          |
| (1,1102) | 1:78:C:TYR:CA  | 1:82:C:ASP:CB  | 3        | 4.54          |
| (1,660)  | 1:52:C:PHE:CB  | 1:56:C:LYS:CA  | 4        | 4.54          |
| (1,660)  | 1:52:C:PHE:CB  | 1:56:C:LYS:CA  | 8        | 4.54          |
| (1,66)   | 1:51:C:LEU:CG  | 1:77:C:LYS:CB  | 3        | 4.5           |
| (1,812)  | 1:71:C:GLY:CA  | 1:66:C:LYS:C   | 5        | 4.49          |
| (1,825)  | 1:70:C:ASP:CB  | 1:51:C:LEU:C   | 5        | 4.48          |
| (1,812)  | 1:71:C:GLY:CA  | 1:66:C:LYS:C   | 8        | 4.48          |
| (1,499)  | 1:33:C:VAL:CB  | 1:91:C:GLN:CG  | 2        | 4.48          |
| (1,434)  | 1:35:C:VAL:CB  | 1:32:C:ARG:CG  | 7        | 4.48          |
| (1,393)  | 1:51:C:LEU:CA  | 1:57:C:TRP:CB  | 4        | 4.48          |
| (1,1440) | 1:33:C:VAL:CG2 | 1:91:C:GLN:CG  | 5        | 4.46          |
| (1,1102) | 1:78:C:TYR:CA  | 1:82:C:ASP:CB  | 5        | 4.46          |
| (1,812)  | 1:71:C:GLY:CA  | 1:66:C:LYS:C   | 10       | 4.46          |
| (1,1282) | 1:94:C:ILE:CB  | 1:38:C:LYS:CB  | 10       | 4.45          |
| (1,815)  | 1:51:C:LEU:CB  | 1:78:C:TYR:C   | 4        | 4.45          |
| (1,499)  | 1:33:C:VAL:CB  | 1:91:C:GLN:CG  | 4        | 4.45          |
| (1,434)  | 1:35:C:VAL:CB  | 1:32:C:ARG:CG  | 1        | 4.43          |
| (1,812)  | 1:71:C:GLY:CA  | 1:66:C:LYS:C   | 2        | 4.42          |
| (1,660)  | 1:52:C:PHE:CB  | 1:56:C:LYS:CA  | 7        | 4.42          |
| (1,393)  | 1:51:C:LEU:CA  | 1:57:C:TRP:CB  | 3        | 4.42          |
| (1,1282) | 1:94:C:ILE:CB  | 1:38:C:LYS:CB  | 8        | 4.38          |
| (1,1143) | 1:77:C:LYS:CA  | 1:83:C:GLU:CB  | 5        | 4.37          |
| (1,393)  | 1:51:C:LEU:CA  | 1:57:C:TRP:CB  | 1        | 4.37          |
| (1,1143) | 1:77:C:LYS:CA  | 1:83:C:GLU:CB  | 3        | 4.36          |
| (1,812)  | 1:71:C:GLY:CA  | 1:66:C:LYS:C   | 3        | 4.34          |
| (1,660)  | 1:52:C:PHE:CB  | 1:56:C:LYS:CA  | 1        | 4.34          |
| (1,1373) | 1:62:C:LEU:CG  | 1:43:C:THR:CG2 | 6        | 4.31          |
| (1,1282) | 1:94:C:ILE:CB  | 1:38:C:LYS:CB  | 7        | 4.3           |
| (1,660)  | 1:52:C:PHE:CB  | 1:56:C:LYS:CA  | 10       | 4.28          |
| (1,651)  | 1:58:C:VAL:CG2 | 1:61:C:ILE:CB  | 2        | 4.27          |
| (1,147)  | 1:40:C:HIS:CA  | 1:36:C:ILE:CG1 | 4        | 4.26          |
| (1,1102) | 1:78:C:TYR:CA  | 1:82:C:ASP:CB  | 10       | 4.25          |
| (1,1143) | 1:77:C:LYS:CA  | 1:83:C:GLU:CB  | 4        | 4.23          |
| (1,651)  | 1:58:C:VAL:CG2 | 1:61:C:ILE:CB  | 5        | 4.23          |
| (1,651)  | 1:58:C:VAL:CG2 | 1:61:C:ILE:CB  | 8        | 4.23          |
| (1,1102) | 1:78:C:TYR:CA  | 1:82:C:ASP:CB  | 6        | 4.22          |
| (1,651)  | 1:58:C:VAL:CG2 | 1:61:C:ILE:CB  | 4        | 4.22          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1143) | 1:77:C:LYS:CA  | 1:83:C:GLU:CB  | 7        | 4.21          |
| (1,1143) | 1:77:C:LYS:CA  | 1:83:C:GLU:CB  | 10       | 4.21          |
| (1,393)  | 1:51:C:LEU:CA  | 1:57:C:TRP:CB  | 8        | 4.21          |
| (1,1166) | 1:41:C:ARG:CA  | 1:87:C:ILE:CD1 | 5        | 4.2           |
| (1,1088) | 1:31:C:SER:CA  | 1:26:C:PRO:CG  | 6        | 4.19          |
| (1,1373) | 1:62:C:LEU:CG  | 1:43:C:THR:CG2 | 2        | 4.18          |
| (1,1143) | 1:77:C:LYS:CA  | 1:83:C:GLU:CB  | 1        | 4.18          |
| (1,651)  | 1:58:C:VAL:CG2 | 1:61:C:ILE:CB  | 6        | 4.18          |
| (1,1166) | 1:41:C:ARG:CA  | 1:87:C:ILE:CD1 | 6        | 4.17          |
| (1,651)  | 1:58:C:VAL:CG2 | 1:61:C:ILE:CB  | 10       | 4.17          |
| (1,1440) | 1:33:C:VAL:CG2 | 1:91:C:GLN:CG  | 4        | 4.16          |
| (1,1143) | 1:77:C:LYS:CA  | 1:83:C:GLU:CB  | 6        | 4.16          |
| (1,1102) | 1:78:C:TYR:CA  | 1:82:C:ASP:CB  | 4        | 4.16          |
| (1,147)  | 1:40:C:HIS:CA  | 1:36:C:ILE:CG1 | 6        | 4.16          |
| (1,1282) | 1:94:C:ILE:CB  | 1:38:C:LYS:CB  | 1        | 4.15          |
| (1,1282) | 1:94:C:ILE:CB  | 1:38:C:LYS:CB  | 6        | 4.14          |
| (1,352)  | 1:31:C:SER:CB  | 1:46:C:TYR:CB  | 9        | 4.14          |
| (1,1143) | 1:77:C:LYS:CA  | 1:83:C:GLU:CB  | 8        | 4.13          |
| (1,1088) | 1:31:C:SER:CA  | 1:26:C:PRO:CG  | 9        | 4.13          |
| (1,635)  | 1:46:C:TYR:CB  | 1:61:C:ILE:CG2 | 5        | 4.13          |
| (1,499)  | 1:33:C:VAL:CB  | 1:91:C:GLN:CG  | 7        | 4.13          |
| (1,352)  | 1:31:C:SER:CB  | 1:46:C:TYR:CB  | 4        | 4.13          |
| (1,352)  | 1:31:C:SER:CB  | 1:46:C:TYR:CB  | 5        | 4.13          |
| (1,815)  | 1:51:C:LEU:CB  | 1:78:C:TYR:C   | 9        | 4.12          |
| (1,352)  | 1:31:C:SER:CB  | 1:46:C:TYR:CB  | 1        | 4.12          |
| (1,352)  | 1:31:C:SER:CB  | 1:46:C:TYR:CB  | 2        | 4.12          |
| (1,368)  | 1:79:C:PHE:CA  | 1:47:C:VAL:CB  | 7        | 4.1           |
| (1,1143) | 1:77:C:LYS:CA  | 1:83:C:GLU:CB  | 9        | 4.08          |
| (1,1102) | 1:78:C:TYR:CA  | 1:82:C:ASP:CB  | 7        | 4.08          |
| (1,1102) | 1:78:C:TYR:CA  | 1:82:C:ASP:CB  | 8        | 4.08          |
| (1,393)  | 1:51:C:LEU:CA  | 1:57:C:TRP:CB  | 10       | 4.08          |
| (1,1373) | 1:62:C:LEU:CG  | 1:43:C:THR:CG2 | 8        | 4.06          |
| (1,635)  | 1:46:C:TYR:CB  | 1:61:C:ILE:CG2 | 7        | 4.06          |
| (1,499)  | 1:33:C:VAL:CB  | 1:91:C:GLN:CG  | 10       | 4.06          |
| (1,147)  | 1:40:C:HIS:CA  | 1:36:C:ILE:CG1 | 3        | 4.06          |
| (1,1088) | 1:31:C:SER:CA  | 1:26:C:PRO:CG  | 1        | 4.05          |
| (1,1088) | 1:31:C:SER:CA  | 1:26:C:PRO:CG  | 10       | 4.05          |
| (1,815)  | 1:51:C:LEU:CB  | 1:78:C:TYR:C   | 10       | 4.05          |
| (1,556)  | 1:68:C:LYS:CD  | 1:77:C:LYS:CG  | 5        | 4.05          |
| (1,46)   | 1:83:C:GLU:CA  | 1:73:C:VAL:CB  | 2        | 4.05          |
| (1,1373) | 1:62:C:LEU:CG  | 1:43:C:THR:CG2 | 4        | 4.04          |
| (1,651)  | 1:58:C:VAL:CG2 | 1:61:C:ILE:CB  | 3        | 4.04          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,434)  | 1:35:C:VAL:CB  | 1:32:C:ARG:CG  | 8        | 4.04          |
| (1,651)  | 1:58:C:VAL:CG2 | 1:61:C:ILE:CB  | 1        | 4.03          |
| (1,556)  | 1:68:C:LYS:CD  | 1:77:C:LYS:CG  | 2        | 4.03          |
| (1,352)  | 1:31:C:SER:CB  | 1:46:C:TYR:CB  | 6        | 4.03          |
| (1,216)  | 1:61:C:ILE:CG1 | 1:40:C:HIS:C   | 9        | 4.03          |
| (1,1373) | 1:62:C:LEU:CG  | 1:43:C:THR:CG2 | 1        | 4.02          |
| (1,147)  | 1:40:C:HIS:CA  | 1:36:C:ILE:CG1 | 8        | 4.02          |
| (1,1282) | 1:94:C:ILE:CB  | 1:38:C:LYS:CB  | 5        | 4.01          |
| (1,352)  | 1:31:C:SER:CB  | 1:46:C:TYR:CB  | 8        | 4.0           |
| (1,352)  | 1:31:C:SER:CB  | 1:46:C:TYR:CB  | 10       | 4.0           |
| (1,147)  | 1:40:C:HIS:CA  | 1:36:C:ILE:CG1 | 7        | 4.0           |
| (1,1440) | 1:33:C:VAL:CG2 | 1:91:C:GLN:CG  | 2        | 3.99          |
| (1,147)  | 1:40:C:HIS:CA  | 1:36:C:ILE:CG1 | 1        | 3.99          |
| (1,1088) | 1:31:C:SER:CA  | 1:26:C:PRO:CG  | 8        | 3.98          |
| (1,651)  | 1:58:C:VAL:CG2 | 1:61:C:ILE:CB  | 7        | 3.98          |
| (1,815)  | 1:51:C:LEU:CB  | 1:78:C:TYR:C   | 8        | 3.97          |
| (1,651)  | 1:58:C:VAL:CG2 | 1:61:C:ILE:CB  | 9        | 3.97          |
| (1,352)  | 1:31:C:SER:CB  | 1:46:C:TYR:CB  | 7        | 3.96          |
| (1,46)   | 1:83:C:GLU:CA  | 1:73:C:VAL:CB  | 4        | 3.96          |
| (1,46)   | 1:83:C:GLU:CA  | 1:73:C:VAL:CB  | 5        | 3.96          |
| (1,147)  | 1:40:C:HIS:CA  | 1:36:C:ILE:CG1 | 10       | 3.95          |
| (1,46)   | 1:83:C:GLU:CA  | 1:73:C:VAL:CB  | 3        | 3.95          |
| (1,1102) | 1:78:C:TYR:CA  | 1:82:C:ASP:CB  | 9        | 3.94          |
| (1,815)  | 1:51:C:LEU:CB  | 1:78:C:TYR:C   | 2        | 3.94          |
| (1,556)  | 1:68:C:LYS:CD  | 1:77:C:LYS:CG  | 6        | 3.94          |
| (1,1102) | 1:78:C:TYR:CA  | 1:82:C:ASP:CB  | 1        | 3.92          |
| (1,556)  | 1:68:C:LYS:CD  | 1:77:C:LYS:CG  | 7        | 3.92          |
| (1,368)  | 1:79:C:PHE:CA  | 1:47:C:VAL:CB  | 1        | 3.92          |
| (1,815)  | 1:51:C:LEU:CB  | 1:78:C:TYR:C   | 1        | 3.91          |
| (1,815)  | 1:51:C:LEU:CB  | 1:78:C:TYR:C   | 7        | 3.9           |
| (1,499)  | 1:33:C:VAL:CB  | 1:91:C:GLN:CG  | 1        | 3.9           |
| (1,556)  | 1:68:C:LYS:CD  | 1:77:C:LYS:CG  | 9        | 3.89          |
| (1,147)  | 1:40:C:HIS:CA  | 1:36:C:ILE:CG1 | 2        | 3.89          |
| (1,1373) | 1:62:C:LEU:CG  | 1:43:C:THR:CG2 | 10       | 3.88          |
| (1,216)  | 1:61:C:ILE:CG1 | 1:40:C:HIS:C   | 5        | 3.86          |
| (1,147)  | 1:40:C:HIS:CA  | 1:36:C:ILE:CG1 | 5        | 3.86          |
| (1,352)  | 1:31:C:SER:CB  | 1:46:C:TYR:CB  | 3        | 3.84          |
| (1,556)  | 1:68:C:LYS:CD  | 1:77:C:LYS:CG  | 3        | 3.83          |
| (1,556)  | 1:68:C:LYS:CD  | 1:77:C:LYS:CG  | 4        | 3.82          |
| (1,368)  | 1:79:C:PHE:CA  | 1:47:C:VAL:CB  | 4        | 3.82          |
| (1,556)  | 1:68:C:LYS:CD  | 1:77:C:LYS:CG  | 8        | 3.81          |
| (1,216)  | 1:61:C:ILE:CG1 | 1:40:C:HIS:C   | 3        | 3.81          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,46)   | 1:83:C:GLU:CA  | 1:73:C:VAL:CB  | 9        | 3.81          |
| (1,815)  | 1:51:C:LEU:CB  | 1:78:C:TYR:C   | 3        | 3.79          |
| (1,368)  | 1:79:C:PHE:CA  | 1:47:C:VAL:CB  | 10       | 3.79          |
| (1,1286) | 1:46:C:TYR:CB  | 1:60:C:VAL:CG1 | 5        | 3.78          |
| (1,46)   | 1:83:C:GLU:CA  | 1:73:C:VAL:CB  | 7        | 3.77          |
| (1,1166) | 1:41:C:ARG:CA  | 1:87:C:ILE:CD1 | 8        | 3.74          |
| (1,635)  | 1:46:C:TYR:CB  | 1:61:C:ILE:CG2 | 3        | 3.74          |
| (1,46)   | 1:83:C:GLU:CA  | 1:73:C:VAL:CB  | 10       | 3.74          |
| (1,767)  | 1:83:C:GLU:CB  | 1:63:C:ASP:CA  | 9        | 3.72          |
| (1,815)  | 1:51:C:LEU:CB  | 1:78:C:TYR:C   | 5        | 3.71          |
| (1,767)  | 1:83:C:GLU:CB  | 1:63:C:ASP:CA  | 10       | 3.71          |
| (1,434)  | 1:35:C:VAL:CB  | 1:32:C:ARG:CG  | 6        | 3.71          |
| (1,1286) | 1:46:C:TYR:CB  | 1:60:C:VAL:CG1 | 3        | 3.69          |
| (1,1088) | 1:31:C:SER:CA  | 1:26:C:PRO:CG  | 4        | 3.69          |
| (1,1106) | 1:78:C:TYR:CA  | 1:74:C:GLN:CG  | 7        | 3.68          |
| (1,815)  | 1:51:C:LEU:CB  | 1:78:C:TYR:C   | 6        | 3.68          |
| (1,533)  | 1:73:C:VAL:CB  | 1:83:C:GLU:CB  | 2        | 3.66          |
| (1,46)   | 1:83:C:GLU:CA  | 1:73:C:VAL:CB  | 1        | 3.66          |
| (1,767)  | 1:83:C:GLU:CB  | 1:63:C:ASP:CA  | 8        | 3.65          |
| (1,635)  | 1:46:C:TYR:CB  | 1:61:C:ILE:CG2 | 1        | 3.64          |
| (1,635)  | 1:46:C:TYR:CB  | 1:61:C:ILE:CG2 | 9        | 3.63          |
| (1,1440) | 1:33:C:VAL:CG2 | 1:91:C:GLN:CG  | 10       | 3.61          |
| (1,1166) | 1:41:C:ARG:CA  | 1:87:C:ILE:CD1 | 7        | 3.61          |
| (1,1106) | 1:78:C:TYR:CA  | 1:74:C:GLN:CG  | 8        | 3.61          |
| (1,368)  | 1:79:C:PHE:CA  | 1:47:C:VAL:CB  | 2        | 3.6           |
| (1,368)  | 1:79:C:PHE:CA  | 1:47:C:VAL:CB  | 8        | 3.6           |
| (1,1088) | 1:31:C:SER:CA  | 1:26:C:PRO:CG  | 7        | 3.59          |
| (1,1106) | 1:78:C:TYR:CA  | 1:74:C:GLN:CG  | 1        | 3.58          |
| (1,1106) | 1:78:C:TYR:CA  | 1:74:C:GLN:CG  | 6        | 3.58          |
| (1,767)  | 1:83:C:GLU:CB  | 1:63:C:ASP:CA  | 5        | 3.58          |
| (1,368)  | 1:79:C:PHE:CA  | 1:47:C:VAL:CB  | 6        | 3.57          |
| (1,216)  | 1:61:C:ILE:CG1 | 1:40:C:HIS:C   | 7        | 3.57          |
| (1,147)  | 1:40:C:HIS:CA  | 1:36:C:ILE:CG1 | 9        | 3.57          |
| (1,46)   | 1:83:C:GLU:CA  | 1:73:C:VAL:CB  | 6        | 3.57          |
| (1,1088) | 1:31:C:SER:CA  | 1:26:C:PRO:CG  | 5        | 3.56          |
| (1,1106) | 1:78:C:TYR:CA  | 1:74:C:GLN:CG  | 3        | 3.55          |
| (1,46)   | 1:83:C:GLU:CA  | 1:73:C:VAL:CB  | 8        | 3.55          |
| (1,1106) | 1:78:C:TYR:CA  | 1:74:C:GLN:CG  | 2        | 3.54          |
| (1,368)  | 1:79:C:PHE:CA  | 1:47:C:VAL:CB  | 5        | 3.54          |
| (1,1286) | 1:46:C:TYR:CB  | 1:60:C:VAL:CG1 | 10       | 3.53          |
| (1,668)  | 1:60:C:VAL:CB  | 1:66:C:LYS:CA  | 4        | 3.53          |
| (1,216)  | 1:61:C:ILE:CG1 | 1:40:C:HIS:C   | 1        | 3.53          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1286) | 1:46:C:TYR:CB  | 1:60:C:VAL:CG1 | 4        | 3.52          |
| (1,496)  | 1:61:C:ILE:CB  | 1:83:C:GLU:CB  | 3        | 3.51          |
| (1,1228) | 1:89:C:VAL:CA  | 1:53:C:ALA:CA  | 7        | 3.5           |
| (1,496)  | 1:61:C:ILE:CB  | 1:83:C:GLU:CB  | 1        | 3.5           |
| (1,692)  | 1:61:C:ILE:CG1 | 1:66:C:LYS:CA  | 1        | 3.48          |
| (1,496)  | 1:61:C:ILE:CB  | 1:83:C:GLU:CB  | 9        | 3.48          |
| (1,434)  | 1:35:C:VAL:CB  | 1:32:C:ARG:CG  | 4        | 3.48          |
| (1,767)  | 1:83:C:GLU:CB  | 1:63:C:ASP:CA  | 7        | 3.47          |
| (1,533)  | 1:73:C:VAL:CB  | 1:83:C:GLU:CB  | 3        | 3.47          |
| (1,1373) | 1:62:C:LEU:CG  | 1:43:C:THR:CG2 | 9        | 3.46          |
| (1,1286) | 1:46:C:TYR:CB  | 1:60:C:VAL:CG1 | 6        | 3.46          |
| (1,368)  | 1:79:C:PHE:CA  | 1:47:C:VAL:CB  | 9        | 3.46          |
| (1,1286) | 1:46:C:TYR:CB  | 1:60:C:VAL:CG1 | 7        | 3.45          |
| (1,1286) | 1:46:C:TYR:CB  | 1:60:C:VAL:CG1 | 9        | 3.45          |
| (1,767)  | 1:83:C:GLU:CB  | 1:63:C:ASP:CA  | 1        | 3.44          |
| (1,556)  | 1:68:C:LYS:CD  | 1:77:C:LYS:CG  | 1        | 3.44          |
| (1,221)  | 1:74:C:GLN:CB  | 1:71:C:GLY:C   | 9        | 3.44          |
| (1,533)  | 1:73:C:VAL:CB  | 1:83:C:GLU:CB  | 5        | 3.43          |
| (1,1286) | 1:46:C:TYR:CB  | 1:60:C:VAL:CG1 | 2        | 3.42          |
| (1,692)  | 1:61:C:ILE:CG1 | 1:66:C:LYS:CA  | 3        | 3.42          |
| (1,368)  | 1:79:C:PHE:CA  | 1:47:C:VAL:CB  | 3        | 3.42          |
| (1,221)  | 1:74:C:GLN:CB  | 1:71:C:GLY:C   | 1        | 3.42          |
| (1,767)  | 1:83:C:GLU:CB  | 1:63:C:ASP:CA  | 4        | 3.41          |
| (1,1286) | 1:46:C:TYR:CB  | 1:60:C:VAL:CG1 | 1        | 3.4           |
| (1,499)  | 1:33:C:VAL:CB  | 1:91:C:GLN:CG  | 9        | 3.4           |
| (1,496)  | 1:61:C:ILE:CB  | 1:83:C:GLU:CB  | 5        | 3.4           |
| (1,221)  | 1:74:C:GLN:CB  | 1:71:C:GLY:C   | 7        | 3.4           |
| (1,1228) | 1:89:C:VAL:CA  | 1:53:C:ALA:CA  | 2        | 3.39          |
| (1,496)  | 1:61:C:ILE:CB  | 1:83:C:GLU:CB  | 7        | 3.39          |
| (1,767)  | 1:83:C:GLU:CB  | 1:63:C:ASP:CA  | 2        | 3.38          |
| (1,701)  | 1:77:C:LYS:CG  | 1:82:C:ASP:CA  | 2        | 3.38          |
| (1,692)  | 1:61:C:ILE:CG1 | 1:66:C:LYS:CA  | 9        | 3.38          |
| (1,692)  | 1:61:C:ILE:CG1 | 1:66:C:LYS:CA  | 7        | 3.37          |
| (1,221)  | 1:74:C:GLN:CB  | 1:71:C:GLY:C   | 8        | 3.37          |
| (1,701)  | 1:77:C:LYS:CG  | 1:82:C:ASP:CA  | 10       | 3.36          |
| (1,533)  | 1:73:C:VAL:CB  | 1:83:C:GLU:CB  | 4        | 3.36          |
| (1,375)  | 1:62:C:LEU:CA  | 1:88:C:PHE:CB  | 2        | 3.36          |
| (1,767)  | 1:83:C:GLU:CB  | 1:63:C:ASP:CA  | 3        | 3.35          |
| (1,221)  | 1:74:C:GLN:CB  | 1:71:C:GLY:C   | 3        | 3.34          |
| (1,221)  | 1:74:C:GLN:CB  | 1:71:C:GLY:C   | 4        | 3.34          |
| (1,767)  | 1:83:C:GLU:CB  | 1:63:C:ASP:CA  | 6        | 3.33          |
| (1,559)  | 1:76:C:ARG:CG  | 1:68:C:LYS:CG  | 3        | 3.33          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,221)  | 1:74:C:GLN:CB  | 1:71:C:GLY:C   | 2        | 3.33          |
| (1,221)  | 1:74:C:GLN:CB  | 1:71:C:GLY:C   | 6        | 3.33          |
| (1,1228) | 1:89:C:VAL:CA  | 1:53:C:ALA:CA  | 6        | 3.31          |
| (1,375)  | 1:62:C:LEU:CA  | 1:88:C:PHE:CB  | 9        | 3.31          |
| (1,1165) | 1:41:C:ARG:CA  | 1:36:C:ILE:CG1 | 4        | 3.29          |
| (1,701)  | 1:77:C:LYS:CG  | 1:82:C:ASP:CA  | 3        | 3.29          |
| (1,692)  | 1:61:C:ILE:CG1 | 1:66:C:LYS:CA  | 5        | 3.29          |
| (1,692)  | 1:61:C:ILE:CG1 | 1:66:C:LYS:CA  | 10       | 3.29          |
| (1,375)  | 1:62:C:LEU:CA  | 1:88:C:PHE:CB  | 1        | 3.29          |
| (1,375)  | 1:62:C:LEU:CA  | 1:88:C:PHE:CB  | 7        | 3.29          |
| (1,375)  | 1:62:C:LEU:CA  | 1:88:C:PHE:CB  | 8        | 3.29          |
| (1,221)  | 1:74:C:GLN:CB  | 1:71:C:GLY:C   | 10       | 3.29          |
| (1,375)  | 1:62:C:LEU:CA  | 1:88:C:PHE:CB  | 5        | 3.28          |
| (1,1228) | 1:89:C:VAL:CA  | 1:53:C:ALA:CA  | 5        | 3.27          |
| (1,593)  | 1:94:C:ILE:CG1 | 1:32:C:ARG:CG  | 3        | 3.27          |
| (1,1074) | 1:83:C:GLU:CB  | 1:80:C:THR:CA  | 1        | 3.26          |
| (1,1074) | 1:83:C:GLU:CB  | 1:80:C:THR:CA  | 8        | 3.26          |
| (1,1074) | 1:83:C:GLU:CB  | 1:80:C:THR:CA  | 9        | 3.26          |
| (1,692)  | 1:61:C:ILE:CG1 | 1:66:C:LYS:CA  | 4        | 3.25          |
| (1,221)  | 1:74:C:GLN:CB  | 1:71:C:GLY:C   | 5        | 3.25          |
| (1,1074) | 1:83:C:GLU:CB  | 1:80:C:THR:CA  | 3        | 3.24          |
| (1,593)  | 1:94:C:ILE:CG1 | 1:32:C:ARG:CG  | 10       | 3.24          |
| (1,1213) | 1:31:C:SER:CA  | 1:26:C:PRO:CA  | 10       | 3.23          |
| (1,1074) | 1:83:C:GLU:CB  | 1:80:C:THR:CA  | 2        | 3.23          |
| (1,533)  | 1:73:C:VAL:CB  | 1:83:C:GLU:CB  | 9        | 3.23          |
| (1,1165) | 1:41:C:ARG:CA  | 1:36:C:ILE:CG1 | 6        | 3.22          |
| (1,1074) | 1:83:C:GLU:CB  | 1:80:C:THR:CA  | 6        | 3.21          |
| (1,701)  | 1:77:C:LYS:CG  | 1:82:C:ASP:CA  | 4        | 3.21          |
| (1,701)  | 1:77:C:LYS:CG  | 1:82:C:ASP:CA  | 5        | 3.21          |
| (1,593)  | 1:94:C:ILE:CG1 | 1:32:C:ARG:CG  | 5        | 3.21          |
| (1,701)  | 1:77:C:LYS:CG  | 1:82:C:ASP:CA  | 6        | 3.2           |
| (1,701)  | 1:77:C:LYS:CG  | 1:51:C:LEU:CA  | 7        | 3.2           |
| (1,692)  | 1:61:C:ILE:CG1 | 1:66:C:LYS:CA  | 6        | 3.2           |
| (1,533)  | 1:73:C:VAL:CB  | 1:83:C:GLU:CB  | 7        | 3.19          |
| (1,375)  | 1:62:C:LEU:CA  | 1:88:C:PHE:CB  | 4        | 3.19          |
| (1,22)   | 1:56:C:LYS:CA  | 1:88:C:PHE:CB  | 4        | 3.19          |
| (1,1286) | 1:46:C:TYR:CB  | 1:60:C:VAL:CG1 | 8        | 3.18          |
| (1,1074) | 1:83:C:GLU:CB  | 1:80:C:THR:CA  | 5        | 3.18          |
| (1,701)  | 1:77:C:LYS:CG  | 1:82:C:ASP:CA  | 1        | 3.18          |
| (1,668)  | 1:60:C:VAL:CB  | 1:66:C:LYS:CA  | 2        | 3.18          |
| (1,533)  | 1:73:C:VAL:CB  | 1:83:C:GLU:CB  | 10       | 3.18          |
| (1,1074) | 1:83:C:GLU:CB  | 1:80:C:THR:CA  | 4        | 3.17          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,559)  | 1:76:C:ARG:CG  | 1:68:C:LYS:CG  | 2        | 3.17          |
| (1,1275) | 1:48:C:GLY:CA  | 1:51:C:LEU:CB  | 9        | 3.16          |
| (1,1213) | 1:31:C:SER:CA  | 1:26:C:PRO:CA  | 6        | 3.16          |
| (1,1166) | 1:41:C:ARG:CA  | 1:87:C:ILE:CD1 | 3        | 3.16          |
| (1,1074) | 1:83:C:GLU:CB  | 1:80:C:THR:CA  | 7        | 3.16          |
| (1,535)  | 1:91:C:GLN:CG  | 1:36:C:ILE:CG1 | 9        | 3.16          |
| (1,22)   | 1:56:C:LYS:CA  | 1:88:C:PHE:CB  | 8        | 3.16          |
| (1,22)   | 1:56:C:LYS:CA  | 1:88:C:PHE:CB  | 2        | 3.15          |
| (1,1275) | 1:48:C:GLY:CA  | 1:51:C:LEU:CB  | 2        | 3.14          |
| (1,1275) | 1:48:C:GLY:CA  | 1:51:C:LEU:CB  | 8        | 3.14          |
| (1,1088) | 1:31:C:SER:CA  | 1:26:C:PRO:CG  | 3        | 3.14          |
| (1,692)  | 1:61:C:ILE:CG1 | 1:66:C:LYS:CA  | 8        | 3.13          |
| (1,216)  | 1:61:C:ILE:CG1 | 1:40:C:HIS:C   | 2        | 3.13          |
| (1,1353) | 1:76:C:ARG:CB  | 1:68:C:LYS:CB  | 2        | 3.12          |
| (1,1353) | 1:76:C:ARG:CB  | 1:68:C:LYS:CB  | 5        | 3.12          |
| (1,1074) | 1:83:C:GLU:CB  | 1:80:C:THR:CA  | 10       | 3.11          |
| (1,1165) | 1:41:C:ARG:CA  | 1:36:C:ILE:CG1 | 3        | 3.1           |
| (1,559)  | 1:76:C:ARG:CG  | 1:68:C:LYS:CG  | 9        | 3.1           |
| (1,1219) | 1:78:C:TYR:CA  | 1:51:C:LEU:CA  | 4        | 3.08          |
| (1,701)  | 1:77:C:LYS:CG  | 1:82:C:ASP:CA  | 8        | 3.08          |
| (1,668)  | 1:60:C:VAL:CB  | 1:66:C:LYS:CA  | 7        | 3.08          |
| (1,668)  | 1:60:C:VAL:CB  | 1:66:C:LYS:CA  | 8        | 3.08          |
| (1,375)  | 1:62:C:LEU:CA  | 1:88:C:PHE:CB  | 3        | 3.08          |
| (1,1275) | 1:48:C:GLY:CA  | 1:51:C:LEU:CB  | 1        | 3.07          |
| (1,1228) | 1:89:C:VAL:CA  | 1:53:C:ALA:CA  | 9        | 3.07          |
| (1,535)  | 1:91:C:GLN:CG  | 1:36:C:ILE:CG1 | 7        | 3.07          |
| (1,216)  | 1:61:C:ILE:CG1 | 1:40:C:HIS:C   | 10       | 3.07          |
| (1,1275) | 1:48:C:GLY:CA  | 1:51:C:LEU:CB  | 4        | 3.06          |
| (1,1275) | 1:48:C:GLY:CA  | 1:51:C:LEU:CB  | 5        | 3.06          |
| (1,701)  | 1:77:C:LYS:CG  | 1:82:C:ASP:CA  | 9        | 3.06          |
| (1,496)  | 1:61:C:ILE:CB  | 1:83:C:GLU:CB  | 10       | 3.06          |
| (1,1275) | 1:48:C:GLY:CA  | 1:51:C:LEU:CB  | 10       | 3.05          |
| (1,1088) | 1:31:C:SER:CA  | 1:26:C:PRO:CG  | 2        | 3.05          |
| (1,668)  | 1:60:C:VAL:CB  | 1:66:C:LYS:CA  | 10       | 3.05          |
| (1,533)  | 1:73:C:VAL:CB  | 1:83:C:GLU:CB  | 1        | 3.05          |
| (1,559)  | 1:76:C:ARG:CG  | 1:68:C:LYS:CG  | 7        | 3.04          |
| (1,375)  | 1:62:C:LEU:CA  | 1:88:C:PHE:CB  | 6        | 3.04          |
| (1,22)   | 1:56:C:LYS:CA  | 1:88:C:PHE:CB  | 1        | 3.04          |
| (1,1275) | 1:48:C:GLY:CA  | 1:51:C:LEU:CB  | 6        | 3.03          |
| (1,692)  | 1:61:C:ILE:CG1 | 1:66:C:LYS:CA  | 2        | 3.03          |
| (1,668)  | 1:60:C:VAL:CB  | 1:66:C:LYS:CA  | 5        | 3.03          |
| (1,1275) | 1:48:C:GLY:CA  | 1:51:C:LEU:CB  | 7        | 3.02          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,961)  | 1:80:C:THR:CB  | 1:73:C:VAL:CG2 | 1        | 3.02          |
| (1,961)  | 1:80:C:THR:CB  | 1:73:C:VAL:CG2 | 7        | 3.02          |
| (1,559)  | 1:76:C:ARG:CG  | 1:68:C:LYS:CG  | 5        | 3.01          |
| (1,22)   | 1:56:C:LYS:CA  | 1:88:C:PHE:CB  | 5        | 3.0           |
| (1,1353) | 1:76:C:ARG:CB  | 1:68:C:LYS:CB  | 4        | 2.99          |
| (1,559)  | 1:76:C:ARG:CG  | 1:68:C:LYS:CG  | 8        | 2.99          |
| (1,533)  | 1:73:C:VAL:CB  | 1:83:C:GLU:CB  | 6        | 2.99          |
| (1,533)  | 1:73:C:VAL:CB  | 1:83:C:GLU:CB  | 8        | 2.99          |
| (1,961)  | 1:80:C:THR:CB  | 1:73:C:VAL:CG2 | 8        | 2.98          |
| (1,668)  | 1:60:C:VAL:CB  | 1:66:C:LYS:CA  | 6        | 2.98          |
| (1,961)  | 1:80:C:THR:CB  | 1:73:C:VAL:CG2 | 4        | 2.97          |
| (1,557)  | 1:36:C:ILE:CG1 | 1:38:C:LYS:CG  | 8        | 2.97          |
| (1,556)  | 1:68:C:LYS:CD  | 1:77:C:LYS:CG  | 10       | 2.97          |
| (1,375)  | 1:62:C:LEU:CA  | 1:88:C:PHE:CB  | 10       | 2.97          |
| (1,1106) | 1:78:C:TYR:CA  | 1:74:C:GLN:CG  | 5        | 2.96          |
| (1,961)  | 1:80:C:THR:CB  | 1:73:C:VAL:CG2 | 9        | 2.96          |
| (1,557)  | 1:36:C:ILE:CG1 | 1:38:C:LYS:CG  | 5        | 2.96          |
| (1,132)  | 1:36:C:ILE:CG1 | 1:40:C:HIS:CA  | 4        | 2.96          |
| (1,1213) | 1:31:C:SER:CA  | 1:26:C:PRO:CA  | 9        | 2.95          |
| (1,961)  | 1:80:C:THR:CB  | 1:73:C:VAL:CG2 | 5        | 2.95          |
| (1,557)  | 1:36:C:ILE:CG1 | 1:38:C:LYS:CG  | 7        | 2.95          |
| (1,22)   | 1:56:C:LYS:CA  | 1:88:C:PHE:CB  | 10       | 2.95          |
| (1,559)  | 1:76:C:ARG:CG  | 1:68:C:LYS:CG  | 6        | 2.94          |
| (1,1275) | 1:48:C:GLY:CA  | 1:51:C:LEU:CB  | 3        | 2.93          |
| (1,1166) | 1:41:C:ARG:CA  | 1:87:C:ILE:CD1 | 9        | 2.93          |
| (1,557)  | 1:68:C:LYS:CD  | 1:66:C:LYS:CG  | 1        | 2.93          |
| (1,557)  | 1:36:C:ILE:CG1 | 1:38:C:LYS:CG  | 6        | 2.93          |
| (1,22)   | 1:56:C:LYS:CA  | 1:88:C:PHE:CB  | 7        | 2.92          |
| (1,496)  | 1:61:C:ILE:CB  | 1:83:C:GLU:CB  | 8        | 2.91          |
| (1,1213) | 1:31:C:SER:CA  | 1:26:C:PRO:CA  | 1        | 2.89          |
| (1,1106) | 1:78:C:TYR:CA  | 1:74:C:GLN:CG  | 10       | 2.89          |
| (1,961)  | 1:80:C:THR:CB  | 1:73:C:VAL:CG2 | 2        | 2.89          |
| (1,961)  | 1:80:C:THR:CB  | 1:73:C:VAL:CG2 | 6        | 2.87          |
| (1,1440) | 1:33:C:VAL:CG2 | 1:91:C:GLN:CG  | 6        | 2.86          |
| (1,1165) | 1:41:C:ARG:CA  | 1:36:C:ILE:CG1 | 8        | 2.86          |
| (1,535)  | 1:91:C:GLN:CG  | 1:36:C:ILE:CG1 | 1        | 2.86          |
| (1,142)  | 1:51:C:LEU:CA  | 1:73:C:VAL:CB  | 7        | 2.86          |
| (1,132)  | 1:36:C:ILE:CG1 | 1:40:C:HIS:CA  | 6        | 2.86          |
| (1,22)   | 1:56:C:LYS:CA  | 1:88:C:PHE:CB  | 9        | 2.86          |
| (1,1228) | 1:89:C:VAL:CA  | 1:53:C:ALA:CA  | 3        | 2.85          |
| (1,961)  | 1:80:C:THR:CB  | 1:73:C:VAL:CG2 | 10       | 2.85          |
| (1,1353) | 1:76:C:ARG:CB  | 1:68:C:LYS:CB  | 3        | 2.84          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,814)  | 1:90:C:ARG:CD  | 1:59:C:GLY:C   | 6        | 2.84          |
| (1,814)  | 1:90:C:ARG:CD  | 1:59:C:GLY:C   | 7        | 2.84          |
| (1,1165) | 1:41:C:ARG:CA  | 1:36:C:ILE:CG1 | 10       | 2.83          |
| (1,1478) | 1:58:C:VAL:CB  | 1:43:C:THR:CB  | 8        | 2.82          |
| (1,961)  | 1:80:C:THR:CB  | 1:73:C:VAL:CG2 | 3        | 2.82          |
| (1,634)  | 1:33:C:VAL:CG2 | 1:41:C:ARG:CD  | 3        | 2.82          |
| (1,359)  | 1:93:C:GLN:CA  | 1:27:C:LEU:CG  | 6        | 2.82          |
| (1,142)  | 1:51:C:LEU:CA  | 1:73:C:VAL:CB  | 2        | 2.82          |
| (1,1219) | 1:78:C:TYR:CA  | 1:51:C:LEU:CA  | 9        | 2.81          |
| (1,1213) | 1:31:C:SER:CA  | 1:26:C:PRO:CA  | 8        | 2.81          |
| (1,496)  | 1:61:C:ILE:CB  | 1:83:C:GLU:CB  | 4        | 2.81          |
| (1,1205) | 1:65:C:ALA:CA  | 1:40:C:HIS:CB  | 10       | 2.8           |
| (1,1165) | 1:41:C:ARG:CA  | 1:36:C:ILE:CG1 | 7        | 2.8           |
| (1,326)  | 1:56:C:LYS:CA  | 1:51:C:LEU:CA  | 10       | 2.8           |
| (1,142)  | 1:51:C:LEU:CA  | 1:73:C:VAL:CB  | 4        | 2.8           |
| (1,668)  | 1:60:C:VAL:CB  | 1:66:C:LYS:CA  | 9        | 2.79          |
| (1,1219) | 1:78:C:TYR:CA  | 1:51:C:LEU:CA  | 10       | 2.78          |
| (1,1478) | 1:58:C:VAL:CB  | 1:43:C:THR:CB  | 2        | 2.77          |
| (1,1165) | 1:41:C:ARG:CA  | 1:36:C:ILE:CG1 | 1        | 2.77          |
| (1,634)  | 1:33:C:VAL:CG2 | 1:41:C:ARG:CD  | 8        | 2.77          |
| (1,22)   | 1:56:C:LYS:CA  | 1:88:C:PHE:CB  | 6        | 2.77          |
| (1,792)  | 1:51:C:LEU:CA  | 1:73:C:VAL:CB  | 7        | 2.76          |
| (1,132)  | 1:36:C:ILE:CG1 | 1:40:C:HIS:CA  | 3        | 2.76          |
| (1,77)   | 1:60:C:VAL:CB  | 1:85:C:HIS:CB  | 4        | 2.76          |
| (1,1353) | 1:76:C:ARG:CB  | 1:68:C:LYS:CB  | 1        | 2.75          |
| (1,359)  | 1:93:C:GLN:CA  | 1:27:C:LEU:CG  | 10       | 2.75          |
| (1,142)  | 1:51:C:LEU:CA  | 1:73:C:VAL:CB  | 10       | 2.75          |
| (1,1301) | 1:82:C:ASP:CB  | 1:68:C:LYS:CG  | 7        | 2.74          |
| (1,1166) | 1:41:C:ARG:CA  | 1:87:C:ILE:CD1 | 4        | 2.74          |
| (1,216)  | 1:61:C:ILE:CG1 | 1:40:C:HIS:C   | 4        | 2.74          |
| (1,1440) | 1:33:C:VAL:CG2 | 1:91:C:GLN:CG  | 8        | 2.73          |
| (1,1353) | 1:76:C:ARG:CB  | 1:68:C:LYS:CB  | 9        | 2.73          |
| (1,814)  | 1:90:C:ARG:CD  | 1:59:C:GLY:C   | 9        | 2.73          |
| (1,1440) | 1:33:C:VAL:CG2 | 1:91:C:GLN:CG  | 3        | 2.72          |
| (1,814)  | 1:90:C:ARG:CD  | 1:59:C:GLY:C   | 1        | 2.72          |
| (1,792)  | 1:51:C:LEU:CA  | 1:73:C:VAL:CB  | 2        | 2.72          |
| (1,142)  | 1:51:C:LEU:CA  | 1:73:C:VAL:CB  | 9        | 2.72          |
| (1,132)  | 1:36:C:ILE:CG1 | 1:40:C:HIS:CA  | 8        | 2.72          |
| (1,668)  | 1:60:C:VAL:CB  | 1:66:C:LYS:CA  | 3        | 2.71          |
| (1,496)  | 1:61:C:ILE:CB  | 1:83:C:GLU:CB  | 2        | 2.71          |
| (1,1478) | 1:58:C:VAL:CB  | 1:43:C:THR:CB  | 1        | 2.7           |
| (1,792)  | 1:51:C:LEU:CA  | 1:73:C:VAL:CB  | 4        | 2.7           |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,707)  | 1:80:C:THR:CG2 | 1:69:C:ASN:CA  | 2        | 2.7           |
| (1,142)  | 1:51:C:LEU:CA  | 1:73:C:VAL:CB  | 6        | 2.7           |
| (1,132)  | 1:36:C:ILE:CG1 | 1:40:C:HIS:CA  | 7        | 2.7           |
| (1,1219) | 1:78:C:TYR:CA  | 1:51:C:LEU:CA  | 2        | 2.69          |
| (1,1219) | 1:78:C:TYR:CA  | 1:51:C:LEU:CA  | 7        | 2.69          |
| (1,1219) | 1:78:C:TYR:CA  | 1:51:C:LEU:CA  | 8        | 2.69          |
| (1,634)  | 1:33:C:VAL:CG2 | 1:41:C:ARG:CD  | 1        | 2.69          |
| (1,326)  | 1:63:C:ASP:CA  | 1:82:C:ASP:CA  | 8        | 2.69          |
| (1,142)  | 1:51:C:LEU:CA  | 1:73:C:VAL:CB  | 1        | 2.69          |
| (1,132)  | 1:36:C:ILE:CG1 | 1:40:C:HIS:CA  | 1        | 2.69          |
| (1,1301) | 1:82:C:ASP:CB  | 1:68:C:LYS:CG  | 3        | 2.67          |
| (1,1228) | 1:89:C:VAL:CA  | 1:53:C:ALA:CA  | 4        | 2.66          |
| (1,668)  | 1:60:C:VAL:CB  | 1:66:C:LYS:CA  | 1        | 2.66          |
| (1,792)  | 1:51:C:LEU:CA  | 1:73:C:VAL:CB  | 10       | 2.65          |
| (1,142)  | 1:51:C:LEU:CA  | 1:73:C:VAL:CB  | 8        | 2.65          |
| (1,132)  | 1:36:C:ILE:CG1 | 1:40:C:HIS:CA  | 10       | 2.65          |
| (1,1228) | 1:89:C:VAL:CA  | 1:53:C:ALA:CA  | 1        | 2.64          |
| (1,1219) | 1:78:C:TYR:CA  | 1:51:C:LEU:CA  | 1        | 2.64          |
| (1,1213) | 1:31:C:SER:CA  | 1:26:C:PRO:CA  | 7        | 2.64          |
| (1,1478) | 1:58:C:VAL:CB  | 1:43:C:THR:CB  | 10       | 2.63          |
| (1,1353) | 1:76:C:ARG:CB  | 1:68:C:LYS:CB  | 10       | 2.63          |
| (1,1301) | 1:82:C:ASP:CB  | 1:68:C:LYS:CG  | 9        | 2.63          |
| (1,1478) | 1:58:C:VAL:CB  | 1:43:C:THR:CB  | 9        | 2.62          |
| (1,1213) | 1:31:C:SER:CA  | 1:26:C:PRO:CA  | 4        | 2.62          |
| (1,792)  | 1:51:C:LEU:CA  | 1:73:C:VAL:CB  | 9        | 2.62          |
| (1,1478) | 1:58:C:VAL:CB  | 1:43:C:THR:CB  | 5        | 2.61          |
| (1,1166) | 1:41:C:ARG:CA  | 1:87:C:ILE:CD1 | 2        | 2.61          |
| (1,814)  | 1:90:C:ARG:CD  | 1:59:C:GLY:C   | 8        | 2.61          |
| (1,814)  | 1:90:C:ARG:CD  | 1:59:C:GLY:C   | 10       | 2.61          |
| (1,496)  | 1:61:C:ILE:CB  | 1:83:C:GLU:CB  | 6        | 2.61          |
| (1,1353) | 1:76:C:ARG:CB  | 1:68:C:LYS:CB  | 7        | 2.6           |
| (1,1106) | 1:78:C:TYR:CA  | 1:74:C:GLN:CG  | 4        | 2.6           |
| (1,814)  | 1:90:C:ARG:CD  | 1:59:C:GLY:C   | 3        | 2.6           |
| (1,792)  | 1:51:C:LEU:CA  | 1:73:C:VAL:CB  | 6        | 2.6           |
| (1,559)  | 1:76:C:ARG:CG  | 1:68:C:LYS:CG  | 4        | 2.6           |
| (1,359)  | 1:93:C:GLN:CA  | 1:27:C:LEU:CG  | 9        | 2.6           |
| (1,1353) | 1:76:C:ARG:CB  | 1:68:C:LYS:CB  | 6        | 2.59          |
| (1,792)  | 1:51:C:LEU:CA  | 1:73:C:VAL:CB  | 1        | 2.59          |
| (1,132)  | 1:36:C:ILE:CG1 | 1:40:C:HIS:CA  | 2        | 2.59          |
| (1,1478) | 1:58:C:VAL:CB  | 1:43:C:THR:CB  | 6        | 2.56          |
| (1,326)  | 1:63:C:ASP:CA  | 1:82:C:ASP:CA  | 9        | 2.56          |
| (1,132)  | 1:36:C:ILE:CG1 | 1:40:C:HIS:CA  | 5        | 2.56          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1478) | 1:58:C:VAL:CB  | 1:43:C:THR:CB  | 7        | 2.55          |
| (1,1351) | 1:29:C:VAL:CB  | 1:26:C:PRO:CG  | 9        | 2.55          |
| (1,1205) | 1:65:C:ALA:CA  | 1:40:C:HIS:CB  | 4        | 2.55          |
| (1,792)  | 1:51:C:LEU:CA  | 1:73:C:VAL:CB  | 8        | 2.55          |
| (1,359)  | 1:93:C:GLN:CA  | 1:27:C:LEU:CG  | 3        | 2.55          |
| (1,1351) | 1:29:C:VAL:CB  | 1:26:C:PRO:CG  | 3        | 2.54          |
| (1,142)  | 1:51:C:LEU:CA  | 1:73:C:VAL:CB  | 5        | 2.54          |
| (1,707)  | 1:80:C:THR:CG2 | 1:69:C:ASN:CA  | 3        | 2.53          |
| (1,707)  | 1:80:C:THR:CG2 | 1:69:C:ASN:CA  | 5        | 2.53          |
| (1,707)  | 1:80:C:THR:CG2 | 1:69:C:ASN:CA  | 9        | 2.53          |
| (1,79)   | 1:85:C:HIS:CB  | 1:66:C:LYS:CB  | 4        | 2.53          |
| (1,52)   | 1:29:C:VAL:CG2 | 1:43:C:THR:CB  | 7        | 2.53          |
| (1,1301) | 1:82:C:ASP:CB  | 1:68:C:LYS:CG  | 6        | 2.52          |
| (1,1353) | 1:76:C:ARG:CB  | 1:68:C:LYS:CB  | 8        | 2.51          |
| (1,1219) | 1:78:C:TYR:CA  | 1:51:C:LEU:CA  | 3        | 2.51          |
| (1,634)  | 1:33:C:VAL:CG2 | 1:41:C:ARG:CD  | 7        | 2.51          |
| (1,22)   | 1:56:C:LYS:CA  | 1:88:C:PHE:CB  | 3        | 2.51          |
| (1,79)   | 1:85:C:HIS:CB  | 1:66:C:LYS:CB  | 7        | 2.5           |
| (1,79)   | 1:85:C:HIS:CB  | 1:66:C:LYS:CB  | 10       | 2.5           |
| (1,1228) | 1:89:C:VAL:CA  | 1:53:C:ALA:CA  | 8        | 2.49          |
| (1,359)  | 1:93:C:GLN:CA  | 1:27:C:LEU:CG  | 7        | 2.49          |
| (1,79)   | 1:85:C:HIS:CB  | 1:66:C:LYS:CB  | 6        | 2.49          |
| (1,1373) | 1:62:C:LEU:CG  | 1:43:C:THR:CG2 | 3        | 2.48          |
| (1,1228) | 1:89:C:VAL:CA  | 1:53:C:ALA:CA  | 10       | 2.48          |
| (1,707)  | 1:80:C:THR:CG2 | 1:69:C:ASN:CA  | 1        | 2.48          |
| (1,707)  | 1:80:C:THR:CG2 | 1:69:C:ASN:CA  | 4        | 2.48          |
| (1,79)   | 1:85:C:HIS:CB  | 1:66:C:LYS:CB  | 1        | 2.48          |
| (1,77)   | 1:60:C:VAL:CB  | 1:85:C:HIS:CB  | 10       | 2.48          |
| (1,1165) | 1:41:C:ARG:CA  | 1:36:C:ILE:CG1 | 2        | 2.47          |
| (1,814)  | 1:90:C:ARG:CD  | 1:59:C:GLY:C   | 5        | 2.47          |
| (1,707)  | 1:80:C:THR:CG2 | 1:69:C:ASN:CA  | 7        | 2.47          |
| (1,707)  | 1:80:C:THR:CG2 | 1:69:C:ASN:CA  | 8        | 2.47          |
| (1,634)  | 1:33:C:VAL:CG2 | 1:41:C:ARG:CD  | 6        | 2.47          |
| (1,359)  | 1:93:C:GLN:CA  | 1:27:C:LEU:CG  | 4        | 2.47          |
| (1,79)   | 1:85:C:HIS:CB  | 1:66:C:LYS:CB  | 5        | 2.47          |
| (1,79)   | 1:85:C:HIS:CB  | 1:66:C:LYS:CB  | 9        | 2.46          |
| (1,1351) | 1:29:C:VAL:CB  | 1:26:C:PRO:CG  | 1        | 2.45          |
| (1,1205) | 1:65:C:ALA:CA  | 1:40:C:HIS:CB  | 2        | 2.45          |
| (1,1219) | 1:78:C:TYR:CA  | 1:51:C:LEU:CA  | 5        | 2.44          |
| (1,814)  | 1:90:C:ARG:CD  | 1:59:C:GLY:C   | 4        | 2.44          |
| (1,792)  | 1:51:C:LEU:CA  | 1:73:C:VAL:CB  | 5        | 2.44          |
| (1,1478) | 1:58:C:VAL:CB  | 1:43:C:THR:CB  | 3        | 2.43          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,359)  | 1:93:C:GLN:CA  | 1:27:C:LEU:CG  | 1        | 2.43          |
| (1,77)   | 1:60:C:VAL:CB  | 1:85:C:HIS:CB  | 2        | 2.43          |
| (1,1219) | 1:78:C:TYR:CA  | 1:51:C:LEU:CA  | 6        | 2.42          |
| (1,707)  | 1:80:C:THR:CG2 | 1:69:C:ASN:CA  | 6        | 2.42          |
| (1,682)  | 1:76:C:ARG:CB  | 1:53:C:ALA:CA  | 3        | 2.42          |
| (1,1205) | 1:65:C:ALA:CA  | 1:40:C:HIS:CB  | 9        | 2.41          |
| (1,359)  | 1:93:C:GLN:CA  | 1:27:C:LEU:CG  | 8        | 2.41          |
| (1,359)  | 1:93:C:GLN:CA  | 1:27:C:LEU:CG  | 2        | 2.4           |
| (1,79)   | 1:85:C:HIS:CB  | 1:66:C:LYS:CB  | 2        | 2.4           |
| (1,326)  | 1:63:C:ASP:CA  | 1:82:C:ASP:CA  | 5        | 2.39          |
| (1,1213) | 1:31:C:SER:CA  | 1:26:C:PRO:CA  | 2        | 2.38          |
| (1,79)   | 1:85:C:HIS:CB  | 1:66:C:LYS:CB  | 8        | 2.38          |
| (1,1351) | 1:29:C:VAL:CB  | 1:26:C:PRO:CG  | 8        | 2.37          |
| (1,1301) | 1:82:C:ASP:CB  | 1:68:C:LYS:CG  | 8        | 2.37          |
| (1,1023) | 1:61:C:ILE:CG1 | 1:82:C:ASP:CA  | 10       | 2.37          |
| (1,557)  | 1:36:C:ILE:CG1 | 1:38:C:LYS:CG  | 2        | 2.37          |
| (1,1213) | 1:31:C:SER:CA  | 1:26:C:PRO:CA  | 3        | 2.36          |
| (1,1190) | 1:32:C:ARG:CA  | 1:95:C:GLN:CG  | 5        | 2.36          |
| (1,79)   | 1:85:C:HIS:CB  | 1:66:C:LYS:CB  | 3        | 2.36          |
| (1,77)   | 1:60:C:VAL:CB  | 1:85:C:HIS:CB  | 8        | 2.36          |
| (1,557)  | 1:36:C:ILE:CG1 | 1:38:C:LYS:CG  | 4        | 2.35          |
| (1,1373) | 1:62:C:LEU:CG  | 1:43:C:THR:CG2 | 5        | 2.34          |
| (1,1205) | 1:65:C:ALA:CA  | 1:40:C:HIS:CB  | 3        | 2.34          |
| (1,1213) | 1:31:C:SER:CA  | 1:26:C:PRO:CA  | 5        | 2.33          |
| (1,1165) | 1:41:C:ARG:CA  | 1:36:C:ILE:CG1 | 5        | 2.33          |
| (1,1049) | 1:45:C:ALA:CB  | 1:28:C:ARG:CA  | 7        | 2.32          |
| (1,557)  | 1:36:C:ILE:CG1 | 1:38:C:LYS:CG  | 9        | 2.31          |
| (1,77)   | 1:60:C:VAL:CB  | 1:85:C:HIS:CB  | 5        | 2.31          |
| (1,707)  | 1:80:C:THR:CG2 | 1:69:C:ASN:CA  | 10       | 2.3           |
| (1,326)  | 1:63:C:ASP:CA  | 1:82:C:ASP:CA  | 1        | 2.3           |
| (1,77)   | 1:60:C:VAL:CB  | 1:85:C:HIS:CB  | 3        | 2.3           |
| (1,557)  | 1:36:C:ILE:CG1 | 1:38:C:LYS:CG  | 3        | 2.29          |
| (1,1301) | 1:82:C:ASP:CB  | 1:68:C:LYS:CG  | 4        | 2.28          |
| (1,132)  | 1:36:C:ILE:CG1 | 1:40:C:HIS:CA  | 9        | 2.27          |
| (1,77)   | 1:60:C:VAL:CB  | 1:85:C:HIS:CB  | 6        | 2.27          |
| (1,1336) | 1:41:C:ARG:CB  | 1:61:C:ILE:CG1 | 3        | 2.26          |
| (1,559)  | 1:76:C:ARG:CG  | 1:68:C:LYS:CG  | 1        | 2.25          |
| (1,326)  | 1:63:C:ASP:CA  | 1:82:C:ASP:CA  | 4        | 2.24          |
| (1,77)   | 1:60:C:VAL:CB  | 1:85:C:HIS:CB  | 1        | 2.24          |
| (1,77)   | 1:60:C:VAL:CB  | 1:85:C:HIS:CB  | 7        | 2.24          |
| (1,1478) | 1:58:C:VAL:CB  | 1:43:C:THR:CB  | 4        | 2.22          |
| (1,326)  | 1:63:C:ASP:CA  | 1:82:C:ASP:CA  | 2        | 2.22          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,326)  | 1:63:C:ASP:CA  | 1:82:C:ASP:CA  | 7        | 2.22          |
| (1,77)   | 1:60:C:VAL:CB  | 1:85:C:HIS:CB  | 9        | 2.22          |
| (1,1373) | 1:62:C:LEU:CG  | 1:43:C:THR:CG2 | 7        | 2.2           |
| (1,1301) | 1:82:C:ASP:CB  | 1:68:C:LYS:CG  | 2        | 2.2           |
| (1,359)  | 1:93:C:GLN:CA  | 1:27:C:LEU:CG  | 5        | 2.2           |
| (1,109)  | 1:40:C:HIS:CB  | 1:64:C:GLU:CA  | 10       | 2.19          |
| (1,557)  | 1:36:C:ILE:CG1 | 1:38:C:LYS:CG  | 10       | 2.18          |
| (1,1301) | 1:82:C:ASP:CB  | 1:68:C:LYS:CG  | 10       | 2.17          |
| (1,535)  | 1:91:C:GLN:CG  | 1:36:C:ILE:CG1 | 10       | 2.17          |
| (1,535)  | 1:91:C:GLN:CG  | 1:36:C:ILE:CG1 | 6        | 2.16          |
| (1,535)  | 1:91:C:GLN:CG  | 1:36:C:ILE:CG1 | 8        | 2.16          |
| (1,1301) | 1:82:C:ASP:CB  | 1:68:C:LYS:CG  | 5        | 2.15          |
| (1,1049) | 1:45:C:ALA:CB  | 1:28:C:ARG:CA  | 6        | 2.15          |
| (1,593)  | 1:94:C:ILE:CG1 | 1:32:C:ARG:CG  | 8        | 2.15          |
| (1,535)  | 1:91:C:GLN:CG  | 1:36:C:ILE:CG1 | 2        | 2.15          |
| (1,326)  | 1:63:C:ASP:CA  | 1:82:C:ASP:CA  | 6        | 2.15          |
| (1,1336) | 1:40:C:HIS:CB  | 1:61:C:ILE:CG1 | 5        | 2.13          |
| (1,1205) | 1:65:C:ALA:CA  | 1:40:C:HIS:CB  | 8        | 2.13          |
| (1,635)  | 1:46:C:TYR:CB  | 1:61:C:ILE:CG2 | 4        | 2.13          |
| (1,593)  | 1:94:C:ILE:CG1 | 1:32:C:ARG:CG  | 6        | 2.11          |
| (1,1049) | 1:45:C:ALA:CB  | 1:28:C:ARG:CA  | 10       | 2.1           |
| (1,635)  | 1:46:C:TYR:CB  | 1:61:C:ILE:CG2 | 6        | 2.1           |
| (1,109)  | 1:40:C:HIS:CB  | 1:64:C:GLU:CA  | 9        | 2.1           |
| (1,1049) | 1:45:C:ALA:CB  | 1:28:C:ARG:CA  | 2        | 2.09          |
| (1,1351) | 1:29:C:VAL:CB  | 1:26:C:PRO:CG  | 4        | 2.08          |
| (1,1205) | 1:65:C:ALA:CA  | 1:40:C:HIS:CB  | 7        | 2.08          |
| (1,617)  | 1:76:C:ARG:CG  | 1:52:C:PHE:CB  | 3        | 2.07          |
| (1,559)  | 1:76:C:ARG:CG  | 1:68:C:LYS:CG  | 10       | 2.07          |
| (1,1049) | 1:45:C:ALA:CB  | 1:28:C:ARG:CA  | 1        | 2.06          |
| (1,1336) | 1:41:C:ARG:CB  | 1:61:C:ILE:CG1 | 9        | 2.05          |
| (1,1049) | 1:45:C:ALA:CB  | 1:28:C:ARG:CA  | 4        | 2.04          |
| (1,1205) | 1:65:C:ALA:CA  | 1:40:C:HIS:CB  | 6        | 2.03          |
| (1,1049) | 1:45:C:ALA:CB  | 1:28:C:ARG:CA  | 8        | 2.03          |
| (1,326)  | 1:63:C:ASP:CA  | 1:82:C:ASP:CA  | 3        | 2.03          |
| (1,1023) | 1:61:C:ILE:CG1 | 1:82:C:ASP:CA  | 8        | 2.02          |
| (1,535)  | 1:91:C:GLN:CG  | 1:36:C:ILE:CG1 | 5        | 2.02          |
| (1,1351) | 1:29:C:VAL:CB  | 1:26:C:PRO:CG  | 6        | 2.01          |
| (1,1205) | 1:65:C:ALA:CA  | 1:40:C:HIS:CB  | 1        | 2.01          |
| (1,1166) | 1:41:C:ARG:CA  | 1:87:C:ILE:CD1 | 1        | 2.01          |
| (1,465)  | 1:87:C:ILE:CA  | 1:94:C:ILE:CD1 | 7        | 2.01          |
| (1,424)  | 1:91:C:GLN:CA  | 1:95:C:GLN:CB  | 9        | 2.01          |
| (1,1049) | 1:45:C:ALA:CB  | 1:28:C:ARG:CA  | 5        | 2.0           |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,682)  | 1:76:C:ARG:CB  | 1:53:C:ALA:CA  | 5        | 2.0           |
| (1,635)  | 1:46:C:TYR:CB  | 1:61:C:ILE:CG2 | 2        | 2.0           |
| (1,216)  | 1:61:C:ILE:CG1 | 1:40:C:HIS:C   | 8        | 2.0           |
| (1,1301) | 1:82:C:ASP:CB  | 1:68:C:LYS:CG  | 1        | 1.99          |
| (1,1049) | 1:45:C:ALA:CB  | 1:28:C:ARG:CA  | 3        | 1.97          |
| (1,424)  | 1:91:C:GLN:CA  | 1:95:C:GLN:CB  | 10       | 1.97          |
| (1,1165) | 1:41:C:ARG:CA  | 1:36:C:ILE:CG1 | 9        | 1.96          |
| (1,1163) | 1:41:C:ARG:CA  | 1:38:C:LYS:CB  | 9        | 1.95          |
| (1,1023) | 1:61:C:ILE:CG1 | 1:82:C:ASP:CA  | 4        | 1.95          |
| (1,535)  | 1:91:C:GLN:CG  | 1:36:C:ILE:CG1 | 3        | 1.95          |
| (1,682)  | 1:76:C:ARG:CB  | 1:53:C:ALA:CA  | 8        | 1.94          |
| (1,593)  | 1:94:C:ILE:CG1 | 1:32:C:ARG:CG  | 2        | 1.94          |
| (1,682)  | 1:76:C:ARG:CB  | 1:53:C:ALA:CA  | 9        | 1.93          |
| (1,682)  | 1:76:C:ARG:CB  | 1:53:C:ALA:CA  | 6        | 1.92          |
| (1,635)  | 1:46:C:TYR:CB  | 1:61:C:ILE:CG2 | 8        | 1.92          |
| (1,465)  | 1:87:C:ILE:CA  | 1:94:C:ILE:CD1 | 1        | 1.92          |
| (1,216)  | 1:61:C:ILE:CG1 | 1:40:C:HIS:C   | 6        | 1.92          |
| (1,384)  | 1:51:C:LEU:CA  | 1:73:C:VAL:CB  | 7        | 1.91          |
| (1,52)   | 1:29:C:VAL:CG2 | 1:43:C:THR:CB  | 4        | 1.91          |
| (1,109)  | 1:40:C:HIS:CB  | 1:64:C:GLU:CA  | 8        | 1.88          |
| (1,1336) | 1:40:C:HIS:CB  | 1:61:C:ILE:CG1 | 1        | 1.87          |
| (1,789)  | 1:74:C:GLN:CG  | 1:52:C:PHE:C   | 8        | 1.87          |
| (1,384)  | 1:51:C:LEU:CA  | 1:73:C:VAL:CB  | 2        | 1.87          |
| (1,112)  | 1:84:C:GLY:CA  | 1:81:C:CYS:C   | 4        | 1.87          |
| (1,846)  | 1:60:C:VAL:CB  | 1:84:C:GLY:C   | 4        | 1.86          |
| (1,682)  | 1:76:C:ARG:CB  | 1:53:C:ALA:CA  | 2        | 1.86          |
| (1,218)  | 1:27:C:LEU:CG  | 1:92:C:SER:C   | 6        | 1.86          |
| (1,112)  | 1:84:C:GLY:CA  | 1:81:C:CYS:C   | 3        | 1.86          |
| (1,112)  | 1:84:C:GLY:CA  | 1:81:C:CYS:C   | 6        | 1.86          |
| (1,109)  | 1:40:C:HIS:CB  | 1:64:C:GLU:CA  | 1        | 1.86          |
| (1,1039) | 1:77:C:LYS:CG  | 1:69:C:ASN:CA  | 2        | 1.85          |
| (1,384)  | 1:51:C:LEU:CA  | 1:73:C:VAL:CB  | 4        | 1.85          |
| (1,109)  | 1:40:C:HIS:CB  | 1:64:C:GLU:CA  | 4        | 1.85          |
| (1,109)  | 1:40:C:HIS:CB  | 1:64:C:GLU:CA  | 7        | 1.85          |
| (1,635)  | 1:46:C:TYR:CB  | 1:61:C:ILE:CG2 | 10       | 1.84          |
| (1,1178) | 1:66:C:LYS:CA  | 1:69:C:ASN:CB  | 4        | 1.83          |
| (1,814)  | 1:90:C:ARG:CD  | 1:59:C:GLY:C   | 2        | 1.83          |
| (1,112)  | 1:84:C:GLY:CA  | 1:81:C:CYS:C   | 9        | 1.83          |
| (1,836)  | 1:33:C:VAL:CB  | 1:91:C:GLN:C   | 6        | 1.82          |
| (1,184)  | 1:33:C:VAL:CB  | 1:91:C:GLN:C   | 6        | 1.82          |
| (1,1178) | 1:76:C:ARG:CA  | 1:69:C:ASN:CB  | 2        | 1.81          |
| (1,1178) | 1:66:C:LYS:CA  | 1:69:C:ASN:CB  | 5        | 1.8           |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,384)  | 1:51:C:LEU:CA  | 1:73:C:VAL:CB  | 10       | 1.8           |
| (1,218)  | 1:27:C:LEU:CG  | 1:92:C:SER:C   | 10       | 1.8           |
| (1,142)  | 1:51:C:LEU:CA  | 1:73:C:VAL:CB  | 3        | 1.8           |
| (1,112)  | 1:84:C:GLY:CA  | 1:81:C:CYS:C   | 1        | 1.8           |
| (1,1336) | 1:40:C:HIS:CB  | 1:61:C:ILE:CG1 | 7        | 1.79          |
| (1,1205) | 1:65:C:ALA:CA  | 1:40:C:HIS:CB  | 5        | 1.79          |
| (1,1178) | 1:66:C:LYS:CA  | 1:69:C:ASN:CB  | 1        | 1.79          |
| (1,682)  | 1:76:C:ARG:CB  | 1:53:C:ALA:CA  | 4        | 1.79          |
| (1,112)  | 1:84:C:GLY:CA  | 1:81:C:CYS:C   | 8        | 1.79          |
| (1,1440) | 1:33:C:VAL:CG2 | 1:91:C:GLN:CG  | 7        | 1.78          |
| (1,1049) | 1:45:C:ALA:CB  | 1:28:C:ARG:CA  | 9        | 1.78          |
| (1,465)  | 1:87:C:ILE:CA  | 1:94:C:ILE:CD1 | 3        | 1.78          |
| (1,112)  | 1:84:C:GLY:CA  | 1:81:C:CYS:C   | 2        | 1.78          |
| (1,112)  | 1:84:C:GLY:CA  | 1:81:C:CYS:C   | 5        | 1.78          |
| (1,109)  | 1:40:C:HIS:CB  | 1:64:C:GLU:CA  | 2        | 1.78          |
| (1,465)  | 1:87:C:ILE:CA  | 1:94:C:ILE:CD1 | 4        | 1.77          |
| (1,465)  | 1:87:C:ILE:CA  | 1:94:C:ILE:CD1 | 8        | 1.77          |
| (1,384)  | 1:51:C:LEU:CA  | 1:73:C:VAL:CB  | 9        | 1.77          |
| (1,218)  | 1:27:C:LEU:CG  | 1:92:C:SER:C   | 9        | 1.77          |
| (1,1440) | 1:33:C:VAL:CG2 | 1:91:C:GLN:CG  | 9        | 1.76          |
| (1,1163) | 1:41:C:ARG:CA  | 1:38:C:LYS:CB  | 2        | 1.76          |
| (1,988)  | 1:69:C:ASN:CB  | 1:74:C:GLN:CA  | 1        | 1.76          |
| (1,173)  | 1:82:C:ASP:CB  | 1:72:C:THR:C   | 4        | 1.76          |
| (1,988)  | 1:69:C:ASN:CB  | 1:74:C:GLN:CA  | 10       | 1.75          |
| (1,384)  | 1:51:C:LEU:CA  | 1:73:C:VAL:CB  | 6        | 1.75          |
| (1,112)  | 1:84:C:GLY:CA  | 1:81:C:CYS:C   | 10       | 1.75          |
| (1,596)  | 1:32:C:ARG:CG  | 1:34:C:GLU:CB  | 5        | 1.74          |
| (1,384)  | 1:51:C:LEU:CA  | 1:73:C:VAL:CB  | 1        | 1.74          |
| (1,1351) | 1:29:C:VAL:CB  | 1:26:C:PRO:CG  | 5        | 1.73          |
| (1,1178) | 1:66:C:LYS:CA  | 1:69:C:ASN:CB  | 7        | 1.73          |
| (1,1039) | 1:77:C:LYS:CG  | 1:69:C:ASN:CA  | 3        | 1.73          |
| (1,836)  | 1:33:C:VAL:CB  | 1:91:C:GLN:C   | 7        | 1.73          |
| (1,596)  | 1:32:C:ARG:CG  | 1:34:C:GLU:CB  | 10       | 1.73          |
| (1,535)  | 1:91:C:GLN:CG  | 1:36:C:ILE:CG1 | 4        | 1.73          |
| (1,184)  | 1:33:C:VAL:CB  | 1:91:C:GLN:C   | 7        | 1.73          |
| (1,173)  | 1:82:C:ASP:CB  | 1:72:C:THR:C   | 2        | 1.73          |
| (1,1178) | 1:66:C:LYS:CA  | 1:69:C:ASN:CB  | 3        | 1.72          |
| (1,1039) | 1:77:C:LYS:CG  | 1:69:C:ASN:CA  | 5        | 1.72          |
| (1,988)  | 1:69:C:ASN:CB  | 1:74:C:GLN:CA  | 4        | 1.72          |
| (1,112)  | 1:84:C:GLY:CA  | 1:81:C:CYS:C   | 7        | 1.72          |
| (1,1178) | 1:66:C:LYS:CA  | 1:69:C:ASN:CB  | 6        | 1.71          |
| (1,1178) | 1:66:C:LYS:CA  | 1:69:C:ASN:CB  | 9        | 1.71          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,173)  | 1:82:C:ASP:CB  | 1:72:C:THR:C   | 10       | 1.71          |
| (1,109)  | 1:40:C:HIS:CB  | 1:64:C:GLU:CA  | 6        | 1.71          |
| (1,792)  | 1:51:C:LEU:CA  | 1:73:C:VAL:CB  | 3        | 1.7           |
| (1,427)  | 1:92:C:SER:CB  | 1:26:C:PRO:CB  | 7        | 1.7           |
| (1,384)  | 1:51:C:LEU:CA  | 1:73:C:VAL:CB  | 8        | 1.7           |
| (1,378)  | 1:41:C:ARG:CA  | 1:60:C:VAL:CB  | 4        | 1.7           |
| (1,173)  | 1:82:C:ASP:CB  | 1:72:C:THR:C   | 5        | 1.7           |
| (1,631)  | 1:63:C:ASP:CB  | 1:41:C:ARG:CD  | 4        | 1.69          |
| (1,199)  | 1:26:C:PRO:CB  | 1:28:C:ARG:C   | 6        | 1.69          |
| (1,65)   | 1:41:C:ARG:CB  | 1:32:C:ARG:CG  | 1        | 1.69          |
| (1,58)   | 1:32:C:ARG:CG  | 1:41:C:ARG:CB  | 1        | 1.69          |
| (1,1178) | 1:66:C:LYS:CA  | 1:69:C:ASN:CB  | 10       | 1.68          |
| (1,1039) | 1:77:C:LYS:CG  | 1:69:C:ASN:CA  | 6        | 1.67          |
| (1,631)  | 1:63:C:ASP:CB  | 1:41:C:ARG:CD  | 6        | 1.67          |
| (1,631)  | 1:63:C:ASP:CB  | 1:41:C:ARG:CD  | 10       | 1.67          |
| (1,199)  | 1:26:C:PRO:CB  | 1:28:C:ARG:C   | 3        | 1.67          |
| (1,1284) | 1:41:C:ARG:CD  | 1:33:C:VAL:CG1 | 5        | 1.66          |
| (1,1039) | 1:77:C:LYS:CG  | 1:69:C:ASN:CA  | 4        | 1.66          |
| (1,1023) | 1:61:C:ILE:CG1 | 1:82:C:ASP:CA  | 2        | 1.66          |
| (1,109)  | 1:40:C:HIS:CB  | 1:64:C:GLU:CA  | 3        | 1.66          |
| (1,65)   | 1:41:C:ARG:CB  | 1:32:C:ARG:CG  | 7        | 1.66          |
| (1,58)   | 1:32:C:ARG:CG  | 1:41:C:ARG:CB  | 7        | 1.66          |
| (1,1163) | 1:41:C:ARG:CA  | 1:38:C:LYS:CB  | 3        | 1.65          |
| (1,1001) | 1:60:C:VAL:CB  | 1:46:C:TYR:CA  | 5        | 1.65          |
| (1,378)  | 1:41:C:ARG:CA  | 1:60:C:VAL:CB  | 10       | 1.65          |
| (1,1039) | 1:77:C:LYS:CG  | 1:69:C:ASN:CA  | 8        | 1.64          |
| (1,427)  | 1:92:C:SER:CB  | 1:26:C:PRO:CB  | 1        | 1.64          |
| (1,427)  | 1:92:C:SER:CB  | 1:26:C:PRO:CB  | 8        | 1.64          |
| (1,173)  | 1:82:C:ASP:CB  | 1:72:C:THR:C   | 7        | 1.64          |
| (1,80)   | 1:34:C:GLU:CB  | 1:32:C:ARG:CB  | 2        | 1.64          |
| (1,836)  | 1:33:C:VAL:CB  | 1:91:C:GLN:C   | 1        | 1.63          |
| (1,682)  | 1:76:C:ARG:CB  | 1:53:C:ALA:CA  | 1        | 1.63          |
| (1,465)  | 1:87:C:ILE:CA  | 1:94:C:ILE:CD1 | 9        | 1.63          |
| (1,427)  | 1:92:C:SER:CB  | 1:26:C:PRO:CB  | 6        | 1.63          |
| (1,378)  | 1:41:C:ARG:CA  | 1:60:C:VAL:CB  | 3        | 1.63          |
| (1,184)  | 1:33:C:VAL:CB  | 1:91:C:GLN:C   | 1        | 1.63          |
| (1,1039) | 1:77:C:LYS:CG  | 1:69:C:ASN:CA  | 1        | 1.62          |
| (1,1163) | 1:41:C:ARG:CA  | 1:38:C:LYS:CB  | 5        | 1.61          |
| (1,1039) | 1:77:C:LYS:CG  | 1:69:C:ASN:CA  | 7        | 1.61          |
| (1,1039) | 1:77:C:LYS:CG  | 1:69:C:ASN:CA  | 10       | 1.61          |
| (1,427)  | 1:92:C:SER:CB  | 1:26:C:PRO:CB  | 4        | 1.61          |
| (1,1178) | 1:66:C:LYS:CA  | 1:69:C:ASN:CB  | 8        | 1.6           |

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| Key      | Atom-1         | Atom-2        | Model ID | Violation (Å) |
|----------|----------------|---------------|----------|---------------|
| (1,1163) | 1:41:C:ARG:CA  | 1:38:C:LYS:CB | 10       | 1.6           |
| (1,846)  | 1:60:C:VAL:CB  | 1:84:C:GLY:C  | 2        | 1.6           |
| (1,593)  | 1:94:C:ILE:CG1 | 1:32:C:ARG:CG | 4        | 1.6           |
| (1,425)  | 1:91:C:GLN:CA  | 1:57:C:TRP:CB | 7        | 1.6           |
| (1,64)   | 1:76:C:ARG:CG  | 1:74:C:GLN:CG | 5        | 1.6           |
| (1,56)   | 1:74:C:GLN:CG  | 1:76:C:ARG:CG | 5        | 1.6           |
| (1,836)  | 1:33:C:VAL:CB  | 1:91:C:GLN:C  | 3        | 1.59          |
| (1,790)  | 1:36:C:ILE:CA  | 1:40:C:HIS:C  | 6        | 1.59          |
| (1,425)  | 1:91:C:GLN:CA  | 1:57:C:TRP:CB | 4        | 1.59          |
| (1,384)  | 1:51:C:LEU:CA  | 1:73:C:VAL:CB | 5        | 1.59          |
| (1,184)  | 1:33:C:VAL:CB  | 1:91:C:GLN:C  | 3        | 1.59          |
| (1,1163) | 1:41:C:ARG:CA  | 1:38:C:LYS:CB | 4        | 1.58          |
| (1,1039) | 1:77:C:LYS:CG  | 1:69:C:ASN:CA | 9        | 1.58          |
| (1,789)  | 1:74:C:GLN:CG  | 1:52:C:PHE:C  | 1        | 1.58          |
| (1,427)  | 1:92:C:SER:CB  | 1:26:C:PRO:CB | 5        | 1.58          |
| (1,1440) | 1:33:C:VAL:CG2 | 1:91:C:GLN:CG | 1        | 1.57          |
| (1,1023) | 1:61:C:ILE:CG1 | 1:82:C:ASP:CA | 1        | 1.57          |
| (1,427)  | 1:92:C:SER:CB  | 1:26:C:PRO:CB | 3        | 1.57          |
| (1,199)  | 1:26:C:PRO:CB  | 1:28:C:ARG:C  | 10       | 1.57          |
| (1,1023) | 1:61:C:ILE:CG1 | 1:82:C:ASP:CA | 6        | 1.56          |
| (1,790)  | 1:36:C:ILE:CA  | 1:40:C:HIS:C  | 4        | 1.56          |
| (1,425)  | 1:91:C:GLN:CA  | 1:57:C:TRP:CB | 5        | 1.56          |
| (1,173)  | 1:82:C:ASP:CB  | 1:72:C:THR:C  | 3        | 1.56          |
| (1,64)   | 1:76:C:ARG:CG  | 1:74:C:GLN:CG | 4        | 1.56          |
| (1,56)   | 1:74:C:GLN:CG  | 1:76:C:ARG:CG | 4        | 1.56          |
| (1,988)  | 1:69:C:ASN:CB  | 1:74:C:GLN:CA | 5        | 1.55          |
| (1,988)  | 1:69:C:ASN:CB  | 1:74:C:GLN:CA | 7        | 1.55          |
| (1,846)  | 1:60:C:VAL:CB  | 1:84:C:GLY:C  | 8        | 1.55          |
| (1,836)  | 1:33:C:VAL:CB  | 1:91:C:GLN:C  | 8        | 1.55          |
| (1,428)  | 1:54:C:THR:CA  | 1:56:C:LYS:CB | 9        | 1.55          |
| (1,378)  | 1:41:C:ARG:CA  | 1:60:C:VAL:CB | 2        | 1.55          |
| (1,367)  | 1:52:C:PHE:CA  | 1:76:C:ARG:CB | 3        | 1.55          |
| (1,184)  | 1:33:C:VAL:CB  | 1:91:C:GLN:C  | 8        | 1.55          |
| (1,1351) | 1:29:C:VAL:CB  | 1:26:C:PRO:CG | 2        | 1.54          |
| (1,1001) | 1:60:C:VAL:CB  | 1:46:C:TYR:CA | 3        | 1.54          |
| (1,64)   | 1:76:C:ARG:CG  | 1:74:C:GLN:CG | 10       | 1.54          |
| (1,56)   | 1:74:C:GLN:CG  | 1:76:C:ARG:CG | 10       | 1.54          |
| (1,791)  | 1:81:C:CYS:CA  | 1:83:C:GLU:CB | 3        | 1.53          |
| (1,427)  | 1:92:C:SER:CB  | 1:26:C:PRO:CB | 9        | 1.53          |
| (1,218)  | 1:27:C:LEU:CG  | 1:92:C:SER:C  | 2        | 1.53          |
| (1,425)  | 1:91:C:GLN:CA  | 1:57:C:TRP:CB | 9        | 1.52          |
| (1,218)  | 1:27:C:LEU:CG  | 1:92:C:SER:C  | 7        | 1.52          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,846)  | 1:60:C:VAL:CB  | 1:84:C:GLY:C   | 10       | 1.51          |
| (1,791)  | 1:81:C:CYS:CA  | 1:83:C:GLU:CB  | 1        | 1.51          |
| (1,791)  | 1:81:C:CYS:CA  | 1:83:C:GLU:CB  | 8        | 1.51          |
| (1,791)  | 1:81:C:CYS:CA  | 1:83:C:GLU:CB  | 9        | 1.51          |
| (1,791)  | 1:81:C:CYS:CA  | 1:83:C:GLU:CB  | 6        | 1.5           |
| (1,634)  | 1:33:C:VAL:CG2 | 1:41:C:ARG:CD  | 9        | 1.5           |
| (1,271)  | 1:41:C:ARG:CA  | 1:43:C:THR:C   | 4        | 1.5           |
| (1,218)  | 1:27:C:LEU:CG  | 1:92:C:SER:C   | 3        | 1.5           |
| (1,64)   | 1:76:C:ARG:CG  | 1:74:C:GLN:CG  | 3        | 1.5           |
| (1,56)   | 1:74:C:GLN:CG  | 1:76:C:ARG:CG  | 3        | 1.5           |
| (1,791)  | 1:81:C:CYS:CA  | 1:83:C:GLU:CB  | 2        | 1.49          |
| (1,791)  | 1:81:C:CYS:CA  | 1:83:C:GLU:CB  | 5        | 1.49          |
| (1,427)  | 1:92:C:SER:CB  | 1:26:C:PRO:CB  | 10       | 1.49          |
| (1,425)  | 1:91:C:GLN:CA  | 1:57:C:TRP:CB  | 3        | 1.49          |
| (1,64)   | 1:76:C:ARG:CG  | 1:74:C:GLN:CG  | 6        | 1.49          |
| (1,56)   | 1:74:C:GLN:CG  | 1:76:C:ARG:CG  | 6        | 1.49          |
| (1,791)  | 1:81:C:CYS:CA  | 1:83:C:GLU:CB  | 4        | 1.48          |
| (1,465)  | 1:87:C:ILE:CA  | 1:94:C:ILE:CD1 | 6        | 1.48          |
| (1,64)   | 1:76:C:ARG:CG  | 1:74:C:GLN:CG  | 2        | 1.48          |
| (1,64)   | 1:76:C:ARG:CG  | 1:74:C:GLN:CG  | 8        | 1.48          |
| (1,56)   | 1:74:C:GLN:CG  | 1:76:C:ARG:CG  | 2        | 1.48          |
| (1,56)   | 1:74:C:GLN:CG  | 1:76:C:ARG:CG  | 8        | 1.48          |
| (1,790)  | 1:36:C:ILE:CA  | 1:40:C:HIS:C   | 3        | 1.47          |
| (1,789)  | 1:74:C:GLN:CG  | 1:52:C:PHE:C   | 3        | 1.47          |
| (1,593)  | 1:94:C:ILE:CG1 | 1:32:C:ARG:CG  | 9        | 1.47          |
| (1,425)  | 1:91:C:GLN:CA  | 1:57:C:TRP:CB  | 1        | 1.47          |
| (1,80)   | 1:34:C:GLU:CB  | 1:32:C:ARG:CB  | 4        | 1.47          |
| (1,65)   | 1:41:C:ARG:CB  | 1:32:C:ARG:CG  | 9        | 1.47          |
| (1,58)   | 1:32:C:ARG:CG  | 1:41:C:ARG:CB  | 9        | 1.47          |
| (1,1001) | 1:60:C:VAL:CB  | 1:46:C:TYR:CA  | 10       | 1.46          |
| (1,791)  | 1:81:C:CYS:CA  | 1:83:C:GLU:CB  | 7        | 1.46          |
| (1,596)  | 1:32:C:ARG:CG  | 1:34:C:GLU:CB  | 3        | 1.46          |
| (1,465)  | 1:87:C:ILE:CA  | 1:94:C:ILE:CD1 | 10       | 1.46          |
| (1,65)   | 1:41:C:ARG:CB  | 1:32:C:ARG:CG  | 2        | 1.46          |
| (1,58)   | 1:32:C:ARG:CG  | 1:41:C:ARG:CB  | 2        | 1.46          |
| (1,791)  | 1:81:C:CYS:CA  | 1:83:C:GLU:CB  | 10       | 1.45          |
| (1,682)  | 1:76:C:ARG:CB  | 1:53:C:ALA:CA  | 10       | 1.45          |
| (1,425)  | 1:91:C:GLN:CA  | 1:57:C:TRP:CB  | 8        | 1.45          |
| (1,65)   | 1:41:C:ARG:CB  | 1:32:C:ARG:CG  | 3        | 1.45          |
| (1,58)   | 1:32:C:ARG:CG  | 1:41:C:ARG:CB  | 3        | 1.45          |
| (1,988)  | 1:69:C:ASN:CB  | 1:74:C:GLN:CA  | 8        | 1.44          |
| (1,271)  | 1:41:C:ARG:CA  | 1:43:C:THR:C   | 10       | 1.44          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,218)  | 1:27:C:LEU:CG  | 1:92:C:SER:C   | 5        | 1.44          |
| (1,80)   | 1:34:C:GLU:CB  | 1:32:C:ARG:CB  | 5        | 1.44          |
| (1,64)   | 1:76:C:ARG:CG  | 1:74:C:GLN:CG  | 7        | 1.44          |
| (1,56)   | 1:74:C:GLN:CG  | 1:76:C:ARG:CG  | 7        | 1.44          |
| (1,131)  | 1:68:C:LYS:CD  | 1:70:C:ASP:CA  | 2        | 1.43          |
| (1,64)   | 1:76:C:ARG:CG  | 1:74:C:GLN:CG  | 1        | 1.43          |
| (1,56)   | 1:74:C:GLN:CG  | 1:76:C:ARG:CG  | 1        | 1.43          |
| (1,1437) | 1:72:C:THR:CG2 | 1:81:C:CYS:CB  | 10       | 1.42          |
| (1,1245) | 1:66:C:LYS:CA  | 1:61:C:ILE:CA  | 7        | 1.42          |
| (1,846)  | 1:60:C:VAL:CB  | 1:84:C:GLY:C   | 5        | 1.42          |
| (1,428)  | 1:54:C:THR:CA  | 1:56:C:LYS:CB  | 3        | 1.42          |
| (1,428)  | 1:54:C:THR:CA  | 1:56:C:LYS:CB  | 5        | 1.42          |
| (1,173)  | 1:82:C:ASP:CB  | 1:72:C:THR:C   | 1        | 1.42          |
| (1,131)  | 1:68:C:LYS:CD  | 1:70:C:ASP:CA  | 9        | 1.42          |
| (1,1001) | 1:60:C:VAL:CB  | 1:46:C:TYR:CA  | 1        | 1.41          |
| (1,485)  | 1:90:C:ARG:CD  | 1:36:C:ILE:CG1 | 2        | 1.41          |
| (1,428)  | 1:54:C:THR:CA  | 1:56:C:LYS:CB  | 2        | 1.41          |
| (1,355)  | 1:63:C:ASP:CA  | 1:60:C:VAL:CB  | 4        | 1.41          |
| (1,131)  | 1:68:C:LYS:CD  | 1:70:C:ASP:CA  | 6        | 1.41          |
| (1,1001) | 1:60:C:VAL:CB  | 1:46:C:TYR:CA  | 4        | 1.4           |
| (1,1001) | 1:60:C:VAL:CB  | 1:46:C:TYR:CA  | 6        | 1.4           |
| (1,763)  | 1:36:C:ILE:CB  | 1:91:C:GLN:CA  | 9        | 1.4           |
| (1,485)  | 1:90:C:ARG:CD  | 1:36:C:ILE:CG1 | 5        | 1.4           |
| (1,131)  | 1:68:C:LYS:CD  | 1:70:C:ASP:CA  | 7        | 1.4           |
| (1,80)   | 1:34:C:GLU:CB  | 1:32:C:ARG:CB  | 10       | 1.4           |
| (1,1121) | 1:43:C:THR:CA  | 1:94:C:ILE:CG2 | 5        | 1.39          |
| (1,1001) | 1:60:C:VAL:CB  | 1:46:C:TYR:CA  | 9        | 1.39          |
| (1,790)  | 1:36:C:ILE:CA  | 1:40:C:HIS:C   | 8        | 1.39          |
| (1,428)  | 1:54:C:THR:CA  | 1:56:C:LYS:CB  | 8        | 1.39          |
| (1,218)  | 1:27:C:LEU:CG  | 1:92:C:SER:C   | 1        | 1.39          |
| (1,218)  | 1:27:C:LEU:CG  | 1:92:C:SER:C   | 4        | 1.39          |
| (1,65)   | 1:41:C:ARG:CB  | 1:32:C:ARG:CG  | 5        | 1.39          |
| (1,58)   | 1:32:C:ARG:CG  | 1:41:C:ARG:CB  | 5        | 1.39          |
| (1,153)  | 1:46:C:TYR:CB  | 1:29:C:VAL:CA  | 4        | 1.38          |
| (1,1437) | 1:72:C:THR:CG2 | 1:81:C:CYS:CB  | 1        | 1.37          |
| (1,1001) | 1:60:C:VAL:CB  | 1:46:C:TYR:CA  | 7        | 1.37          |
| (1,988)  | 1:69:C:ASN:CB  | 1:74:C:GLN:CA  | 6        | 1.37          |
| (1,790)  | 1:36:C:ILE:CA  | 1:40:C:HIS:C   | 10       | 1.37          |
| (1,763)  | 1:36:C:ILE:CB  | 1:91:C:GLN:CA  | 8        | 1.37          |
| (1,355)  | 1:63:C:ASP:CA  | 1:60:C:VAL:CB  | 8        | 1.37          |
| (1,1190) | 1:32:C:ARG:CA  | 1:95:C:GLN:CG  | 2        | 1.36          |
| (1,846)  | 1:60:C:VAL:CB  | 1:84:C:GLY:C   | 7        | 1.36          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,616)  | 1:36:C:ILE:CG1 | 1:95:C:GLN:CG  | 4        | 1.36          |
| (1,425)  | 1:91:C:GLN:CA  | 1:57:C:TRP:CB  | 2        | 1.36          |
| (1,173)  | 1:82:C:ASP:CB  | 1:72:C:THR:C   | 6        | 1.36          |
| (1,141)  | 1:28:C:ARG:CA  | 1:47:C:VAL:CB  | 7        | 1.36          |
| (1,131)  | 1:68:C:LYS:CD  | 1:70:C:ASP:CA  | 8        | 1.36          |
| (1,65)   | 1:41:C:ARG:CB  | 1:32:C:ARG:CG  | 10       | 1.36          |
| (1,58)   | 1:32:C:ARG:CG  | 1:41:C:ARG:CB  | 10       | 1.36          |
| (1,1163) | 1:41:C:ARG:CA  | 1:38:C:LYS:CB  | 8        | 1.35          |
| (1,1023) | 1:61:C:ILE:CG1 | 1:82:C:ASP:CA  | 3        | 1.35          |
| (1,790)  | 1:36:C:ILE:CA  | 1:40:C:HIS:C   | 7        | 1.35          |
| (1,428)  | 1:54:C:THR:CA  | 1:56:C:LYS:CB  | 6        | 1.34          |
| (1,1163) | 1:41:C:ARG:CA  | 1:38:C:LYS:CB  | 7        | 1.33          |
| (1,1106) | 1:78:C:TYR:CA  | 1:74:C:GLN:CG  | 9        | 1.33          |
| (1,988)  | 1:69:C:ASN:CB  | 1:74:C:GLN:CA  | 9        | 1.33          |
| (1,790)  | 1:36:C:ILE:CA  | 1:40:C:HIS:C   | 1        | 1.33          |
| (1,789)  | 1:74:C:GLN:CG  | 1:52:C:PHE:C   | 6        | 1.33          |
| (1,485)  | 1:90:C:ARG:CD  | 1:36:C:ILE:CG1 | 7        | 1.33          |
| (1,435)  | 1:92:C:SER:CB  | 1:27:C:LEU:CG  | 6        | 1.33          |
| (1,424)  | 1:91:C:GLN:CA  | 1:95:C:GLN:CB  | 2        | 1.33          |
| (1,310)  | 1:80:C:THR:CB  | 1:70:C:ASP:CA  | 5        | 1.33          |
| (1,199)  | 1:26:C:PRO:CB  | 1:28:C:ARG:C   | 9        | 1.33          |
| (1,131)  | 1:68:C:LYS:CD  | 1:70:C:ASP:CA  | 3        | 1.33          |
| (1,131)  | 1:68:C:LYS:CD  | 1:70:C:ASP:CA  | 4        | 1.33          |
| (1,1437) | 1:72:C:THR:CG2 | 1:81:C:CYS:CB  | 7        | 1.32          |
| (1,1001) | 1:60:C:VAL:CB  | 1:46:C:TYR:CA  | 2        | 1.32          |
| (1,846)  | 1:60:C:VAL:CB  | 1:84:C:GLY:C   | 6        | 1.32          |
| (1,1437) | 1:72:C:THR:CG2 | 1:81:C:CYS:CB  | 4        | 1.31          |
| (1,1174) | 1:76:C:ARG:CA  | 1:46:C:TYR:CB  | 3        | 1.31          |
| (1,593)  | 1:94:C:ILE:CG1 | 1:32:C:ARG:CG  | 1        | 1.31          |
| (1,485)  | 1:90:C:ARG:CD  | 1:36:C:ILE:CG1 | 9        | 1.31          |
| (1,485)  | 1:90:C:ARG:CD  | 1:36:C:ILE:CG1 | 10       | 1.31          |
| (1,435)  | 1:92:C:SER:CB  | 1:27:C:LEU:CG  | 9        | 1.31          |
| (1,153)  | 1:46:C:TYR:CB  | 1:29:C:VAL:CA  | 5        | 1.31          |
| (1,1351) | 1:29:C:VAL:CB  | 1:26:C:PRO:CG  | 7        | 1.3           |
| (1,1245) | 1:66:C:LYS:CA  | 1:61:C:ILE:CA  | 5        | 1.3           |
| (1,763)  | 1:36:C:ILE:CB  | 1:91:C:GLN:CA  | 5        | 1.3           |
| (1,593)  | 1:94:C:ILE:CG1 | 1:32:C:ARG:CG  | 7        | 1.3           |
| (1,485)  | 1:90:C:ARG:CD  | 1:36:C:ILE:CG1 | 6        | 1.3           |
| (1,271)  | 1:41:C:ARG:CA  | 1:43:C:THR:C   | 2        | 1.3           |
| (1,199)  | 1:26:C:PRO:CB  | 1:28:C:ARG:C   | 1        | 1.3           |
| (1,199)  | 1:26:C:PRO:CB  | 1:28:C:ARG:C   | 8        | 1.3           |
| (1,173)  | 1:82:C:ASP:CB  | 1:72:C:THR:C   | 9        | 1.3           |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,141)  | 1:28:C:ARG:CA  | 1:47:C:VAL:CB  | 4        | 1.3           |
| (1,109)  | 1:40:C:HIS:CB  | 1:64:C:GLU:CA  | 5        | 1.3           |
| (1,1351) | 1:29:C:VAL:CB  | 1:26:C:PRO:CG  | 10       | 1.29          |
| (1,1245) | 1:66:C:LYS:CA  | 1:61:C:ILE:CA  | 9        | 1.29          |
| (1,564)  | 1:87:C:ILE:CD1 | 1:61:C:ILE:CG2 | 3        | 1.29          |
| (1,465)  | 1:87:C:ILE:CA  | 1:94:C:ILE:CD1 | 2        | 1.29          |
| (1,428)  | 1:54:C:THR:CA  | 1:56:C:LYS:CB  | 4        | 1.29          |
| (1,153)  | 1:46:C:TYR:CB  | 1:29:C:VAL:CA  | 2        | 1.29          |
| (1,199)  | 1:26:C:PRO:CB  | 1:28:C:ARG:C   | 2        | 1.28          |
| (1,153)  | 1:46:C:TYR:CB  | 1:29:C:VAL:CA  | 1        | 1.28          |
| (1,80)   | 1:34:C:GLU:CB  | 1:32:C:ARG:CB  | 9        | 1.28          |
| (1,1284) | 1:41:C:ARG:CD  | 1:33:C:VAL:CG1 | 2        | 1.27          |
| (1,1121) | 1:43:C:THR:CA  | 1:94:C:ILE:CG2 | 2        | 1.27          |
| (1,763)  | 1:36:C:ILE:CB  | 1:91:C:GLN:CA  | 6        | 1.27          |
| (1,422)  | 1:43:C:THR:CA  | 1:41:C:ARG:CB  | 10       | 1.27          |
| (1,355)  | 1:63:C:ASP:CA  | 1:60:C:VAL:CB  | 2        | 1.27          |
| (1,199)  | 1:26:C:PRO:CB  | 1:28:C:ARG:C   | 4        | 1.27          |
| (1,153)  | 1:46:C:TYR:CB  | 1:29:C:VAL:CA  | 7        | 1.27          |
| (1,153)  | 1:46:C:TYR:CB  | 1:29:C:VAL:CA  | 10       | 1.27          |
| (1,846)  | 1:60:C:VAL:CB  | 1:84:C:GLY:C   | 3        | 1.26          |
| (1,435)  | 1:92:C:SER:CB  | 1:27:C:LEU:CG  | 10       | 1.26          |
| (1,428)  | 1:54:C:THR:CA  | 1:56:C:LYS:CB  | 7        | 1.26          |
| (1,131)  | 1:68:C:LYS:CD  | 1:70:C:ASP:CA  | 5        | 1.26          |
| (1,1245) | 1:66:C:LYS:CA  | 1:61:C:ILE:CA  | 1        | 1.25          |
| (1,1023) | 1:61:C:ILE:CG1 | 1:82:C:ASP:CA  | 9        | 1.25          |
| (1,763)  | 1:36:C:ILE:CB  | 1:91:C:GLN:CA  | 7        | 1.25          |
| (1,763)  | 1:36:C:ILE:CB  | 1:91:C:GLN:CA  | 10       | 1.25          |
| (1,634)  | 1:33:C:VAL:CG2 | 1:41:C:ARG:CD  | 2        | 1.25          |
| (1,427)  | 1:92:C:SER:CB  | 1:26:C:PRO:CB  | 2        | 1.25          |
| (1,425)  | 1:91:C:GLN:CA  | 1:57:C:TRP:CB  | 6        | 1.25          |
| (1,378)  | 1:41:C:ARG:CA  | 1:60:C:VAL:CB  | 5        | 1.25          |
| (1,218)  | 1:27:C:LEU:CG  | 1:92:C:SER:C   | 8        | 1.25          |
| (1,141)  | 1:28:C:ARG:CA  | 1:47:C:VAL:CB  | 10       | 1.25          |
| (1,1163) | 1:41:C:ARG:CA  | 1:38:C:LYS:CB  | 6        | 1.24          |
| (1,763)  | 1:36:C:ILE:CB  | 1:91:C:GLN:CA  | 3        | 1.24          |
| (1,631)  | 1:63:C:ASP:CB  | 1:41:C:ARG:CD  | 9        | 1.24          |
| (1,428)  | 1:54:C:THR:CA  | 1:56:C:LYS:CB  | 1        | 1.24          |
| (1,153)  | 1:46:C:TYR:CB  | 1:29:C:VAL:CA  | 9        | 1.24          |
| (1,1437) | 1:72:C:THR:CG2 | 1:81:C:CYS:CB  | 6        | 1.23          |
| (1,1437) | 1:72:C:THR:CG2 | 1:81:C:CYS:CB  | 9        | 1.23          |
| (1,1163) | 1:41:C:ARG:CA  | 1:38:C:LYS:CB  | 1        | 1.23          |
| (1,1109) | 1:87:C:ILE:CA  | 1:57:C:TRP:CB  | 4        | 1.23          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,634)  | 1:33:C:VAL:CG2 | 1:41:C:ARG:CD  | 5        | 1.23          |
| (1,564)  | 1:87:C:ILE:CD1 | 1:61:C:ILE:CG2 | 7        | 1.23          |
| (1,378)  | 1:41:C:ARG:CA  | 1:60:C:VAL:CB  | 6        | 1.23          |
| (1,153)  | 1:46:C:TYR:CB  | 1:29:C:VAL:CA  | 6        | 1.23          |
| (1,424)  | 1:91:C:GLN:CA  | 1:95:C:GLN:CB  | 5        | 1.22          |
| (1,1437) | 1:72:C:THR:CG2 | 1:81:C:CYS:CB  | 8        | 1.21          |
| (1,1284) | 1:41:C:ARG:CD  | 1:33:C:VAL:CG1 | 4        | 1.21          |
| (1,846)  | 1:60:C:VAL:CB  | 1:84:C:GLY:C   | 9        | 1.21          |
| (1,763)  | 1:36:C:ILE:CB  | 1:91:C:GLN:CA  | 1        | 1.21          |
| (1,564)  | 1:87:C:ILE:CD1 | 1:61:C:ILE:CG2 | 1        | 1.21          |
| (1,166)  | 1:29:C:VAL:CG2 | 1:31:C:SER:CB  | 7        | 1.21          |
| (1,1245) | 1:66:C:LYS:CA  | 1:61:C:ILE:CA  | 3        | 1.2           |
| (1,378)  | 1:41:C:ARG:CA  | 1:60:C:VAL:CB  | 8        | 1.2           |
| (1,374)  | 1:41:C:ARG:CA  | 1:32:C:ARG:CG  | 9        | 1.2           |
| (1,149)  | 1:85:C:HIS:CA  | 1:83:C:GLU:CB  | 3        | 1.2           |
| (1,1391) | 1:58:C:VAL:CG1 | 1:56:C:LYS:CB  | 3        | 1.19          |
| (1,870)  | 1:68:C:LYS:CD  | 1:84:C:GLY:C   | 2        | 1.19          |
| (1,870)  | 1:68:C:LYS:CD  | 1:84:C:GLY:C   | 5        | 1.19          |
| (1,790)  | 1:36:C:ILE:CA  | 1:40:C:HIS:C   | 5        | 1.19          |
| (1,485)  | 1:90:C:ARG:CD  | 1:36:C:ILE:CG1 | 1        | 1.19          |
| (1,425)  | 1:91:C:GLN:CA  | 1:57:C:TRP:CB  | 10       | 1.19          |
| (1,173)  | 1:82:C:ASP:CB  | 1:72:C:THR:C   | 8        | 1.19          |
| (1,18)   | 1:51:C:LEU:CG  | 1:53:C:ALA:C   | 8        | 1.19          |
| (1,1437) | 1:72:C:THR:CG2 | 1:81:C:CYS:CB  | 5        | 1.18          |
| (1,1109) | 1:87:C:ILE:CA  | 1:57:C:TRP:CB  | 2        | 1.18          |
| (1,865)  | 1:76:C:ARG:CB  | 1:52:C:PHE:C   | 3        | 1.18          |
| (1,149)  | 1:85:C:HIS:CA  | 1:83:C:GLU:CB  | 7        | 1.18          |
| (1,141)  | 1:28:C:ARG:CA  | 1:47:C:VAL:CB  | 2        | 1.17          |
| (1,1466) | 1:61:C:ILE:CB  | 1:41:C:ARG:CA  | 10       | 1.16          |
| (1,1245) | 1:66:C:LYS:CA  | 1:61:C:ILE:CA  | 4        | 1.16          |
| (1,846)  | 1:60:C:VAL:CB  | 1:84:C:GLY:C   | 1        | 1.16          |
| (1,428)  | 1:54:C:THR:CA  | 1:56:C:LYS:CB  | 10       | 1.16          |
| (1,1336) | 1:41:C:ARG:CB  | 1:61:C:ILE:CG1 | 10       | 1.15          |
| (1,1280) | 1:30:C:GLY:CA  | 1:27:C:LEU:CG  | 1        | 1.15          |
| (1,1023) | 1:61:C:ILE:CG1 | 1:82:C:ASP:CA  | 7        | 1.15          |
| (1,870)  | 1:68:C:LYS:CD  | 1:84:C:GLY:C   | 4        | 1.15          |
| (1,763)  | 1:36:C:ILE:CB  | 1:91:C:GLN:CA  | 2        | 1.15          |
| (1,763)  | 1:36:C:ILE:CB  | 1:91:C:GLN:CA  | 4        | 1.15          |
| (1,555)  | 1:85:C:HIS:CB  | 1:68:C:LYS:CG  | 3        | 1.15          |
| (1,149)  | 1:85:C:HIS:CA  | 1:83:C:GLU:CB  | 8        | 1.15          |
| (1,18)   | 1:51:C:LEU:CG  | 1:53:C:ALA:C   | 2        | 1.15          |
| (1,485)  | 1:90:C:ARG:CD  | 1:36:C:ILE:CG1 | 8        | 1.14          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,149)  | 1:85:C:HIS:CA  | 1:83:C:GLU:CB  | 9        | 1.14          |
| (1,631)  | 1:63:C:ASP:CB  | 1:41:C:ARG:CD  | 5        | 1.13          |
| (1,153)  | 1:46:C:TYR:CB  | 1:29:C:VAL:CA  | 3        | 1.13          |
| (1,18)   | 1:51:C:LEU:CG  | 1:53:C:ALA:C   | 1        | 1.13          |
| (1,1426) | 1:29:C:VAL:CG2 | 1:27:C:LEU:CG  | 3        | 1.12          |
| (1,1391) | 1:58:C:VAL:CG1 | 1:56:C:LYS:CB  | 2        | 1.12          |
| (1,1280) | 1:30:C:GLY:CA  | 1:27:C:LEU:CG  | 3        | 1.12          |
| (1,1023) | 1:61:C:ILE:CG1 | 1:82:C:ASP:CA  | 5        | 1.12          |
| (1,836)  | 1:33:C:VAL:CB  | 1:91:C:GLN:C   | 9        | 1.12          |
| (1,422)  | 1:43:C:THR:CA  | 1:41:C:ARG:CB  | 2        | 1.12          |
| (1,355)  | 1:63:C:ASP:CA  | 1:60:C:VAL:CB  | 7        | 1.12          |
| (1,310)  | 1:80:C:THR:CB  | 1:70:C:ASP:CA  | 2        | 1.12          |
| (1,184)  | 1:33:C:VAL:CB  | 1:91:C:GLN:C   | 9        | 1.12          |
| (1,153)  | 1:46:C:TYR:CB  | 1:29:C:VAL:CA  | 8        | 1.12          |
| (1,149)  | 1:85:C:HIS:CA  | 1:83:C:GLU:CB  | 1        | 1.12          |
| (1,149)  | 1:85:C:HIS:CA  | 1:83:C:GLU:CB  | 6        | 1.12          |
| (1,92)   | 1:33:C:VAL:C   | 1:40:C:HIS:CA  | 2        | 1.12          |
| (1,92)   | 1:33:C:VAL:C   | 1:40:C:HIS:CA  | 9        | 1.12          |
| (1,80)   | 1:34:C:GLU:CB  | 1:32:C:ARG:CB  | 1        | 1.12          |
| (1,80)   | 1:34:C:GLU:CB  | 1:32:C:ARG:CB  | 7        | 1.12          |
| (1,18)   | 1:51:C:LEU:CG  | 1:53:C:ALA:C   | 4        | 1.12          |
| (1,1391) | 1:58:C:VAL:CG1 | 1:56:C:LYS:CB  | 6        | 1.11          |
| (1,1195) | 1:70:C:ASP:CA  | 1:76:C:ARG:CB  | 3        | 1.11          |
| (1,1109) | 1:87:C:ILE:CA  | 1:57:C:TRP:CB  | 8        | 1.11          |
| (1,789)  | 1:74:C:GLN:CG  | 1:52:C:PHE:C   | 10       | 1.11          |
| (1,258)  | 1:70:C:ASP:CA  | 1:83:C:GLU:C   | 4        | 1.11          |
| (1,149)  | 1:85:C:HIS:CA  | 1:83:C:GLU:CB  | 4        | 1.11          |
| (1,80)   | 1:34:C:GLU:CB  | 1:32:C:ARG:CB  | 3        | 1.11          |
| (1,1391) | 1:58:C:VAL:CG1 | 1:56:C:LYS:CB  | 7        | 1.1           |
| (1,1245) | 1:66:C:LYS:CA  | 1:61:C:ILE:CA  | 10       | 1.1           |
| (1,1001) | 1:60:C:VAL:CB  | 1:46:C:TYR:CA  | 8        | 1.1           |
| (1,988)  | 1:69:C:ASN:CB  | 1:74:C:GLN:CA  | 2        | 1.1           |
| (1,92)   | 1:33:C:VAL:C   | 1:40:C:HIS:CA  | 5        | 1.1           |
| (1,43)   | 1:40:C:HIS:CA  | 1:34:C:GLU:CB  | 5        | 1.1           |
| (1,1391) | 1:58:C:VAL:CG1 | 1:56:C:LYS:CB  | 5        | 1.09          |
| (1,634)  | 1:33:C:VAL:CG2 | 1:41:C:ARG:CD  | 4        | 1.09          |
| (1,149)  | 1:85:C:HIS:CA  | 1:83:C:GLU:CB  | 2        | 1.09          |
| (1,149)  | 1:85:C:HIS:CA  | 1:83:C:GLU:CB  | 5        | 1.09          |
| (1,555)  | 1:85:C:HIS:CB  | 1:68:C:LYS:CG  | 8        | 1.08          |
| (1,485)  | 1:90:C:ARG:CD  | 1:36:C:ILE:CG1 | 3        | 1.08          |
| (1,422)  | 1:43:C:THR:CA  | 1:41:C:ARG:CB  | 4        | 1.08          |
| (1,258)  | 1:70:C:ASP:CA  | 1:83:C:GLU:C   | 6        | 1.08          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,258)  | 1:70:C:ASP:CA  | 1:83:C:GLU:C   | 9        | 1.08          |
| (1,149)  | 1:85:C:HIS:CA  | 1:83:C:GLU:CB  | 10       | 1.08          |
| (1,1437) | 1:72:C:THR:CG2 | 1:81:C:CYS:CB  | 2        | 1.07          |
| (1,1426) | 1:29:C:VAL:CG2 | 1:27:C:LEU:CG  | 1        | 1.07          |
| (1,1336) | 1:41:C:ARG:CB  | 1:61:C:ILE:CG1 | 2        | 1.07          |
| (1,1195) | 1:70:C:ASP:CA  | 1:76:C:ARG:CB  | 2        | 1.07          |
| (1,988)  | 1:69:C:ASN:CB  | 1:74:C:GLN:CA  | 3        | 1.07          |
| (1,790)  | 1:36:C:ILE:CA  | 1:40:C:HIS:C   | 2        | 1.07          |
| (1,789)  | 1:74:C:GLN:CG  | 1:52:C:PHE:C   | 5        | 1.07          |
| (1,616)  | 1:36:C:ILE:CG1 | 1:95:C:GLN:CG  | 8        | 1.07          |
| (1,555)  | 1:85:C:HIS:CB  | 1:68:C:LYS:CG  | 6        | 1.07          |
| (1,422)  | 1:43:C:THR:CA  | 1:41:C:ARG:CB  | 8        | 1.07          |
| (1,310)  | 1:80:C:THR:CB  | 1:70:C:ASP:CA  | 10       | 1.07          |
| (1,43)   | 1:40:C:HIS:CA  | 1:34:C:GLU:CB  | 8        | 1.07          |
| (1,18)   | 1:51:C:LEU:CG  | 1:53:C:ALA:C   | 9        | 1.07          |
| (1,1174) | 1:76:C:ARG:CA  | 1:46:C:TYR:CB  | 9        | 1.06          |
| (1,310)  | 1:80:C:THR:CB  | 1:70:C:ASP:CA  | 7        | 1.06          |
| (1,106)  | 1:40:C:HIS:C   | 1:33:C:VAL:CB  | 2        | 1.06          |
| (1,80)   | 1:34:C:GLU:CB  | 1:32:C:ARG:CB  | 8        | 1.06          |
| (1,1109) | 1:87:C:ILE:CA  | 1:57:C:TRP:CB  | 10       | 1.05          |
| (1,836)  | 1:33:C:VAL:CB  | 1:91:C:GLN:C   | 5        | 1.05          |
| (1,823)  | 1:82:C:ASP:CB  | 1:79:C:PHE:C   | 3        | 1.05          |
| (1,689)  | 1:76:C:ARG:CG  | 1:70:C:ASP:CA  | 3        | 1.05          |
| (1,682)  | 1:76:C:ARG:CB  | 1:53:C:ALA:CA  | 7        | 1.05          |
| (1,422)  | 1:43:C:THR:CA  | 1:41:C:ARG:CB  | 1        | 1.05          |
| (1,422)  | 1:43:C:THR:CA  | 1:41:C:ARG:CB  | 5        | 1.05          |
| (1,405)  | 1:70:C:ASP:CA  | 1:76:C:ARG:CG  | 3        | 1.05          |
| (1,310)  | 1:80:C:THR:CB  | 1:70:C:ASP:CA  | 9        | 1.05          |
| (1,258)  | 1:70:C:ASP:CA  | 1:83:C:GLU:C   | 5        | 1.05          |
| (1,184)  | 1:33:C:VAL:CB  | 1:91:C:GLN:C   | 5        | 1.05          |
| (1,43)   | 1:40:C:HIS:CA  | 1:34:C:GLU:CB  | 1        | 1.05          |
| (1,1190) | 1:32:C:ARG:CA  | 1:95:C:GLN:CG  | 9        | 1.04          |
| (1,616)  | 1:36:C:ILE:CG1 | 1:95:C:GLN:CG  | 3        | 1.04          |
| (1,355)  | 1:63:C:ASP:CA  | 1:60:C:VAL:CB  | 9        | 1.04          |
| (1,258)  | 1:70:C:ASP:CA  | 1:83:C:GLU:C   | 7        | 1.04          |
| (1,18)   | 1:51:C:LEU:CG  | 1:53:C:ALA:C   | 3        | 1.04          |
| (1,1280) | 1:30:C:GLY:CA  | 1:27:C:LEU:CG  | 8        | 1.03          |
| (1,733)  | 1:58:C:VAL:CG1 | 1:92:C:SER:CA  | 7        | 1.03          |
| (1,310)  | 1:80:C:THR:CB  | 1:70:C:ASP:CA  | 4        | 1.03          |
| (1,310)  | 1:80:C:THR:CB  | 1:70:C:ASP:CA  | 8        | 1.03          |
| (1,43)   | 1:40:C:HIS:CA  | 1:34:C:GLU:CB  | 6        | 1.03          |
| (1,43)   | 1:40:C:HIS:CA  | 1:34:C:GLU:CB  | 7        | 1.03          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,823)  | 1:82:C:ASP:CB  | 1:79:C:PHE:C   | 2        | 1.02          |
| (1,374)  | 1:41:C:ARG:CA  | 1:32:C:ARG:CG  | 2        | 1.02          |
| (1,1391) | 1:58:C:VAL:CG1 | 1:56:C:LYS:CB  | 9        | 1.01          |
| (1,1174) | 1:76:C:ARG:CA  | 1:46:C:TYR:CB  | 1        | 1.01          |
| (1,797)  | 1:62:C:LEU:CG  | 1:66:C:LYS:CA  | 8        | 1.01          |
| (1,555)  | 1:85:C:HIS:CB  | 1:68:C:LYS:CG  | 9        | 1.01          |
| (1,422)  | 1:43:C:THR:CA  | 1:41:C:ARG:CB  | 6        | 1.01          |
| (1,355)  | 1:63:C:ASP:CA  | 1:60:C:VAL:CB  | 1        | 1.01          |
| (1,310)  | 1:80:C:THR:CB  | 1:70:C:ASP:CA  | 1        | 1.01          |
| (1,258)  | 1:70:C:ASP:CA  | 1:83:C:GLU:C   | 8        | 1.01          |
| (1,80)   | 1:34:C:GLU:CB  | 1:32:C:ARG:CB  | 6        | 1.01          |
| (1,43)   | 1:40:C:HIS:CA  | 1:34:C:GLU:CB  | 2        | 1.01          |
| (1,43)   | 1:40:C:HIS:CA  | 1:34:C:GLU:CB  | 4        | 1.01          |
| (1,378)  | 1:41:C:ARG:CA  | 1:60:C:VAL:CB  | 1        | 1.0           |
| (1,355)  | 1:63:C:ASP:CA  | 1:60:C:VAL:CB  | 5        | 1.0           |
| (1,258)  | 1:70:C:ASP:CA  | 1:83:C:GLU:C   | 1        | 1.0           |
| (1,44)   | 1:57:C:TRP:CA  | 1:47:C:VAL:CB  | 5        | 1.0           |
| (1,1466) | 1:61:C:ILE:CB  | 1:41:C:ARG:CA  | 2        | 0.99          |
| (1,1426) | 1:29:C:VAL:CG2 | 1:27:C:LEU:CG  | 8        | 0.99          |
| (1,1391) | 1:58:C:VAL:CG1 | 1:56:C:LYS:CB  | 8        | 0.99          |
| (1,1280) | 1:30:C:GLY:CA  | 1:27:C:LEU:CG  | 7        | 0.99          |
| (1,465)  | 1:87:C:ILE:CA  | 1:94:C:ILE:CD1 | 5        | 0.99          |
| (1,374)  | 1:41:C:ARG:CA  | 1:32:C:ARG:CG  | 7        | 0.99          |
| (1,310)  | 1:80:C:THR:CB  | 1:70:C:ASP:CA  | 6        | 0.99          |
| (1,1391) | 1:58:C:VAL:CG1 | 1:56:C:LYS:CB  | 10       | 0.98          |
| (1,1174) | 1:76:C:ARG:CA  | 1:46:C:TYR:CB  | 8        | 0.98          |
| (1,901)  | 1:94:C:ILE:CD1 | 1:87:C:ILE:C   | 7        | 0.98          |
| (1,733)  | 1:58:C:VAL:CG1 | 1:92:C:SER:CA  | 4        | 0.98          |
| (1,564)  | 1:87:C:ILE:CD1 | 1:61:C:ILE:CG2 | 9        | 0.98          |
| (1,435)  | 1:92:C:SER:CB  | 1:27:C:LEU:CG  | 7        | 0.98          |
| (1,1437) | 1:72:C:THR:CG2 | 1:81:C:CYS:CB  | 3        | 0.97          |
| (1,1245) | 1:66:C:LYS:CA  | 1:61:C:ILE:CA  | 6        | 0.97          |
| (1,1109) | 1:87:C:ILE:CA  | 1:57:C:TRP:CB  | 5        | 0.97          |
| (1,823)  | 1:82:C:ASP:CB  | 1:79:C:PHE:C   | 5        | 0.97          |
| (1,733)  | 1:58:C:VAL:CG1 | 1:92:C:SER:CA  | 9        | 0.97          |
| (1,258)  | 1:70:C:ASP:CA  | 1:83:C:GLU:C   | 10       | 0.97          |
| (1,166)  | 1:29:C:VAL:CG2 | 1:31:C:SER:CB  | 9        | 0.97          |
| (1,141)  | 1:28:C:ARG:CA  | 1:47:C:VAL:CB  | 3        | 0.97          |
| (1,137)  | 1:32:C:ARG:CG  | 1:31:C:SER:CB  | 8        | 0.97          |
| (1,44)   | 1:57:C:TRP:CA  | 1:47:C:VAL:CB  | 6        | 0.97          |
| (1,1280) | 1:30:C:GLY:CA  | 1:27:C:LEU:CG  | 2        | 0.96          |
| (1,1280) | 1:30:C:GLY:CA  | 1:27:C:LEU:CG  | 4        | 0.96          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1174) | 1:76:C:ARG:CA  | 1:46:C:TYR:CB  | 6        | 0.96          |
| (1,1121) | 1:43:C:THR:CA  | 1:94:C:ILE:CG2 | 8        | 0.96          |
| (1,564)  | 1:87:C:ILE:CD1 | 1:61:C:ILE:CG2 | 4        | 0.96          |
| (1,374)  | 1:41:C:ARG:CA  | 1:32:C:ARG:CG  | 1        | 0.96          |
| (1,310)  | 1:80:C:THR:CB  | 1:70:C:ASP:CA  | 3        | 0.96          |
| (1,1121) | 1:43:C:THR:CA  | 1:94:C:ILE:CG2 | 6        | 0.95          |
| (1,797)  | 1:62:C:LEU:CG  | 1:66:C:LYS:CA  | 6        | 0.95          |
| (1,555)  | 1:85:C:HIS:CB  | 1:68:C:LYS:CG  | 4        | 0.95          |
| (1,555)  | 1:85:C:HIS:CB  | 1:68:C:LYS:CG  | 5        | 0.95          |
| (1,156)  | 1:61:C:ILE:CB  | 1:45:C:ALA:CB  | 4        | 0.95          |
| (1,137)  | 1:32:C:ARG:CG  | 1:31:C:SER:CB  | 4        | 0.95          |
| (1,974)  | 1:37:C:GLY:CA  | 1:93:C:GLN:CA  | 4        | 0.94          |
| (1,379)  | 1:64:C:GLU:CA  | 1:85:C:HIS:CB  | 2        | 0.94          |
| (1,355)  | 1:63:C:ASP:CA  | 1:60:C:VAL:CB  | 6        | 0.94          |
| (1,271)  | 1:41:C:ARG:CA  | 1:43:C:THR:C   | 5        | 0.94          |
| (1,258)  | 1:70:C:ASP:CA  | 1:83:C:GLU:C   | 3        | 0.94          |
| (1,166)  | 1:29:C:VAL:CG2 | 1:31:C:SER:CB  | 5        | 0.94          |
| (1,156)  | 1:61:C:ILE:CB  | 1:45:C:ALA:CB  | 5        | 0.94          |
| (1,92)   | 1:33:C:VAL:C   | 1:40:C:HIS:CA  | 4        | 0.94          |
| (1,1245) | 1:66:C:LYS:CA  | 1:61:C:ILE:CA  | 8        | 0.93          |
| (1,1174) | 1:76:C:ARG:CA  | 1:46:C:TYR:CB  | 7        | 0.93          |
| (1,823)  | 1:82:C:ASP:CB  | 1:79:C:PHE:C   | 10       | 0.93          |
| (1,631)  | 1:63:C:ASP:CB  | 1:41:C:ARG:CD  | 3        | 0.93          |
| (1,564)  | 1:87:C:ILE:CD1 | 1:61:C:ILE:CG2 | 5        | 0.93          |
| (1,374)  | 1:41:C:ARG:CA  | 1:32:C:ARG:CG  | 3        | 0.93          |
| (1,141)  | 1:28:C:ARG:CA  | 1:47:C:VAL:CB  | 8        | 0.93          |
| (1,1174) | 1:76:C:ARG:CA  | 1:46:C:TYR:CB  | 5        | 0.92          |
| (1,733)  | 1:58:C:VAL:CG1 | 1:92:C:SER:CA  | 3        | 0.92          |
| (1,422)  | 1:43:C:THR:CA  | 1:41:C:ARG:CB  | 3        | 0.92          |
| (1,379)  | 1:64:C:GLU:CA  | 1:85:C:HIS:CB  | 10       | 0.92          |
| (1,374)  | 1:41:C:ARG:CA  | 1:32:C:ARG:CG  | 5        | 0.92          |
| (1,271)  | 1:41:C:ARG:CA  | 1:43:C:THR:C   | 3        | 0.92          |
| (1,199)  | 1:26:C:PRO:CB  | 1:28:C:ARG:C   | 7        | 0.92          |
| (1,166)  | 1:29:C:VAL:CG2 | 1:31:C:SER:CB  | 2        | 0.92          |
| (1,166)  | 1:29:C:VAL:CG2 | 1:31:C:SER:CB  | 8        | 0.92          |
| (1,137)  | 1:32:C:ARG:CG  | 1:31:C:SER:CB  | 6        | 0.92          |
| (1,92)   | 1:33:C:VAL:C   | 1:40:C:HIS:CA  | 10       | 0.92          |
| (1,1245) | 1:66:C:LYS:CA  | 1:61:C:ILE:CA  | 2        | 0.91          |
| (1,564)  | 1:87:C:ILE:CD1 | 1:61:C:ILE:CG2 | 6        | 0.91          |
| (1,422)  | 1:43:C:THR:CA  | 1:41:C:ARG:CB  | 9        | 0.91          |
| (1,166)  | 1:29:C:VAL:CG2 | 1:31:C:SER:CB  | 10       | 0.91          |
| (1,106)  | 1:40:C:HIS:C   | 1:33:C:VAL:CB  | 9        | 0.91          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1391) | 1:58:C:VAL:CG1 | 1:56:C:LYS:CB  | 1        | 0.9           |
| (1,1121) | 1:43:C:THR:CA  | 1:94:C:ILE:CG2 | 9        | 0.9           |
| (1,797)  | 1:62:C:LEU:CG  | 1:66:C:LYS:CA  | 7        | 0.9           |
| (1,789)  | 1:74:C:GLN:CG  | 1:52:C:PHE:C   | 9        | 0.9           |
| (1,379)  | 1:64:C:GLU:CA  | 1:85:C:HIS:CB  | 8        | 0.9           |
| (1,271)  | 1:41:C:ARG:CA  | 1:43:C:THR:C   | 9        | 0.9           |
| (1,166)  | 1:29:C:VAL:CG2 | 1:31:C:SER:CB  | 1        | 0.9           |
| (1,106)  | 1:40:C:HIS:C   | 1:33:C:VAL:CB  | 5        | 0.9           |
| (1,1121) | 1:43:C:THR:CA  | 1:94:C:ILE:CG2 | 1        | 0.89          |
| (1,1121) | 1:43:C:THR:CA  | 1:94:C:ILE:CG2 | 7        | 0.89          |
| (1,156)  | 1:61:C:ILE:CB  | 1:45:C:ALA:CB  | 6        | 0.89          |
| (1,18)   | 1:51:C:LEU:CG  | 1:53:C:ALA:C   | 6        | 0.89          |
| (1,1391) | 1:58:C:VAL:CG1 | 1:56:C:LYS:CB  | 4        | 0.88          |
| (1,1280) | 1:30:C:GLY:CA  | 1:27:C:LEU:CG  | 5        | 0.88          |
| (1,823)  | 1:82:C:ASP:CB  | 1:79:C:PHE:C   | 4        | 0.88          |
| (1,797)  | 1:62:C:LEU:CG  | 1:66:C:LYS:CA  | 10       | 0.88          |
| (1,733)  | 1:58:C:VAL:CG1 | 1:92:C:SER:CA  | 5        | 0.88          |
| (1,555)  | 1:85:C:HIS:CB  | 1:68:C:LYS:CG  | 2        | 0.88          |
| (1,555)  | 1:85:C:HIS:CB  | 1:68:C:LYS:CG  | 7        | 0.88          |
| (1,435)  | 1:92:C:SER:CB  | 1:27:C:LEU:CG  | 2        | 0.88          |
| (1,18)   | 1:51:C:LEU:CG  | 1:53:C:ALA:C   | 7        | 0.88          |
| (1,18)   | 1:51:C:LEU:CG  | 1:53:C:ALA:C   | 10       | 0.88          |
| (1,797)  | 1:62:C:LEU:CG  | 1:66:C:LYS:CA  | 9        | 0.87          |
| (1,199)  | 1:26:C:PRO:CB  | 1:28:C:ARG:C   | 5        | 0.87          |
| (1,1121) | 1:43:C:THR:CA  | 1:94:C:ILE:CG2 | 4        | 0.86          |
| (1,901)  | 1:94:C:ILE:CD1 | 1:87:C:ILE:C   | 1        | 0.86          |
| (1,733)  | 1:58:C:VAL:CG1 | 1:92:C:SER:CA  | 1        | 0.86          |
| (1,689)  | 1:76:C:ARG:CG  | 1:70:C:ASP:CA  | 2        | 0.86          |
| (1,485)  | 1:90:C:ARG:CD  | 1:36:C:ILE:CG1 | 4        | 0.86          |
| (1,405)  | 1:70:C:ASP:CA  | 1:76:C:ARG:CG  | 2        | 0.86          |
| (1,379)  | 1:64:C:GLU:CA  | 1:85:C:HIS:CB  | 5        | 0.86          |
| (1,378)  | 1:41:C:ARG:CA  | 1:60:C:VAL:CB  | 7        | 0.86          |
| (1,355)  | 1:63:C:ASP:CA  | 1:60:C:VAL:CB  | 10       | 0.86          |
| (1,106)  | 1:40:C:HIS:C   | 1:33:C:VAL:CB  | 10       | 0.86          |
| (1,18)   | 1:51:C:LEU:CG  | 1:53:C:ALA:C   | 5        | 0.86          |
| (1,1109) | 1:87:C:ILE:CA  | 1:57:C:TRP:CB  | 1        | 0.85          |
| (1,640)  | 1:45:C:ALA:CB  | 1:61:C:ILE:CB  | 4        | 0.85          |
| (1,424)  | 1:91:C:GLN:CA  | 1:95:C:GLN:CB  | 1        | 0.85          |
| (1,422)  | 1:43:C:THR:CA  | 1:41:C:ARG:CB  | 7        | 0.85          |
| (1,384)  | 1:51:C:LEU:CA  | 1:73:C:VAL:CB  | 3        | 0.85          |
| (1,52)   | 1:29:C:VAL:CG2 | 1:43:C:THR:CB  | 9        | 0.85          |
| (1,52)   | 1:29:C:VAL:CG2 | 1:43:C:THR:CB  | 10       | 0.85          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,43)   | 1:40:C:HIS:CA  | 1:34:C:GLU:CB  | 9        | 0.85          |
| (1,1174) | 1:76:C:ARG:CA  | 1:46:C:TYR:CB  | 2        | 0.84          |
| (1,1174) | 1:76:C:ARG:CA  | 1:46:C:TYR:CB  | 10       | 0.84          |
| (1,852)  | 1:56:C:LYS:CB  | 1:53:C:ALA:C   | 2        | 0.84          |
| (1,836)  | 1:33:C:VAL:CB  | 1:91:C:GLN:C   | 4        | 0.84          |
| (1,823)  | 1:82:C:ASP:CB  | 1:79:C:PHE:C   | 6        | 0.84          |
| (1,640)  | 1:45:C:ALA:CB  | 1:61:C:ILE:CB  | 5        | 0.84          |
| (1,616)  | 1:36:C:ILE:CG1 | 1:95:C:GLN:CG  | 6        | 0.84          |
| (1,271)  | 1:41:C:ARG:CA  | 1:43:C:THR:C   | 1        | 0.84          |
| (1,271)  | 1:41:C:ARG:CA  | 1:43:C:THR:C   | 6        | 0.84          |
| (1,184)  | 1:33:C:VAL:CB  | 1:91:C:GLN:C   | 4        | 0.84          |
| (1,92)   | 1:33:C:VAL:C   | 1:40:C:HIS:CA  | 8        | 0.84          |
| (1,379)  | 1:64:C:GLU:CA  | 1:85:C:HIS:CB  | 1        | 0.83          |
| (1,379)  | 1:64:C:GLU:CA  | 1:85:C:HIS:CB  | 9        | 0.83          |
| (1,271)  | 1:41:C:ARG:CA  | 1:43:C:THR:C   | 8        | 0.83          |
| (1,141)  | 1:28:C:ARG:CA  | 1:47:C:VAL:CB  | 9        | 0.83          |
| (1,47)   | 1:88:C:PHE:CA  | 1:60:C:VAL:CB  | 1        | 0.83          |
| (1,43)   | 1:40:C:HIS:CA  | 1:34:C:GLU:CB  | 3        | 0.83          |
| (1,1063) | 1:89:C:VAL:CG2 | 1:34:C:GLU:CA  | 10       | 0.82          |
| (1,823)  | 1:82:C:ASP:CB  | 1:79:C:PHE:C   | 7        | 0.82          |
| (1,631)  | 1:63:C:ASP:CB  | 1:41:C:ARG:CD  | 7        | 0.82          |
| (1,435)  | 1:92:C:SER:CB  | 1:27:C:LEU:CG  | 5        | 0.82          |
| (1,355)  | 1:63:C:ASP:CA  | 1:60:C:VAL:CB  | 3        | 0.82          |
| (1,166)  | 1:29:C:VAL:CG2 | 1:31:C:SER:CB  | 6        | 0.82          |
| (1,44)   | 1:57:C:TRP:CA  | 1:47:C:VAL:CB  | 2        | 0.82          |
| (1,1426) | 1:29:C:VAL:CG2 | 1:27:C:LEU:CG  | 4        | 0.81          |
| (1,797)  | 1:62:C:LEU:CG  | 1:66:C:LYS:CA  | 5        | 0.81          |
| (1,733)  | 1:58:C:VAL:CG1 | 1:92:C:SER:CA  | 6        | 0.81          |
| (1,92)   | 1:33:C:VAL:C   | 1:40:C:HIS:CA  | 1        | 0.81          |
| (1,43)   | 1:40:C:HIS:CA  | 1:34:C:GLU:CB  | 10       | 0.81          |
| (1,1426) | 1:29:C:VAL:CG2 | 1:27:C:LEU:CG  | 2        | 0.8           |
| (1,1399) | 1:29:C:VAL:CG1 | 1:27:C:LEU:CD1 | 6        | 0.8           |
| (1,1399) | 1:29:C:VAL:CG1 | 1:27:C:LEU:CD1 | 7        | 0.8           |
| (1,1121) | 1:43:C:THR:CA  | 1:94:C:ILE:CG2 | 10       | 0.8           |
| (1,974)  | 1:37:C:GLY:CA  | 1:93:C:GLN:CA  | 3        | 0.8           |
| (1,852)  | 1:56:C:LYS:CB  | 1:53:C:ALA:C   | 9        | 0.8           |
| (1,823)  | 1:82:C:ASP:CB  | 1:79:C:PHE:C   | 1        | 0.8           |
| (1,823)  | 1:82:C:ASP:CB  | 1:79:C:PHE:C   | 8        | 0.8           |
| (1,653)  | 1:61:C:ILE:CG1 | 1:87:C:ILE:CB  | 1        | 0.8           |
| (1,435)  | 1:92:C:SER:CB  | 1:27:C:LEU:CG  | 1        | 0.8           |
| (1,435)  | 1:92:C:SER:CB  | 1:27:C:LEU:CG  | 3        | 0.8           |
| (1,1426) | 1:29:C:VAL:CG2 | 1:27:C:LEU:CG  | 5        | 0.79          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,852)  | 1:56:C:LYS:CB  | 1:53:C:ALA:C   | 5        | 0.79          |
| (1,852)  | 1:56:C:LYS:CB  | 1:53:C:ALA:C   | 6        | 0.79          |
| (1,836)  | 1:33:C:VAL:CB  | 1:91:C:GLN:C   | 2        | 0.79          |
| (1,823)  | 1:82:C:ASP:CB  | 1:79:C:PHE:C   | 9        | 0.79          |
| (1,640)  | 1:45:C:ALA:CB  | 1:61:C:ILE:CB  | 6        | 0.79          |
| (1,631)  | 1:63:C:ASP:CB  | 1:41:C:ARG:CD  | 1        | 0.79          |
| (1,184)  | 1:33:C:VAL:CB  | 1:91:C:GLN:C   | 2        | 0.79          |
| (1,156)  | 1:61:C:ILE:CB  | 1:45:C:ALA:CB  | 2        | 0.79          |
| (1,1109) | 1:87:C:ILE:CA  | 1:57:C:TRP:CB  | 6        | 0.78          |
| (1,1109) | 1:87:C:ILE:CA  | 1:57:C:TRP:CB  | 7        | 0.77          |
| (1,852)  | 1:56:C:LYS:CB  | 1:53:C:ALA:C   | 3        | 0.77          |
| (1,794)  | 1:76:C:ARG:CG  | 1:51:C:LEU:CA  | 4        | 0.77          |
| (1,631)  | 1:63:C:ASP:CB  | 1:41:C:ARG:CD  | 2        | 0.77          |
| (1,166)  | 1:29:C:VAL:CG2 | 1:31:C:SER:CB  | 3        | 0.77          |
| (1,92)   | 1:33:C:VAL:C   | 1:40:C:HIS:CA  | 7        | 0.77          |
| (1,1466) | 1:61:C:ILE:CB  | 1:41:C:ARG:CA  | 4        | 0.76          |
| (1,1270) | 1:86:C:GLY:CA  | 1:83:C:GLU:CB  | 2        | 0.76          |
| (1,974)  | 1:37:C:GLY:CA  | 1:93:C:GLN:CA  | 2        | 0.76          |
| (1,374)  | 1:41:C:ARG:CA  | 1:32:C:ARG:CG  | 10       | 0.76          |
| (1,47)   | 1:88:C:PHE:CA  | 1:60:C:VAL:CB  | 2        | 0.76          |
| (1,733)  | 1:58:C:VAL:CG1 | 1:92:C:SER:CA  | 2        | 0.75          |
| (1,156)  | 1:61:C:ILE:CB  | 1:45:C:ALA:CB  | 7        | 0.75          |
| (1,105)  | 1:44:C:VAL:C   | 1:60:C:VAL:CB  | 7        | 0.75          |
| (1,105)  | 1:44:C:VAL:C   | 1:60:C:VAL:CB  | 9        | 0.75          |
| (1,1270) | 1:86:C:GLY:CA  | 1:83:C:GLU:CB  | 5        | 0.74          |
| (1,1121) | 1:43:C:THR:CA  | 1:94:C:ILE:CG2 | 3        | 0.74          |
| (1,901)  | 1:94:C:ILE:CD1 | 1:87:C:ILE:C   | 8        | 0.74          |
| (1,634)  | 1:33:C:VAL:CG2 | 1:41:C:ARG:CD  | 10       | 0.74          |
| (1,617)  | 1:76:C:ARG:CG  | 1:52:C:PHE:CB  | 9        | 0.74          |
| (1,367)  | 1:52:C:PHE:CA  | 1:76:C:ARG:CB  | 9        | 0.74          |
| (1,258)  | 1:70:C:ASP:CA  | 1:83:C:GLU:C   | 2        | 0.74          |
| (1,44)   | 1:57:C:TRP:CA  | 1:47:C:VAL:CB  | 1        | 0.74          |
| (1,1109) | 1:87:C:ILE:CA  | 1:57:C:TRP:CB  | 9        | 0.73          |
| (1,797)  | 1:62:C:LEU:CG  | 1:66:C:LYS:CA  | 4        | 0.73          |
| (1,653)  | 1:61:C:ILE:CG1 | 1:87:C:ILE:CB  | 3        | 0.73          |
| (1,564)  | 1:87:C:ILE:CD1 | 1:61:C:ILE:CG2 | 10       | 0.73          |
| (1,166)  | 1:29:C:VAL:CG2 | 1:31:C:SER:CB  | 4        | 0.73          |
| (1,47)   | 1:88:C:PHE:CA  | 1:60:C:VAL:CB  | 5        | 0.73          |
| (1,47)   | 1:88:C:PHE:CA  | 1:60:C:VAL:CB  | 7        | 0.73          |
| (1,1270) | 1:86:C:GLY:CA  | 1:83:C:GLU:CB  | 3        | 0.72          |
| (1,874)  | 1:62:C:LEU:CG  | 1:67:C:GLY:C   | 8        | 0.72          |
| (1,564)  | 1:87:C:ILE:CD1 | 1:61:C:ILE:CG2 | 2        | 0.72          |

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| Key      | Atom-1         | Atom-2        | Model ID | Violation (Å) |
|----------|----------------|---------------|----------|---------------|
| (1,156)  | 1:61:C:ILE:CB  | 1:45:C:ALA:CB | 3        | 0.72          |
| (1,156)  | 1:61:C:ILE:CB  | 1:45:C:ALA:CB | 10       | 0.72          |
| (1,1109) | 1:87:C:ILE:CA  | 1:57:C:TRP:CB | 3        | 0.71          |
| (1,901)  | 1:94:C:ILE:CD1 | 1:87:C:ILE:C  | 4        | 0.71          |
| (1,789)  | 1:74:C:GLN:CG  | 1:52:C:PHE:C  | 4        | 0.71          |
| (1,379)  | 1:64:C:GLU:CA  | 1:85:C:HIS:CB | 3        | 0.71          |
| (1,379)  | 1:64:C:GLU:CA  | 1:85:C:HIS:CB | 6        | 0.71          |
| (1,156)  | 1:61:C:ILE:CB  | 1:45:C:ALA:CB | 8        | 0.71          |
| (1,874)  | 1:62:C:LEU:CG  | 1:67:C:GLY:C  | 10       | 0.7           |
| (1,653)  | 1:61:C:ILE:CG1 | 1:87:C:ILE:CB | 4        | 0.7           |
| (1,424)  | 1:91:C:GLN:CA  | 1:95:C:GLN:CB | 7        | 0.7           |
| (1,156)  | 1:61:C:ILE:CB  | 1:45:C:ALA:CB | 1        | 0.7           |
| (1,1270) | 1:86:C:GLY:CA  | 1:83:C:GLU:CB | 9        | 0.69          |
| (1,901)  | 1:94:C:ILE:CD1 | 1:87:C:ILE:C  | 3        | 0.69          |
| (1,640)  | 1:45:C:ALA:CB  | 1:61:C:ILE:CB | 2        | 0.69          |
| (1,616)  | 1:36:C:ILE:CG1 | 1:95:C:GLN:CG | 1        | 0.69          |
| (1,106)  | 1:40:C:HIS:C   | 1:33:C:VAL:CB | 4        | 0.69          |
| (1,1195) | 1:70:C:ASP:CA  | 1:76:C:ARG:CB | 1        | 0.68          |
| (1,790)  | 1:36:C:ILE:CA  | 1:40:C:HIS:C  | 9        | 0.68          |
| (1,727)  | 1:51:C:LEU:CG  | 1:54:C:THR:CA | 6        | 0.68          |
| (1,92)   | 1:33:C:VAL:C   | 1:40:C:HIS:CA | 3        | 0.68          |
| (1,1270) | 1:86:C:GLY:CA  | 1:83:C:GLU:CB | 8        | 0.67          |
| (1,1119) | 1:43:C:THR:CA  | 1:29:C:VAL:CB | 7        | 0.67          |
| (1,789)  | 1:74:C:GLN:CG  | 1:52:C:PHE:C  | 7        | 0.67          |
| (1,367)  | 1:52:C:PHE:CA  | 1:76:C:ARG:CB | 4        | 0.67          |
| (1,367)  | 1:52:C:PHE:CA  | 1:76:C:ARG:CB | 5        | 0.67          |
| (1,47)   | 1:88:C:PHE:CA  | 1:60:C:VAL:CB | 8        | 0.67          |
| (1,1270) | 1:86:C:GLY:CA  | 1:83:C:GLU:CB | 7        | 0.66          |
| (1,1270) | 1:86:C:GLY:CA  | 1:83:C:GLU:CB | 10       | 0.66          |
| (1,1195) | 1:70:C:ASP:CA  | 1:76:C:ARG:CB | 9        | 0.66          |
| (1,874)  | 1:62:C:LEU:CG  | 1:67:C:GLY:C  | 6        | 0.66          |
| (1,727)  | 1:51:C:LEU:CG  | 1:54:C:THR:CA | 7        | 0.66          |
| (1,789)  | 1:74:C:GLN:CG  | 1:52:C:PHE:C  | 2        | 0.65          |
| (1,640)  | 1:45:C:ALA:CB  | 1:61:C:ILE:CB | 7        | 0.65          |
| (1,616)  | 1:36:C:ILE:CG1 | 1:95:C:GLN:CG | 7        | 0.65          |
| (1,435)  | 1:92:C:SER:CB  | 1:27:C:LEU:CG | 4        | 0.65          |
| (1,424)  | 1:91:C:GLN:CA  | 1:95:C:GLN:CB | 6        | 0.65          |
| (1,141)  | 1:28:C:ARG:CA  | 1:47:C:VAL:CB | 1        | 0.65          |
| (1,92)   | 1:33:C:VAL:C   | 1:40:C:HIS:CA | 6        | 0.65          |
| (1,1270) | 1:86:C:GLY:CA  | 1:83:C:GLU:CB | 1        | 0.64          |
| (1,1270) | 1:86:C:GLY:CA  | 1:83:C:GLU:CB | 6        | 0.64          |
| (1,1174) | 1:76:C:ARG:CA  | 1:46:C:TYR:CB | 4        | 0.64          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,662)  | 1:68:C:LYS:CB  | 1:82:C:ASP:CA  | 2        | 0.64          |
| (1,653)  | 1:61:C:ILE:CG1 | 1:87:C:ILE:CB  | 2        | 0.64          |
| (1,653)  | 1:61:C:ILE:CG1 | 1:87:C:ILE:CB  | 6        | 0.64          |
| (1,564)  | 1:87:C:ILE:CD1 | 1:61:C:ILE:CG2 | 8        | 0.64          |
| (1,47)   | 1:88:C:PHE:CA  | 1:60:C:VAL:CB  | 6        | 0.64          |
| (1,1195) | 1:70:C:ASP:CA  | 1:76:C:ARG:CB  | 4        | 0.63          |
| (1,1195) | 1:70:C:ASP:CA  | 1:76:C:ARG:CB  | 6        | 0.63          |
| (1,874)  | 1:62:C:LEU:CG  | 1:67:C:GLY:C   | 5        | 0.63          |
| (1,662)  | 1:68:C:LYS:CB  | 1:82:C:ASP:CA  | 4        | 0.63          |
| (1,662)  | 1:68:C:LYS:CB  | 1:82:C:ASP:CA  | 5        | 0.63          |
| (1,444)  | 1:36:C:ILE:CA  | 1:89:C:VAL:CG1 | 10       | 0.63          |
| (1,379)  | 1:64:C:GLU:CA  | 1:85:C:HIS:CB  | 4        | 0.63          |
| (1,733)  | 1:58:C:VAL:CG1 | 1:92:C:SER:CA  | 8        | 0.62          |
| (1,662)  | 1:68:C:LYS:CB  | 1:82:C:ASP:CA  | 3        | 0.62          |
| (1,640)  | 1:45:C:ALA:CB  | 1:61:C:ILE:CB  | 3        | 0.62          |
| (1,640)  | 1:45:C:ALA:CB  | 1:61:C:ILE:CB  | 10       | 0.62          |
| (1,1399) | 1:29:C:VAL:CG1 | 1:27:C:LEU:CD1 | 5        | 0.61          |
| (1,1399) | 1:29:C:VAL:CG1 | 1:27:C:LEU:CD1 | 10       | 0.61          |
| (1,901)  | 1:94:C:ILE:CD1 | 1:87:C:ILE:C   | 9        | 0.61          |
| (1,794)  | 1:76:C:ARG:CG  | 1:51:C:LEU:CA  | 9        | 0.61          |
| (1,727)  | 1:51:C:LEU:CG  | 1:54:C:THR:CA  | 2        | 0.61          |
| (1,640)  | 1:45:C:ALA:CB  | 1:61:C:ILE:CB  | 8        | 0.61          |
| (1,379)  | 1:64:C:GLU:CA  | 1:85:C:HIS:CB  | 7        | 0.61          |
| (1,141)  | 1:28:C:ARG:CA  | 1:47:C:VAL:CB  | 5        | 0.61          |
| (1,47)   | 1:88:C:PHE:CA  | 1:60:C:VAL:CB  | 3        | 0.61          |
| (1,1195) | 1:70:C:ASP:CA  | 1:76:C:ARG:CB  | 7        | 0.6           |
| (1,1195) | 1:70:C:ASP:CA  | 1:76:C:ARG:CB  | 8        | 0.6           |
| (1,727)  | 1:51:C:LEU:CG  | 1:54:C:THR:CA  | 8        | 0.6           |
| (1,640)  | 1:45:C:ALA:CB  | 1:61:C:ILE:CB  | 1        | 0.6           |
| (1,271)  | 1:41:C:ARG:CA  | 1:43:C:THR:C   | 7        | 0.6           |
| (1,1063) | 1:89:C:VAL:CG2 | 1:34:C:GLU:CA  | 2        | 0.59          |
| (1,974)  | 1:37:C:GLY:CA  | 1:93:C:GLN:CA  | 5        | 0.59          |
| (1,727)  | 1:51:C:LEU:CG  | 1:54:C:THR:CA  | 1        | 0.59          |
| (1,598)  | 1:91:C:GLN:CB  | 1:56:C:LYS:CB  | 9        | 0.59          |
| (1,473)  | 1:70:C:ASP:CA  | 1:72:C:THR:CG2 | 1        | 0.59          |
| (1,45)   | 1:62:C:LEU:CA  | 1:60:C:VAL:CB  | 4        | 0.59          |
| (1,1270) | 1:86:C:GLY:CA  | 1:83:C:GLU:CB  | 4        | 0.58          |
| (1,852)  | 1:56:C:LYS:CB  | 1:53:C:ALA:C   | 8        | 0.58          |
| (1,473)  | 1:70:C:ASP:CA  | 1:72:C:THR:CG2 | 9        | 0.58          |
| (1,47)   | 1:88:C:PHE:CA  | 1:60:C:VAL:CB  | 4        | 0.58          |
| (1,47)   | 1:88:C:PHE:CA  | 1:60:C:VAL:CB  | 9        | 0.58          |
| (1,1399) | 1:29:C:VAL:CG1 | 1:27:C:LEU:CD1 | 1        | 0.57          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,727)  | 1:51:C:LEU:CG  | 1:54:C:THR:CA  | 5        | 0.57          |
| (1,617)  | 1:76:C:ARG:CG  | 1:52:C:PHE:CB  | 5        | 0.57          |
| (1,602)  | 1:90:C:ARG:CG  | 1:58:C:VAL:CB  | 6        | 0.57          |
| (1,473)  | 1:70:C:ASP:CA  | 1:72:C:THR:CG2 | 4        | 0.57          |
| (1,473)  | 1:70:C:ASP:CA  | 1:72:C:THR:CG2 | 7        | 0.57          |
| (1,473)  | 1:70:C:ASP:CA  | 1:72:C:THR:CG2 | 8        | 0.57          |
| (1,473)  | 1:70:C:ASP:CA  | 1:72:C:THR:CG2 | 10       | 0.57          |
| (1,424)  | 1:91:C:GLN:CA  | 1:95:C:GLN:CB  | 8        | 0.57          |
| (1,231)  | 1:29:C:VAL:CG1 | 1:47:C:VAL:C   | 7        | 0.57          |
| (1,105)  | 1:44:C:VAL:C   | 1:60:C:VAL:CB  | 1        | 0.57          |
| (1,105)  | 1:44:C:VAL:C   | 1:60:C:VAL:CB  | 5        | 0.57          |
| (1,47)   | 1:88:C:PHE:CA  | 1:60:C:VAL:CB  | 10       | 0.57          |
| (1,653)  | 1:61:C:ILE:CG1 | 1:87:C:ILE:CB  | 7        | 0.56          |
| (1,653)  | 1:61:C:ILE:CG1 | 1:87:C:ILE:CB  | 10       | 0.56          |
| (1,617)  | 1:76:C:ARG:CG  | 1:52:C:PHE:CB  | 6        | 0.56          |
| (1,156)  | 1:61:C:ILE:CB  | 1:45:C:ALA:CB  | 9        | 0.56          |
| (1,1431) | 1:49:C:ALA:CB  | 1:51:C:LEU:CB  | 8        | 0.55          |
| (1,874)  | 1:62:C:LEU:CG  | 1:67:C:GLY:C   | 9        | 0.55          |
| (1,852)  | 1:56:C:LYS:CB  | 1:53:C:ALA:C   | 7        | 0.55          |
| (1,794)  | 1:76:C:ARG:CG  | 1:51:C:LEU:CA  | 3        | 0.55          |
| (1,727)  | 1:51:C:LEU:CG  | 1:54:C:THR:CA  | 4        | 0.55          |
| (1,727)  | 1:51:C:LEU:CG  | 1:54:C:THR:CA  | 10       | 0.55          |
| (1,653)  | 1:61:C:ILE:CG1 | 1:87:C:ILE:CB  | 8        | 0.55          |
| (1,473)  | 1:70:C:ASP:CA  | 1:72:C:THR:CG2 | 3        | 0.55          |
| (1,473)  | 1:70:C:ASP:CA  | 1:72:C:THR:CG2 | 6        | 0.55          |
| (1,367)  | 1:52:C:PHE:CA  | 1:76:C:ARG:CB  | 8        | 0.55          |
| (1,662)  | 1:68:C:LYS:CB  | 1:82:C:ASP:CA  | 7        | 0.54          |
| (1,473)  | 1:70:C:ASP:CA  | 1:72:C:THR:CG2 | 2        | 0.54          |
| (1,473)  | 1:70:C:ASP:CA  | 1:72:C:THR:CG2 | 5        | 0.54          |
| (1,367)  | 1:52:C:PHE:CA  | 1:76:C:ARG:CB  | 6        | 0.54          |
| (1,52)   | 1:29:C:VAL:CG2 | 1:43:C:THR:CB  | 1        | 0.54          |
| (1,1195) | 1:70:C:ASP:CA  | 1:76:C:ARG:CB  | 5        | 0.53          |
| (1,852)  | 1:56:C:LYS:CB  | 1:53:C:ALA:C   | 4        | 0.53          |
| (1,689)  | 1:76:C:ARG:CG  | 1:70:C:ASP:CA  | 7        | 0.53          |
| (1,405)  | 1:70:C:ASP:CA  | 1:76:C:ARG:CG  | 7        | 0.53          |
| (1,1365) | 1:76:C:ARG:CG  | 1:52:C:PHE:CB  | 3        | 0.52          |
| (1,836)  | 1:33:C:VAL:CB  | 1:91:C:GLN:C   | 10       | 0.52          |
| (1,184)  | 1:33:C:VAL:CB  | 1:91:C:GLN:C   | 10       | 0.52          |
| (1,131)  | 1:68:C:LYS:CD  | 1:70:C:ASP:CA  | 1        | 0.52          |
| (1,57)   | 1:74:C:GLN:CG  | 1:51:C:LEU:CG  | 4        | 0.52          |
| (1,52)   | 1:29:C:VAL:CG2 | 1:43:C:THR:CB  | 2        | 0.52          |
| (1,44)   | 1:57:C:TRP:CA  | 1:47:C:VAL:CB  | 8        | 0.52          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,865)  | 1:76:C:ARG:CB  | 1:52:C:PHE:C   | 9        | 0.51          |
| (1,435)  | 1:92:C:SER:CB  | 1:27:C:LEU:CG  | 8        | 0.51          |
| (1,378)  | 1:41:C:ARG:CA  | 1:60:C:VAL:CB  | 9        | 0.51          |
| (1,874)  | 1:62:C:LEU:CG  | 1:67:C:GLY:C   | 2        | 0.5           |
| (1,617)  | 1:76:C:ARG:CG  | 1:52:C:PHE:CB  | 2        | 0.5           |
| (1,44)   | 1:57:C:TRP:CA  | 1:47:C:VAL:CB  | 10       | 0.5           |
| (1,1336) | 1:41:C:ARG:CB  | 1:61:C:ILE:CG1 | 4        | 0.49          |
| (1,1195) | 1:70:C:ASP:CA  | 1:76:C:ARG:CB  | 10       | 0.49          |
| (1,870)  | 1:68:C:LYS:CD  | 1:84:C:GLY:C   | 6        | 0.49          |
| (1,689)  | 1:76:C:ARG:CG  | 1:70:C:ASP:CA  | 8        | 0.48          |
| (1,477)  | 1:71:C:GLY:CA  | 1:82:C:ASP:CB  | 10       | 0.48          |
| (1,405)  | 1:70:C:ASP:CA  | 1:76:C:ARG:CG  | 8        | 0.48          |
| (1,105)  | 1:44:C:VAL:C   | 1:60:C:VAL:CB  | 3        | 0.48          |
| (1,78)   | 1:57:C:TRP:CB  | 1:90:C:ARG:CB  | 8        | 0.48          |
| (1,52)   | 1:29:C:VAL:CG2 | 1:43:C:THR:CB  | 5        | 0.48          |
| (1,1336) | 1:41:C:ARG:CB  | 1:61:C:ILE:CG1 | 8        | 0.47          |
| (1,1284) | 1:41:C:ARG:CD  | 1:33:C:VAL:CG1 | 10       | 0.47          |
| (1,870)  | 1:68:C:LYS:CD  | 1:84:C:GLY:C   | 7        | 0.47          |
| (1,870)  | 1:68:C:LYS:CD  | 1:84:C:GLY:C   | 9        | 0.47          |
| (1,797)  | 1:62:C:LEU:CG  | 1:66:C:LYS:CA  | 2        | 0.47          |
| (1,727)  | 1:51:C:LEU:CG  | 1:54:C:THR:CA  | 9        | 0.47          |
| (1,662)  | 1:68:C:LYS:CB  | 1:82:C:ASP:CA  | 10       | 0.47          |
| (1,602)  | 1:90:C:ARG:CG  | 1:58:C:VAL:CB  | 10       | 0.47          |
| (1,424)  | 1:91:C:GLN:CA  | 1:95:C:GLN:CB  | 3        | 0.47          |
| (1,1431) | 1:49:C:ALA:CB  | 1:51:C:LEU:CB  | 4        | 0.46          |
| (1,874)  | 1:62:C:LEU:CG  | 1:67:C:GLY:C   | 4        | 0.46          |
| (1,870)  | 1:68:C:LYS:CD  | 1:84:C:GLY:C   | 8        | 0.46          |
| (1,865)  | 1:76:C:ARG:CB  | 1:52:C:PHE:C   | 5        | 0.46          |
| (1,640)  | 1:45:C:ALA:CB  | 1:61:C:ILE:CB  | 9        | 0.46          |
| (1,596)  | 1:32:C:ARG:CG  | 1:34:C:GLU:CB  | 2        | 0.46          |
| (1,52)   | 1:29:C:VAL:CG2 | 1:43:C:THR:CB  | 3        | 0.46          |
| (1,52)   | 1:29:C:VAL:CG2 | 1:43:C:THR:CB  | 8        | 0.46          |
| (1,45)   | 1:62:C:LEU:CA  | 1:60:C:VAL:CB  | 2        | 0.46          |
| (1,1431) | 1:49:C:ALA:CB  | 1:51:C:LEU:CB  | 1        | 0.45          |
| (1,1431) | 1:49:C:ALA:CB  | 1:51:C:LEU:CB  | 10       | 0.45          |
| (1,1119) | 1:43:C:THR:CA  | 1:29:C:VAL:CB  | 9        | 0.45          |
| (1,1119) | 1:43:C:THR:CA  | 1:29:C:VAL:CB  | 10       | 0.45          |
| (1,653)  | 1:61:C:ILE:CG1 | 1:87:C:ILE:CB  | 9        | 0.45          |
| (1,367)  | 1:52:C:PHE:CA  | 1:76:C:ARG:CB  | 2        | 0.45          |
| (1,141)  | 1:28:C:ARG:CA  | 1:47:C:VAL:CB  | 6        | 0.45          |
| (1,852)  | 1:56:C:LYS:CB  | 1:53:C:ALA:C   | 1        | 0.44          |
| (1,662)  | 1:68:C:LYS:CB  | 1:82:C:ASP:CA  | 9        | 0.44          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,602)  | 1:90:C:ARG:CG  | 1:58:C:VAL:CB  | 9        | 0.44          |
| (1,78)   | 1:57:C:TRP:CB  | 1:90:C:ARG:CB  | 9        | 0.44          |
| (1,44)   | 1:57:C:TRP:CA  | 1:47:C:VAL:CB  | 7        | 0.44          |
| (1,1399) | 1:29:C:VAL:CG1 | 1:27:C:LEU:CD1 | 2        | 0.43          |
| (1,1393) | 1:89:C:VAL:CG1 | 1:62:C:LEU:CB  | 9        | 0.43          |
| (1,1354) | 1:83:C:GLU:CB  | 1:68:C:LYS:CD  | 1        | 0.43          |
| (1,1144) | 1:93:C:GLN:CA  | 1:27:C:LEU:CD1 | 4        | 0.43          |
| (1,1063) | 1:89:C:VAL:CG2 | 1:34:C:GLU:CA  | 5        | 0.43          |
| (1,689)  | 1:76:C:ARG:CG  | 1:70:C:ASP:CA  | 6        | 0.43          |
| (1,405)  | 1:70:C:ASP:CA  | 1:76:C:ARG:CG  | 6        | 0.43          |
| (1,351)  | 1:29:C:VAL:CA  | 1:46:C:TYR:CB  | 4        | 0.43          |
| (1,106)  | 1:40:C:HIS:C   | 1:33:C:VAL:CB  | 1        | 0.43          |
| (1,78)   | 1:57:C:TRP:CB  | 1:90:C:ARG:CB  | 1        | 0.43          |
| (1,45)   | 1:62:C:LEU:CA  | 1:60:C:VAL:CB  | 8        | 0.43          |
| (1,1421) | 1:29:C:VAL:CG2 | 1:27:C:LEU:CD1 | 1        | 0.42          |
| (1,1144) | 1:93:C:GLN:CA  | 1:27:C:LEU:CD1 | 3        | 0.42          |
| (1,689)  | 1:76:C:ARG:CG  | 1:70:C:ASP:CA  | 9        | 0.42          |
| (1,617)  | 1:76:C:ARG:CG  | 1:52:C:PHE:CB  | 8        | 0.42          |
| (1,405)  | 1:70:C:ASP:CA  | 1:76:C:ARG:CG  | 9        | 0.42          |
| (1,44)   | 1:57:C:TRP:CA  | 1:47:C:VAL:CB  | 9        | 0.42          |
| (1,1421) | 1:29:C:VAL:CG2 | 1:27:C:LEU:CD1 | 4        | 0.41          |
| (1,865)  | 1:76:C:ARG:CB  | 1:52:C:PHE:C   | 4        | 0.41          |
| (1,727)  | 1:51:C:LEU:CG  | 1:54:C:THR:CA  | 3        | 0.41          |
| (1,78)   | 1:57:C:TRP:CB  | 1:90:C:ARG:CB  | 7        | 0.41          |
| (1,1431) | 1:49:C:ALA:CB  | 1:51:C:LEU:CB  | 2        | 0.4           |
| (1,901)  | 1:94:C:ILE:CD1 | 1:87:C:ILE:C   | 6        | 0.4           |
| (1,797)  | 1:62:C:LEU:CG  | 1:66:C:LYS:CA  | 1        | 0.4           |
| (1,653)  | 1:61:C:ILE:CG1 | 1:87:C:ILE:CB  | 5        | 0.4           |
| (1,602)  | 1:90:C:ARG:CG  | 1:58:C:VAL:CB  | 3        | 0.4           |
| (1,245)  | 1:72:C:THR:CG2 | 1:78:C:TYR:C   | 8        | 0.4           |
| (1,78)   | 1:57:C:TRP:CB  | 1:90:C:ARG:CB  | 5        | 0.4           |
| (1,1466) | 1:61:C:ILE:CB  | 1:41:C:ARG:CA  | 3        | 0.39          |
| (1,1431) | 1:49:C:ALA:CB  | 1:51:C:LEU:CB  | 9        | 0.39          |
| (1,1280) | 1:30:C:GLY:CA  | 1:27:C:LEU:CG  | 9        | 0.39          |
| (1,901)  | 1:94:C:ILE:CD1 | 1:87:C:ILE:C   | 10       | 0.39          |
| (1,105)  | 1:44:C:VAL:C   | 1:60:C:VAL:CB  | 10       | 0.39          |
| (1,1421) | 1:29:C:VAL:CG2 | 1:27:C:LEU:CD1 | 3        | 0.38          |
| (1,1393) | 1:89:C:VAL:CG1 | 1:62:C:LEU:CB  | 8        | 0.38          |
| (1,1144) | 1:93:C:GLN:CA  | 1:27:C:LEU:CD1 | 9        | 0.38          |
| (1,870)  | 1:68:C:LYS:CD  | 1:84:C:GLY:C   | 3        | 0.38          |
| (1,508)  | 1:36:C:ILE:CB  | 1:89:C:VAL:CG2 | 8        | 0.38          |
| (1,245)  | 1:72:C:THR:CG2 | 1:78:C:TYR:C   | 2        | 0.38          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,245)  | 1:72:C:THR:CG2 | 1:78:C:TYR:C   | 5        | 0.38          |
| (1,245)  | 1:72:C:THR:CG2 | 1:78:C:TYR:C   | 6        | 0.38          |
| (1,106)  | 1:40:C:HIS:C   | 1:33:C:VAL:CB  | 8        | 0.38          |
| (2,62)   | 1:65:C:ALA:H   | 1:84:C:GLY:O   | 2        | 0.37          |
| (1,1399) | 1:29:C:VAL:CG1 | 1:27:C:LEU:CD1 | 9        | 0.37          |
| (1,1336) | 1:41:C:ARG:CB  | 1:61:C:ILE:CG1 | 6        | 0.37          |
| (1,974)  | 1:37:C:GLY:CA  | 1:93:C:GLN:CA  | 6        | 0.37          |
| (1,874)  | 1:62:C:LEU:CG  | 1:67:C:GLY:C   | 7        | 0.37          |
| (1,865)  | 1:76:C:ARG:CB  | 1:52:C:PHE:C   | 8        | 0.37          |
| (1,794)  | 1:76:C:ARG:CG  | 1:51:C:LEU:CA  | 8        | 0.37          |
| (1,231)  | 1:29:C:VAL:CG1 | 1:47:C:VAL:C   | 10       | 0.37          |
| (1,159)  | 1:62:C:LEU:CA  | 1:61:C:ILE:CG2 | 10       | 0.37          |
| (2,62)   | 1:65:C:ALA:H   | 1:84:C:GLY:O   | 9        | 0.36          |
| (1,1470) | 1:89:C:VAL:CG2 | 1:36:C:ILE:CA  | 2        | 0.36          |
| (1,1431) | 1:49:C:ALA:CB  | 1:51:C:LEU:CB  | 7        | 0.36          |
| (1,1421) | 1:29:C:VAL:CG2 | 1:27:C:LEU:CD1 | 6        | 0.36          |
| (1,1399) | 1:29:C:VAL:CG1 | 1:27:C:LEU:CD1 | 3        | 0.36          |
| (1,1393) | 1:89:C:VAL:CG1 | 1:62:C:LEU:CB  | 7        | 0.36          |
| (1,1104) | 1:87:C:ILE:CA  | 1:84:C:GLY:CA  | 8        | 0.36          |
| (1,662)  | 1:68:C:LYS:CB  | 1:82:C:ASP:CA  | 6        | 0.36          |
| (1,598)  | 1:27:C:LEU:CG  | 1:95:C:GLN:CB  | 10       | 0.36          |
| (1,508)  | 1:36:C:ILE:CB  | 1:89:C:VAL:CG2 | 9        | 0.36          |
| (1,351)  | 1:29:C:VAL:CA  | 1:46:C:TYR:CB  | 5        | 0.36          |
| (1,245)  | 1:72:C:THR:CG2 | 1:78:C:TYR:C   | 4        | 0.36          |
| (1,245)  | 1:72:C:THR:CG2 | 1:78:C:TYR:C   | 9        | 0.36          |
| (1,1393) | 1:89:C:VAL:CG1 | 1:62:C:LEU:CB  | 10       | 0.35          |
| (1,662)  | 1:68:C:LYS:CB  | 1:82:C:ASP:CA  | 8        | 0.35          |
| (1,477)  | 1:71:C:GLY:CA  | 1:82:C:ASP:CB  | 2        | 0.35          |
| (1,245)  | 1:72:C:THR:CG2 | 1:78:C:TYR:C   | 10       | 0.35          |
| (1,44)   | 1:57:C:TRP:CA  | 1:47:C:VAL:CB  | 3        | 0.35          |
| (1,44)   | 1:57:C:TRP:CA  | 1:47:C:VAL:CB  | 4        | 0.35          |
| (1,1470) | 1:89:C:VAL:CG2 | 1:36:C:ILE:CA  | 5        | 0.34          |
| (1,1393) | 1:89:C:VAL:CG1 | 1:62:C:LEU:CB  | 1        | 0.34          |
| (1,1144) | 1:93:C:GLN:CA  | 1:27:C:LEU:CD1 | 1        | 0.34          |
| (1,1063) | 1:89:C:VAL:CG2 | 1:34:C:GLU:CA  | 4        | 0.34          |
| (1,865)  | 1:76:C:ARG:CB  | 1:52:C:PHE:C   | 6        | 0.34          |
| (1,662)  | 1:68:C:LYS:CB  | 1:82:C:ASP:CA  | 1        | 0.34          |
| (1,508)  | 1:36:C:ILE:CB  | 1:89:C:VAL:CG2 | 5        | 0.34          |
| (1,508)  | 1:36:C:ILE:CB  | 1:89:C:VAL:CG2 | 7        | 0.34          |
| (1,351)  | 1:29:C:VAL:CA  | 1:46:C:TYR:CB  | 2        | 0.34          |
| (1,245)  | 1:72:C:THR:CG2 | 1:78:C:TYR:C   | 1        | 0.34          |
| (1,159)  | 1:62:C:LEU:CA  | 1:61:C:ILE:CG2 | 6        | 0.34          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,78)   | 1:57:C:TRP:CB  | 1:90:C:ARG:CB  | 10       | 0.34          |
| (1,60)   | 1:32:C:ARG:CB  | 1:34:C:GLU:CB  | 2        | 0.34          |
| (1,59)   | 1:32:C:ARG:CB  | 1:34:C:GLU:CB  | 2        | 0.34          |
| (1,14)   | 1:46:C:TYR:CB  | 1:77:C:LYS:CB  | 7        | 0.34          |
| (2,58)   | 1:85:C:HIS:H   | 1:82:C:ASP:O   | 10       | 0.33          |
| (2,28)   | 1:49:C:ALA:H   | 1:55:C:GLY:O   | 4        | 0.33          |
| (2,28)   | 1:49:C:ALA:H   | 1:55:C:GLY:O   | 6        | 0.33          |
| (2,28)   | 1:49:C:ALA:H   | 1:55:C:GLY:O   | 8        | 0.33          |
| (2,28)   | 1:49:C:ALA:H   | 1:55:C:GLY:O   | 9        | 0.33          |
| (1,1431) | 1:49:C:ALA:CB  | 1:51:C:LEU:CB  | 5        | 0.33          |
| (1,1421) | 1:29:C:VAL:CG2 | 1:27:C:LEU:CD1 | 8        | 0.33          |
| (1,1399) | 1:29:C:VAL:CG1 | 1:27:C:LEU:CD1 | 8        | 0.33          |
| (1,1119) | 1:43:C:THR:CA  | 1:29:C:VAL:CB  | 1        | 0.33          |
| (1,590)  | 1:62:C:LEU:CG  | 1:85:C:HIS:CB  | 10       | 0.33          |
| (1,477)  | 1:71:C:GLY:CA  | 1:82:C:ASP:CB  | 5        | 0.33          |
| (1,351)  | 1:29:C:VAL:CA  | 1:46:C:TYR:CB  | 1        | 0.33          |
| (1,245)  | 1:72:C:THR:CG2 | 1:78:C:TYR:C   | 3        | 0.33          |
| (1,78)   | 1:57:C:TRP:CB  | 1:90:C:ARG:CB  | 6        | 0.33          |
| (1,1185) | 1:69:C:ASN:CA  | 1:77:C:LYS:CB  | 2        | 0.32          |
| (1,1104) | 1:87:C:ILE:CA  | 1:84:C:GLY:CA  | 5        | 0.32          |
| (1,918)  | 1:85:C:HIS:CA  | 1:63:C:ASP:CG  | 7        | 0.32          |
| (1,637)  | 1:73:C:VAL:CG1 | 1:69:C:ASN:CB  | 5        | 0.32          |
| (1,351)  | 1:29:C:VAL:CA  | 1:46:C:TYR:CB  | 7        | 0.32          |
| (1,351)  | 1:29:C:VAL:CA  | 1:46:C:TYR:CB  | 10       | 0.32          |
| (2,62)   | 1:65:C:ALA:H   | 1:84:C:GLY:O   | 1        | 0.31          |
| (2,62)   | 1:65:C:ALA:H   | 1:84:C:GLY:O   | 8        | 0.31          |
| (2,58)   | 1:85:C:HIS:H   | 1:82:C:ASP:O   | 5        | 0.31          |
| (1,1470) | 1:89:C:VAL:CG2 | 1:36:C:ILE:CA  | 4        | 0.31          |
| (1,1144) | 1:93:C:GLN:CA  | 1:27:C:LEU:CD1 | 2        | 0.31          |
| (1,1104) | 1:87:C:ILE:CA  | 1:84:C:GLY:CA  | 2        | 0.31          |
| (1,872)  | 1:27:C:LEU:CG  | 1:92:C:SER:C   | 6        | 0.31          |
| (1,794)  | 1:76:C:ARG:CG  | 1:51:C:LEU:CA  | 2        | 0.31          |
| (1,598)  | 1:27:C:LEU:CG  | 1:95:C:GLN:CB  | 5        | 0.31          |
| (1,508)  | 1:36:C:ILE:CB  | 1:89:C:VAL:CG2 | 1        | 0.31          |
| (1,245)  | 1:72:C:THR:CG2 | 1:78:C:TYR:C   | 7        | 0.31          |
| (1,106)  | 1:40:C:HIS:C   | 1:33:C:VAL:CB  | 7        | 0.31          |
| (1,78)   | 1:57:C:TRP:CB  | 1:90:C:ARG:CB  | 2        | 0.31          |
| (2,62)   | 1:65:C:ALA:H   | 1:84:C:GLY:O   | 5        | 0.3           |
| (2,58)   | 1:85:C:HIS:H   | 1:82:C:ASP:O   | 2        | 0.3           |
| (2,28)   | 1:49:C:ALA:H   | 1:55:C:GLY:O   | 2        | 0.3           |
| (2,28)   | 1:49:C:ALA:H   | 1:55:C:GLY:O   | 5        | 0.3           |
| (1,1104) | 1:87:C:ILE:CA  | 1:84:C:GLY:CA  | 7        | 0.3           |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1104) | 1:87:C:ILE:CA  | 1:84:C:GLY:CA  | 9        | 0.3           |
| (1,637)  | 1:73:C:VAL:CG1 | 1:69:C:ASN:CB  | 10       | 0.3           |
| (1,493)  | 1:69:C:ASN:CB  | 1:77:C:LYS:CB  | 5        | 0.3           |
| (2,58)   | 1:85:C:HIS:H   | 1:82:C:ASP:O   | 7        | 0.29          |
| (2,28)   | 1:49:C:ALA:H   | 1:55:C:GLY:O   | 3        | 0.29          |
| (2,28)   | 1:49:C:ALA:H   | 1:55:C:GLY:O   | 7        | 0.29          |
| (1,1431) | 1:49:C:ALA:CB  | 1:51:C:LEU:CB  | 6        | 0.29          |
| (1,1393) | 1:89:C:VAL:CG1 | 1:62:C:LEU:CB  | 6        | 0.29          |
| (1,974)  | 1:37:C:GLY:CA  | 1:93:C:GLN:CA  | 9        | 0.29          |
| (1,689)  | 1:76:C:ARG:CG  | 1:70:C:ASP:CA  | 5        | 0.29          |
| (1,631)  | 1:63:C:ASP:CB  | 1:41:C:ARG:CD  | 8        | 0.29          |
| (1,602)  | 1:90:C:ARG:CG  | 1:58:C:VAL:CB  | 1        | 0.29          |
| (1,602)  | 1:90:C:ARG:CG  | 1:58:C:VAL:CB  | 7        | 0.29          |
| (1,405)  | 1:70:C:ASP:CA  | 1:76:C:ARG:CG  | 5        | 0.29          |
| (1,367)  | 1:52:C:PHE:CA  | 1:76:C:ARG:CB  | 1        | 0.29          |
| (1,351)  | 1:29:C:VAL:CA  | 1:46:C:TYR:CB  | 9        | 0.29          |
| (1,290)  | 1:31:C:SER:CB  | 1:43:C:THR:C   | 8        | 0.29          |
| (1,231)  | 1:29:C:VAL:CG1 | 1:47:C:VAL:C   | 2        | 0.29          |
| (1,106)  | 1:40:C:HIS:C   | 1:33:C:VAL:CB  | 3        | 0.29          |
| (2,28)   | 1:49:C:ALA:H   | 1:55:C:GLY:O   | 10       | 0.28          |
| (1,1421) | 1:29:C:VAL:CG2 | 1:27:C:LEU:CD1 | 2        | 0.28          |
| (1,1421) | 1:29:C:VAL:CG2 | 1:27:C:LEU:CD1 | 10       | 0.28          |
| (1,1144) | 1:93:C:GLN:CA  | 1:27:C:LEU:CD1 | 5        | 0.28          |
| (1,1144) | 1:93:C:GLN:CA  | 1:27:C:LEU:CD1 | 7        | 0.28          |
| (1,865)  | 1:76:C:ARG:CB  | 1:52:C:PHE:C   | 2        | 0.28          |
| (1,616)  | 1:36:C:ILE:CG1 | 1:95:C:GLN:CG  | 2        | 0.28          |
| (1,351)  | 1:29:C:VAL:CA  | 1:46:C:TYR:CB  | 6        | 0.28          |
| (1,290)  | 1:31:C:SER:CB  | 1:43:C:THR:C   | 1        | 0.28          |
| (1,290)  | 1:31:C:SER:CB  | 1:43:C:THR:C   | 6        | 0.28          |
| (1,290)  | 1:31:C:SER:CB  | 1:43:C:THR:C   | 9        | 0.28          |
| (1,159)  | 1:62:C:LEU:CA  | 1:61:C:ILE:CG2 | 8        | 0.28          |
| (1,105)  | 1:44:C:VAL:C   | 1:60:C:VAL:CB  | 6        | 0.28          |
| (1,78)   | 1:57:C:TRP:CB  | 1:90:C:ARG:CB  | 4        | 0.28          |
| (2,58)   | 1:85:C:HIS:H   | 1:82:C:ASP:O   | 8        | 0.27          |
| (2,40)   | 1:84:C:GLY:H   | 1:67:C:GLY:O   | 3        | 0.27          |
| (1,1296) | 1:88:C:PHE:CB  | 1:58:C:VAL:CG2 | 8        | 0.27          |
| (1,1190) | 1:32:C:ARG:CA  | 1:95:C:GLN:CG  | 10       | 0.27          |
| (1,901)  | 1:94:C:ILE:CD1 | 1:87:C:ILE:C   | 2        | 0.27          |
| (1,637)  | 1:73:C:VAL:CG1 | 1:69:C:ASN:CB  | 3        | 0.27          |
| (1,606)  | 1:38:C:LYS:CG  | 1:40:C:HIS:CB  | 5        | 0.27          |
| (1,493)  | 1:69:C:ASN:CB  | 1:77:C:LYS:CB  | 2        | 0.27          |
| (1,477)  | 1:71:C:GLY:CA  | 1:82:C:ASP:CB  | 4        | 0.27          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,231)  | 1:29:C:VAL:CG1 | 1:47:C:VAL:C   | 5        | 0.27          |
| (1,35)   | 1:73:C:VAL:CA  | 1:71:C:GLY:CA  | 1        | 0.27          |
| (1,14)   | 1:46:C:TYR:CB  | 1:77:C:LYS:CB  | 1        | 0.27          |
| (2,62)   | 1:65:C:ALA:H   | 1:84:C:GLY:O   | 3        | 0.26          |
| (2,62)   | 1:65:C:ALA:H   | 1:84:C:GLY:O   | 10       | 0.26          |
| (2,58)   | 1:85:C:HIS:H   | 1:82:C:ASP:O   | 4        | 0.26          |
| (2,28)   | 1:49:C:ALA:H   | 1:55:C:GLY:O   | 1        | 0.26          |
| (1,1421) | 1:29:C:VAL:CG2 | 1:27:C:LEU:CD1 | 5        | 0.26          |
| (1,1293) | 1:88:C:PHE:CB  | 1:90:C:ARG:CB  | 8        | 0.26          |
| (1,1293) | 1:88:C:PHE:CB  | 1:90:C:ARG:CB  | 9        | 0.26          |
| (1,1144) | 1:93:C:GLN:CA  | 1:27:C:LEU:CD1 | 8        | 0.26          |
| (1,974)  | 1:37:C:GLY:CA  | 1:93:C:GLN:CA  | 8        | 0.26          |
| (1,874)  | 1:62:C:LEU:CG  | 1:67:C:GLY:C   | 1        | 0.26          |
| (1,852)  | 1:56:C:LYS:CB  | 1:53:C:ALA:C   | 10       | 0.26          |
| (1,697)  | 1:74:C:GLN:CB  | 1:77:C:LYS:CA  | 9        | 0.26          |
| (1,617)  | 1:76:C:ARG:CG  | 1:52:C:PHE:CB  | 4        | 0.26          |
| (1,606)  | 1:38:C:LYS:CG  | 1:40:C:HIS:CB  | 8        | 0.26          |
| (1,508)  | 1:36:C:ILE:CB  | 1:89:C:VAL:CG2 | 2        | 0.26          |
| (1,477)  | 1:71:C:GLY:CA  | 1:82:C:ASP:CB  | 7        | 0.26          |
| (1,159)  | 1:62:C:LEU:CA  | 1:61:C:ILE:CG2 | 2        | 0.26          |
| (1,105)  | 1:44:C:VAL:C   | 1:60:C:VAL:CB  | 8        | 0.26          |
| (1,67)   | 1:68:C:LYS:CG  | 1:83:C:GLU:CB  | 1        | 0.26          |
| (1,35)   | 1:73:C:VAL:CA  | 1:71:C:GLY:CA  | 4        | 0.26          |
| (1,1393) | 1:89:C:VAL:CG1 | 1:62:C:LEU:CB  | 5        | 0.25          |
| (1,1314) | 1:60:C:VAL:CB  | 1:43:C:THR:CG2 | 1        | 0.25          |
| (1,1104) | 1:87:C:ILE:CA  | 1:84:C:GLY:CA  | 4        | 0.25          |
| (1,1104) | 1:87:C:ILE:CA  | 1:84:C:GLY:CA  | 6        | 0.25          |
| (1,1104) | 1:87:C:ILE:CA  | 1:84:C:GLY:CA  | 10       | 0.25          |
| (1,872)  | 1:27:C:LEU:CG  | 1:92:C:SER:C   | 10       | 0.25          |
| (1,733)  | 1:89:C:VAL:CG1 | 1:92:C:SER:CA  | 10       | 0.25          |
| (1,689)  | 1:76:C:ARG:CG  | 1:70:C:ASP:CA  | 1        | 0.25          |
| (1,606)  | 1:38:C:LYS:CG  | 1:40:C:HIS:CB  | 6        | 0.25          |
| (1,602)  | 1:90:C:ARG:CG  | 1:58:C:VAL:CB  | 8        | 0.25          |
| (1,508)  | 1:36:C:ILE:CB  | 1:89:C:VAL:CG2 | 6        | 0.25          |
| (1,493)  | 1:69:C:ASN:CB  | 1:77:C:LYS:CB  | 1        | 0.25          |
| (1,493)  | 1:69:C:ASN:CB  | 1:77:C:LYS:CB  | 4        | 0.25          |
| (1,405)  | 1:70:C:ASP:CA  | 1:76:C:ARG:CG  | 1        | 0.25          |
| (1,231)  | 1:29:C:VAL:CG1 | 1:47:C:VAL:C   | 9        | 0.25          |
| (1,78)   | 1:57:C:TRP:CB  | 1:90:C:ARG:CB  | 3        | 0.25          |
| (1,52)   | 1:29:C:VAL:CG2 | 1:43:C:THR:CB  | 6        | 0.25          |
| (2,58)   | 1:85:C:HIS:H   | 1:82:C:ASP:O   | 1        | 0.24          |
| (2,14)   | 1:61:C:ILE:H   | 1:43:C:THR:O   | 6        | 0.24          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (2,14)   | 1:61:C:ILE:H   | 1:43:C:THR:O   | 7        | 0.24          |
| (1,1393) | 1:89:C:VAL:CG1 | 1:62:C:LEU:CB  | 2        | 0.24          |
| (1,1296) | 1:88:C:PHE:CB  | 1:58:C:VAL:CG2 | 2        | 0.24          |
| (1,1280) | 1:30:C:GLY:CA  | 1:27:C:LEU:CG  | 6        | 0.24          |
| (1,1119) | 1:43:C:THR:CA  | 1:29:C:VAL:CB  | 8        | 0.24          |
| (1,797)  | 1:62:C:LEU:CG  | 1:66:C:LYS:CA  | 3        | 0.24          |
| (1,616)  | 1:36:C:ILE:CG1 | 1:95:C:GLN:CG  | 10       | 0.24          |
| (1,558)  | 1:76:C:ARG:CG  | 1:74:C:GLN:CB  | 9        | 0.24          |
| (1,493)  | 1:69:C:ASN:CB  | 1:77:C:LYS:CB  | 7        | 0.24          |
| (1,477)  | 1:71:C:GLY:CA  | 1:82:C:ASP:CB  | 3        | 0.24          |
| (1,72)   | 1:61:C:ILE:CG1 | 1:60:C:VAL:CB  | 7        | 0.24          |
| (2,14)   | 1:61:C:ILE:H   | 1:43:C:THR:O   | 8        | 0.23          |
| (1,1470) | 1:89:C:VAL:CG2 | 1:36:C:ILE:CA  | 3        | 0.23          |
| (1,1470) | 1:89:C:VAL:CG2 | 1:36:C:ILE:CA  | 8        | 0.23          |
| (1,1433) | 1:72:C:THR:CG2 | 1:73:C:VAL:CG1 | 5        | 0.23          |
| (1,1419) | 1:62:C:LEU:CD1 | 1:67:C:GLY:CA  | 1        | 0.23          |
| (1,1293) | 1:88:C:PHE:CB  | 1:90:C:ARG:CB  | 6        | 0.23          |
| (1,1119) | 1:43:C:THR:CA  | 1:29:C:VAL:CB  | 3        | 0.23          |
| (1,1119) | 1:43:C:THR:CA  | 1:29:C:VAL:CB  | 5        | 0.23          |
| (1,974)  | 1:37:C:GLY:CA  | 1:93:C:GLN:CA  | 10       | 0.23          |
| (1,637)  | 1:73:C:VAL:CG1 | 1:69:C:ASN:CB  | 4        | 0.23          |
| (1,589)  | 1:58:C:VAL:CG1 | 1:57:C:TRP:CB  | 10       | 0.23          |
| (1,500)  | 1:79:C:PHE:CB  | 1:77:C:LYS:CB  | 2        | 0.23          |
| (1,500)  | 1:79:C:PHE:CB  | 1:77:C:LYS:CB  | 8        | 0.23          |
| (1,231)  | 1:29:C:VAL:CG1 | 1:47:C:VAL:C   | 3        | 0.23          |
| (1,159)  | 1:62:C:LEU:CA  | 1:61:C:ILE:CG2 | 4        | 0.23          |
| (1,105)  | 1:44:C:VAL:C   | 1:60:C:VAL:CB  | 2        | 0.23          |
| (1,105)  | 1:44:C:VAL:C   | 1:60:C:VAL:CB  | 4        | 0.23          |
| (1,61)   | 1:32:C:ARG:CB  | 1:41:C:ARG:CB  | 6        | 0.23          |
| (1,35)   | 1:73:C:VAL:CA  | 1:71:C:GLY:CA  | 9        | 0.23          |
| (2,62)   | 1:65:C:ALA:H   | 1:84:C:GLY:O   | 4        | 0.22          |
| (2,34)   | 1:86:C:GLY:H   | 1:60:C:VAL:O   | 4        | 0.22          |
| (2,13)   | 1:61:C:ILE:N   | 1:43:C:THR:O   | 6        | 0.22          |
| (2,13)   | 1:61:C:ILE:N   | 1:43:C:THR:O   | 7        | 0.22          |
| (2,13)   | 1:61:C:ILE:N   | 1:43:C:THR:O   | 8        | 0.22          |
| (1,1466) | 1:61:C:ILE:CB  | 1:41:C:ARG:CA  | 6        | 0.22          |
| (1,1433) | 1:72:C:THR:CG2 | 1:73:C:VAL:CG1 | 6        | 0.22          |
| (1,1432) | 1:72:C:THR:CG2 | 1:70:C:ASP:CB  | 9        | 0.22          |
| (1,1314) | 1:60:C:VAL:CB  | 1:43:C:THR:CG2 | 6        | 0.22          |
| (1,1241) | 1:52:C:PHE:CA  | 1:49:C:ALA:CA  | 3        | 0.22          |
| (1,1240) | 1:52:C:PHE:CA  | 1:49:C:ALA:CA  | 3        | 0.22          |
| (1,1185) | 1:69:C:ASN:CA  | 1:77:C:LYS:CB  | 3        | 0.22          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1185) | 1:69:C:ASN:CA  | 1:77:C:LYS:CB  | 5        | 0.22          |
| (1,918)  | 1:85:C:HIS:CA  | 1:63:C:ASP:CG  | 6        | 0.22          |
| (1,913)  | 1:83:C:GLU:CA  | 1:86:C:GLY:C   | 5        | 0.22          |
| (1,872)  | 1:27:C:LEU:CG  | 1:92:C:SER:C   | 9        | 0.22          |
| (1,689)  | 1:76:C:ARG:CG  | 1:70:C:ASP:CA  | 4        | 0.22          |
| (1,598)  | 1:27:C:LEU:CG  | 1:95:C:GLN:CB  | 2        | 0.22          |
| (1,589)  | 1:58:C:VAL:CG1 | 1:57:C:TRP:CB  | 8        | 0.22          |
| (1,531)  | 1:32:C:ARG:CB  | 1:27:C:LEU:CD1 | 4        | 0.22          |
| (1,500)  | 1:79:C:PHE:CB  | 1:77:C:LYS:CB  | 6        | 0.22          |
| (1,493)  | 1:69:C:ASN:CB  | 1:77:C:LYS:CB  | 6        | 0.22          |
| (1,444)  | 1:36:C:ILE:CA  | 1:89:C:VAL:CG1 | 3        | 0.22          |
| (1,444)  | 1:36:C:ILE:CA  | 1:89:C:VAL:CG1 | 6        | 0.22          |
| (1,405)  | 1:70:C:ASP:CA  | 1:76:C:ARG:CG  | 4        | 0.22          |
| (1,290)  | 1:31:C:SER:CB  | 1:43:C:THR:C   | 4        | 0.22          |
| (1,54)   | 1:91:C:GLN:CG  | 1:90:C:ARG:CG  | 9        | 0.22          |
| (1,14)   | 1:46:C:TYR:CB  | 1:77:C:LYS:CB  | 6        | 0.22          |
| (2,58)   | 1:85:C:HIS:H   | 1:82:C:ASP:O   | 6        | 0.21          |
| (1,1466) | 1:61:C:ILE:CB  | 1:41:C:ARG:CA  | 5        | 0.21          |
| (1,1433) | 1:72:C:THR:CG2 | 1:73:C:VAL:CG1 | 2        | 0.21          |
| (1,1433) | 1:72:C:THR:CG2 | 1:73:C:VAL:CG1 | 8        | 0.21          |
| (1,1432) | 1:72:C:THR:CG2 | 1:70:C:ASP:CB  | 8        | 0.21          |
| (1,1426) | 1:29:C:VAL:CG2 | 1:27:C:LEU:CG  | 9        | 0.21          |
| (1,1421) | 1:29:C:VAL:CG2 | 1:27:C:LEU:CD1 | 9        | 0.21          |
| (1,1293) | 1:88:C:PHE:CB  | 1:90:C:ARG:CB  | 1        | 0.21          |
| (1,1119) | 1:43:C:THR:CA  | 1:29:C:VAL:CB  | 6        | 0.21          |
| (1,913)  | 1:83:C:GLU:CA  | 1:86:C:GLY:C   | 2        | 0.21          |
| (1,646)  | 1:58:C:VAL:CG2 | 1:46:C:TYR:CB  | 5        | 0.21          |
| (1,637)  | 1:73:C:VAL:CG1 | 1:69:C:ASN:CB  | 8        | 0.21          |
| (1,606)  | 1:38:C:LYS:CG  | 1:40:C:HIS:CB  | 7        | 0.21          |
| (1,602)  | 1:90:C:ARG:CG  | 1:58:C:VAL:CB  | 4        | 0.21          |
| (1,493)  | 1:69:C:ASN:CB  | 1:77:C:LYS:CB  | 8        | 0.21          |
| (1,477)  | 1:71:C:GLY:CA  | 1:82:C:ASP:CB  | 6        | 0.21          |
| (1,231)  | 1:29:C:VAL:CG1 | 1:47:C:VAL:C   | 8        | 0.21          |
| (1,137)  | 1:32:C:ARG:CG  | 1:31:C:SER:CB  | 5        | 0.21          |
| (1,110)  | 1:70:C:ASP:CA  | 1:68:C:LYS:CG  | 8        | 0.21          |
| (1,61)   | 1:32:C:ARG:CB  | 1:41:C:ARG:CB  | 8        | 0.21          |
| (1,35)   | 1:73:C:VAL:CA  | 1:71:C:GLY:CA  | 3        | 0.21          |
| (1,35)   | 1:73:C:VAL:CA  | 1:71:C:GLY:CA  | 7        | 0.21          |
| (1,35)   | 1:73:C:VAL:CA  | 1:71:C:GLY:CA  | 10       | 0.21          |
| (2,40)   | 1:84:C:GLY:H   | 1:67:C:GLY:O   | 8        | 0.2           |
| (2,14)   | 1:61:C:ILE:H   | 1:43:C:THR:O   | 2        | 0.2           |
| (1,1466) | 1:61:C:ILE:CB  | 1:41:C:ARG:CA  | 8        | 0.2           |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1432) | 1:72:C:THR:CG2 | 1:70:C:ASP:CB  | 1        | 0.2           |
| (1,1432) | 1:72:C:THR:CG2 | 1:70:C:ASP:CB  | 10       | 0.2           |
| (1,1314) | 1:60:C:VAL:CB  | 1:43:C:THR:CG2 | 8        | 0.2           |
| (1,1296) | 1:88:C:PHE:CB  | 1:58:C:VAL:CG2 | 4        | 0.2           |
| (1,1291) | 1:90:C:ARG:CD  | 1:94:C:ILE:CB  | 1        | 0.2           |
| (1,718)  | 1:72:C:THR:CG2 | 1:78:C:TYR:CA  | 5        | 0.2           |
| (1,589)  | 1:58:C:VAL:CG1 | 1:57:C:TRP:CB  | 6        | 0.2           |
| (1,589)  | 1:58:C:VAL:CG1 | 1:57:C:TRP:CB  | 9        | 0.2           |
| (1,531)  | 1:32:C:ARG:CB  | 1:27:C:LEU:CD1 | 3        | 0.2           |
| (1,531)  | 1:32:C:ARG:CB  | 1:27:C:LEU:CD1 | 6        | 0.2           |
| (1,480)  | 1:94:C:ILE:CB  | 1:90:C:ARG:CD  | 1        | 0.2           |
| (1,231)  | 1:29:C:VAL:CG1 | 1:47:C:VAL:C   | 6        | 0.2           |
| (1,110)  | 1:70:C:ASP:CA  | 1:68:C:LYS:CG  | 9        | 0.2           |
| (1,72)   | 1:61:C:ILE:CG1 | 1:60:C:VAL:CB  | 5        | 0.2           |
| (1,14)   | 1:46:C:TYR:CB  | 1:77:C:LYS:CB  | 4        | 0.2           |
| (2,62)   | 1:65:C:ALA:H   | 1:84:C:GLY:O   | 6        | 0.19          |
| (2,62)   | 1:65:C:ALA:H   | 1:84:C:GLY:O   | 7        | 0.19          |
| (2,58)   | 1:85:C:HIS:H   | 1:82:C:ASP:O   | 3        | 0.19          |
| (2,58)   | 1:85:C:HIS:H   | 1:82:C:ASP:O   | 9        | 0.19          |
| (2,40)   | 1:84:C:GLY:H   | 1:67:C:GLY:O   | 7        | 0.19          |
| (2,40)   | 1:84:C:GLY:H   | 1:67:C:GLY:O   | 9        | 0.19          |
| (2,12)   | 1:33:C:VAL:H   | 1:42:C:GLY:O   | 7        | 0.19          |
| (1,1433) | 1:72:C:THR:CG2 | 1:73:C:VAL:CG1 | 3        | 0.19          |
| (1,1432) | 1:72:C:THR:CG2 | 1:70:C:ASP:CB  | 2        | 0.19          |
| (1,1432) | 1:72:C:THR:CG2 | 1:70:C:ASP:CB  | 3        | 0.19          |
| (1,1432) | 1:72:C:THR:CG2 | 1:70:C:ASP:CB  | 5        | 0.19          |
| (1,1369) | 1:32:C:ARG:CG  | 1:34:C:GLU:CB  | 5        | 0.19          |
| (1,974)  | 1:37:C:GLY:CA  | 1:93:C:GLN:CA  | 1        | 0.19          |
| (1,843)  | 1:73:C:VAL:CB  | 1:52:C:PHE:C   | 9        | 0.19          |
| (1,637)  | 1:73:C:VAL:CG1 | 1:69:C:ASN:CB  | 2        | 0.19          |
| (1,637)  | 1:73:C:VAL:CG1 | 1:69:C:ASN:CB  | 6        | 0.19          |
| (1,531)  | 1:32:C:ARG:CB  | 1:27:C:LEU:CD1 | 2        | 0.19          |
| (1,508)  | 1:36:C:ILE:CB  | 1:89:C:VAL:CG2 | 3        | 0.19          |
| (1,444)  | 1:36:C:ILE:CA  | 1:89:C:VAL:CG1 | 9        | 0.19          |
| (1,110)  | 1:70:C:ASP:CA  | 1:68:C:LYS:CG  | 3        | 0.19          |
| (1,81)   | 1:34:C:GLU:CB  | 1:40:C:HIS:C   | 4        | 0.19          |
| (1,72)   | 1:61:C:ILE:CG1 | 1:60:C:VAL:CB  | 9        | 0.19          |
| (1,54)   | 1:91:C:GLN:CG  | 1:90:C:ARG:CG  | 1        | 0.19          |
| (1,45)   | 1:62:C:LEU:CA  | 1:60:C:VAL:CB  | 7        | 0.19          |
| (1,35)   | 1:73:C:VAL:CA  | 1:71:C:GLY:CA  | 2        | 0.19          |
| (1,35)   | 1:73:C:VAL:CA  | 1:71:C:GLY:CA  | 8        | 0.19          |
| (2,14)   | 1:61:C:ILE:H   | 1:43:C:THR:O   | 10       | 0.18          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (2,13)   | 1:61:C:ILE:N   | 1:43:C:THR:O   | 2        | 0.18          |
| (1,1470) | 1:89:C:VAL:CG2 | 1:36:C:ILE:CA  | 1        | 0.18          |
| (1,1470) | 1:89:C:VAL:CG2 | 1:36:C:ILE:CA  | 9        | 0.18          |
| (1,1433) | 1:72:C:THR:CG2 | 1:73:C:VAL:CG1 | 7        | 0.18          |
| (1,1432) | 1:72:C:THR:CG2 | 1:70:C:ASP:CB  | 4        | 0.18          |
| (1,1426) | 1:29:C:VAL:CG2 | 1:27:C:LEU:CG  | 6        | 0.18          |
| (1,1369) | 1:32:C:ARG:CG  | 1:34:C:GLU:CB  | 10       | 0.18          |
| (1,1354) | 1:83:C:GLU:CB  | 1:68:C:LYS:CD  | 10       | 0.18          |
| (1,1241) | 1:52:C:PHE:CA  | 1:49:C:ALA:CA  | 6        | 0.18          |
| (1,1240) | 1:52:C:PHE:CA  | 1:49:C:ALA:CA  | 6        | 0.18          |
| (1,918)  | 1:85:C:HIS:CA  | 1:63:C:ASP:CG  | 3        | 0.18          |
| (1,913)  | 1:83:C:GLU:CA  | 1:86:C:GLY:C   | 7        | 0.18          |
| (1,589)  | 1:58:C:VAL:CG1 | 1:57:C:TRP:CB  | 3        | 0.18          |
| (1,531)  | 1:32:C:ARG:CB  | 1:27:C:LEU:CD1 | 10       | 0.18          |
| (1,500)  | 1:79:C:PHE:CB  | 1:77:C:LYS:CB  | 10       | 0.18          |
| (1,493)  | 1:69:C:ASN:CB  | 1:77:C:LYS:CB  | 3        | 0.18          |
| (1,493)  | 1:69:C:ASN:CB  | 1:77:C:LYS:CB  | 10       | 0.18          |
| (1,351)  | 1:29:C:VAL:CA  | 1:46:C:TYR:CB  | 3        | 0.18          |
| (2,40)   | 1:84:C:GLY:H   | 1:67:C:GLY:O   | 4        | 0.17          |
| (2,22)   | 1:53:C:ALA:H   | 1:50:C:THR:O   | 8        | 0.17          |
| (1,1470) | 1:89:C:VAL:CG2 | 1:36:C:ILE:CA  | 7        | 0.17          |
| (1,1433) | 1:72:C:THR:CG2 | 1:73:C:VAL:CG1 | 9        | 0.17          |
| (1,1433) | 1:72:C:THR:CG2 | 1:73:C:VAL:CG1 | 10       | 0.17          |
| (1,1432) | 1:72:C:THR:CG2 | 1:70:C:ASP:CB  | 6        | 0.17          |
| (1,1393) | 1:89:C:VAL:CG1 | 1:62:C:LEU:CB  | 3        | 0.17          |
| (1,1355) | 1:85:C:HIS:CB  | 1:71:C:GLY:CA  | 4        | 0.17          |
| (1,1338) | 1:93:C:GLN:CB  | 1:58:C:VAL:CG2 | 10       | 0.17          |
| (1,1296) | 1:88:C:PHE:CB  | 1:58:C:VAL:CG2 | 10       | 0.17          |
| (1,1280) | 1:30:C:GLY:CA  | 1:27:C:LEU:CG  | 10       | 0.17          |
| (1,1274) | 1:37:C:GLY:CA  | 1:93:C:GLN:CG  | 10       | 0.17          |
| (1,1185) | 1:69:C:ASN:CA  | 1:77:C:LYS:CB  | 4        | 0.17          |
| (1,1185) | 1:69:C:ASN:CA  | 1:77:C:LYS:CB  | 6        | 0.17          |
| (1,1158) | 1:79:C:PHE:CA  | 1:72:C:THR:CG2 | 8        | 0.17          |
| (1,1083) | 1:80:C:THR:CA  | 1:61:C:ILE:CB  | 9        | 0.17          |
| (1,1063) | 1:89:C:VAL:CG2 | 1:34:C:GLU:CA  | 3        | 0.17          |
| (1,974)  | 1:37:C:GLY:CA  | 1:93:C:GLN:CA  | 7        | 0.17          |
| (1,913)  | 1:83:C:GLU:CA  | 1:86:C:GLY:C   | 8        | 0.17          |
| (1,913)  | 1:83:C:GLU:CA  | 1:86:C:GLY:C   | 9        | 0.17          |
| (1,794)  | 1:76:C:ARG:CG  | 1:51:C:LEU:CA  | 1        | 0.17          |
| (1,723)  | 1:72:C:THR:CG2 | 1:79:C:PHE:CA  | 8        | 0.17          |
| (1,718)  | 1:72:C:THR:CG2 | 1:78:C:TYR:CA  | 9        | 0.17          |
| (1,637)  | 1:73:C:VAL:CG1 | 1:69:C:ASN:CB  | 7        | 0.17          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,589)  | 1:58:C:VAL:CG1 | 1:57:C:TRP:CB  | 4        | 0.17          |
| (1,531)  | 1:32:C:ARG:CB  | 1:27:C:LEU:CD1 | 8        | 0.17          |
| (1,500)  | 1:79:C:PHE:CB  | 1:77:C:LYS:CB  | 5        | 0.17          |
| (1,500)  | 1:79:C:PHE:CB  | 1:77:C:LYS:CB  | 9        | 0.17          |
| (1,351)  | 1:29:C:VAL:CA  | 1:46:C:TYR:CB  | 8        | 0.17          |
| (1,137)  | 1:32:C:ARG:CG  | 1:31:C:SER:CB  | 10       | 0.17          |
| (1,89)   | 1:55:C:GLY:C   | 1:50:C:THR:CA  | 8        | 0.17          |
| (1,60)   | 1:32:C:ARG:CB  | 1:34:C:GLU:CB  | 4        | 0.17          |
| (1,59)   | 1:32:C:ARG:CB  | 1:34:C:GLU:CB  | 4        | 0.17          |
| (1,35)   | 1:73:C:VAL:CA  | 1:71:C:GLY:CA  | 6        | 0.17          |
| (1,14)   | 1:46:C:TYR:CB  | 1:77:C:LYS:CB  | 3        | 0.17          |
| (1,1)    | 1:26:C:PRO:CG  | 1:28:C:ARG:C   | 9        | 0.17          |
| (2,72)   | 1:94:C:ILE:H   | 1:90:C:ARG:O   | 10       | 0.16          |
| (2,40)   | 1:84:C:GLY:H   | 1:67:C:GLY:O   | 5        | 0.16          |
| (2,14)   | 1:61:C:ILE:H   | 1:43:C:THR:O   | 4        | 0.16          |
| (2,13)   | 1:61:C:ILE:N   | 1:43:C:THR:O   | 10       | 0.16          |
| (1,1432) | 1:72:C:THR:CG2 | 1:70:C:ASP:CB  | 7        | 0.16          |
| (1,1426) | 1:29:C:VAL:CG2 | 1:27:C:LEU:CG  | 10       | 0.16          |
| (1,1400) | 1:33:C:VAL:CG1 | 1:95:C:GLN:CB  | 7        | 0.16          |
| (1,1400) | 1:33:C:VAL:CG1 | 1:95:C:GLN:CB  | 9        | 0.16          |
| (1,1314) | 1:60:C:VAL:CB  | 1:43:C:THR:CG2 | 9        | 0.16          |
| (1,1296) | 1:88:C:PHE:CB  | 1:58:C:VAL:CG2 | 5        | 0.16          |
| (1,1293) | 1:88:C:PHE:CB  | 1:90:C:ARG:CB  | 5        | 0.16          |
| (1,1293) | 1:88:C:PHE:CB  | 1:90:C:ARG:CB  | 7        | 0.16          |
| (1,1291) | 1:90:C:ARG:CD  | 1:94:C:ILE:CB  | 4        | 0.16          |
| (1,1291) | 1:90:C:ARG:CD  | 1:94:C:ILE:CB  | 8        | 0.16          |
| (1,1158) | 1:79:C:PHE:CA  | 1:72:C:THR:CG2 | 6        | 0.16          |
| (1,843)  | 1:73:C:VAL:CB  | 1:52:C:PHE:C   | 3        | 0.16          |
| (1,723)  | 1:72:C:THR:CG2 | 1:79:C:PHE:CA  | 6        | 0.16          |
| (1,718)  | 1:72:C:THR:CG2 | 1:78:C:TYR:CA  | 1        | 0.16          |
| (1,718)  | 1:72:C:THR:CG2 | 1:78:C:TYR:CA  | 8        | 0.16          |
| (1,602)  | 1:90:C:ARG:CG  | 1:58:C:VAL:CB  | 5        | 0.16          |
| (1,590)  | 1:62:C:LEU:CG  | 1:85:C:HIS:CB  | 6        | 0.16          |
| (1,508)  | 1:36:C:ILE:CB  | 1:89:C:VAL:CG2 | 4        | 0.16          |
| (1,500)  | 1:79:C:PHE:CB  | 1:77:C:LYS:CB  | 1        | 0.16          |
| (1,493)  | 1:69:C:ASN:CB  | 1:77:C:LYS:CB  | 9        | 0.16          |
| (1,480)  | 1:94:C:ILE:CB  | 1:90:C:ARG:CD  | 4        | 0.16          |
| (1,480)  | 1:94:C:ILE:CB  | 1:90:C:ARG:CD  | 8        | 0.16          |
| (1,290)  | 1:31:C:SER:CB  | 1:43:C:THR:C   | 7        | 0.16          |
| (1,290)  | 1:31:C:SER:CB  | 1:43:C:THR:C   | 10       | 0.16          |
| (1,110)  | 1:70:C:ASP:CA  | 1:68:C:LYS:CG  | 6        | 0.16          |
| (1,110)  | 1:70:C:ASP:CA  | 1:68:C:LYS:CG  | 7        | 0.16          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,89)   | 1:55:C:GLY:C   | 1:50:C:THR:CA  | 2        | 0.16          |
| (1,14)   | 1:46:C:TYR:CB  | 1:77:C:LYS:CB  | 5        | 0.16          |
| (1,14)   | 1:46:C:TYR:CB  | 1:77:C:LYS:CB  | 9        | 0.16          |
| (2,40)   | 1:84:C:GLY:H   | 1:67:C:GLY:O   | 2        | 0.15          |
| (2,40)   | 1:84:C:GLY:H   | 1:67:C:GLY:O   | 6        | 0.15          |
| (1,1433) | 1:72:C:THR:CG2 | 1:73:C:VAL:CG1 | 4        | 0.15          |
| (1,1431) | 1:49:C:ALA:CB  | 1:51:C:LEU:CB  | 3        | 0.15          |
| (1,1393) | 1:89:C:VAL:CG1 | 1:62:C:LEU:CB  | 4        | 0.15          |
| (1,1355) | 1:85:C:HIS:CB  | 1:71:C:GLY:CA  | 9        | 0.15          |
| (1,1296) | 1:88:C:PHE:CB  | 1:58:C:VAL:CG2 | 1        | 0.15          |
| (1,1296) | 1:88:C:PHE:CB  | 1:58:C:VAL:CG2 | 9        | 0.15          |
| (1,1291) | 1:90:C:ARG:CD  | 1:94:C:ILE:CB  | 3        | 0.15          |
| (1,1185) | 1:69:C:ASN:CA  | 1:77:C:LYS:CB  | 1        | 0.15          |
| (1,718)  | 1:72:C:THR:CG2 | 1:78:C:TYR:CA  | 4        | 0.15          |
| (1,718)  | 1:72:C:THR:CG2 | 1:78:C:TYR:CA  | 10       | 0.15          |
| (1,672)  | 1:34:C:GLU:CB  | 1:40:C:HIS:CA  | 5        | 0.15          |
| (1,500)  | 1:79:C:PHE:CB  | 1:77:C:LYS:CB  | 3        | 0.15          |
| (1,500)  | 1:79:C:PHE:CB  | 1:77:C:LYS:CB  | 7        | 0.15          |
| (1,480)  | 1:94:C:ILE:CB  | 1:90:C:ARG:CD  | 3        | 0.15          |
| (1,367)  | 1:52:C:PHE:CA  | 1:76:C:ARG:CB  | 10       | 0.15          |
| (1,290)  | 1:31:C:SER:CB  | 1:43:C:THR:C   | 2        | 0.15          |
| (1,290)  | 1:31:C:SER:CB  | 1:43:C:THR:C   | 5        | 0.15          |
| (1,231)  | 1:29:C:VAL:CG1 | 1:47:C:VAL:C   | 1        | 0.15          |
| (2,22)   | 1:53:C:ALA:H   | 1:50:C:THR:O   | 4        | 0.14          |
| (2,18)   | 1:59:C:GLY:H   | 1:46:C:TYR:O   | 5        | 0.14          |
| (1,1470) | 1:89:C:VAL:CG2 | 1:36:C:ILE:CA  | 6        | 0.14          |
| (1,1355) | 1:85:C:HIS:CB  | 1:71:C:GLY:CA  | 8        | 0.14          |
| (1,1293) | 1:88:C:PHE:CB  | 1:90:C:ARG:CB  | 2        | 0.14          |
| (1,1291) | 1:90:C:ARG:CD  | 1:94:C:ILE:CB  | 7        | 0.14          |
| (1,1241) | 1:52:C:PHE:CA  | 1:49:C:ALA:CA  | 7        | 0.14          |
| (1,1241) | 1:52:C:PHE:CA  | 1:49:C:ALA:CA  | 9        | 0.14          |
| (1,1241) | 1:52:C:PHE:CA  | 1:49:C:ALA:CA  | 10       | 0.14          |
| (1,1240) | 1:52:C:PHE:CA  | 1:49:C:ALA:CA  | 7        | 0.14          |
| (1,1240) | 1:52:C:PHE:CA  | 1:49:C:ALA:CA  | 9        | 0.14          |
| (1,1240) | 1:52:C:PHE:CA  | 1:49:C:ALA:CA  | 10       | 0.14          |
| (1,1185) | 1:69:C:ASN:CA  | 1:77:C:LYS:CB  | 7        | 0.14          |
| (1,1185) | 1:69:C:ASN:CA  | 1:77:C:LYS:CB  | 8        | 0.14          |
| (1,1104) | 1:87:C:ILE:CA  | 1:84:C:GLY:CA  | 3        | 0.14          |
| (1,1083) | 1:80:C:THR:CA  | 1:61:C:ILE:CB  | 1        | 0.14          |
| (1,913)  | 1:83:C:GLU:CA  | 1:86:C:GLY:C   | 6        | 0.14          |
| (1,718)  | 1:72:C:THR:CG2 | 1:78:C:TYR:CA  | 2        | 0.14          |
| (1,618)  | 1:61:C:ILE:CG1 | 1:60:C:VAL:CB  | 7        | 0.14          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,589)  | 1:58:C:VAL:CG1 | 1:57:C:TRP:CB  | 1        | 0.14          |
| (1,480)  | 1:94:C:ILE:CB  | 1:90:C:ARG:CD  | 7        | 0.14          |
| (1,60)   | 1:32:C:ARG:CB  | 1:34:C:GLU:CB  | 5        | 0.14          |
| (1,59)   | 1:32:C:ARG:CB  | 1:34:C:GLU:CB  | 5        | 0.14          |
| (1,35)   | 1:73:C:VAL:CA  | 1:71:C:GLY:CA  | 5        | 0.14          |
| (2,40)   | 1:84:C:GLY:H   | 1:67:C:GLY:O   | 1        | 0.13          |
| (2,22)   | 1:53:C:ALA:H   | 1:50:C:THR:O   | 2        | 0.13          |
| (2,22)   | 1:53:C:ALA:H   | 1:50:C:THR:O   | 6        | 0.13          |
| (1,1355) | 1:85:C:HIS:CB  | 1:71:C:GLY:CA  | 6        | 0.13          |
| (1,1296) | 1:88:C:PHE:CB  | 1:58:C:VAL:CG2 | 7        | 0.13          |
| (1,1291) | 1:90:C:ARG:CD  | 1:94:C:ILE:CB  | 2        | 0.13          |
| (1,1291) | 1:90:C:ARG:CD  | 1:94:C:ILE:CB  | 6        | 0.13          |
| (1,1241) | 1:52:C:PHE:CA  | 1:49:C:ALA:CA  | 5        | 0.13          |
| (1,1240) | 1:52:C:PHE:CA  | 1:49:C:ALA:CA  | 5        | 0.13          |
| (1,1158) | 1:79:C:PHE:CA  | 1:72:C:THR:CG2 | 2        | 0.13          |
| (1,1158) | 1:79:C:PHE:CA  | 1:72:C:THR:CG2 | 5        | 0.13          |
| (1,1158) | 1:79:C:PHE:CA  | 1:72:C:THR:CG2 | 9        | 0.13          |
| (1,1063) | 1:89:C:VAL:CG2 | 1:34:C:GLU:CA  | 6        | 0.13          |
| (1,1063) | 1:89:C:VAL:CG2 | 1:34:C:GLU:CA  | 8        | 0.13          |
| (1,918)  | 1:85:C:HIS:CA  | 1:63:C:ASP:CG  | 4        | 0.13          |
| (1,870)  | 1:68:C:LYS:CD  | 1:84:C:GLY:C   | 10       | 0.13          |
| (1,723)  | 1:72:C:THR:CG2 | 1:79:C:PHE:CA  | 2        | 0.13          |
| (1,723)  | 1:72:C:THR:CG2 | 1:79:C:PHE:CA  | 5        | 0.13          |
| (1,723)  | 1:72:C:THR:CG2 | 1:79:C:PHE:CA  | 9        | 0.13          |
| (1,718)  | 1:72:C:THR:CG2 | 1:78:C:TYR:CA  | 6        | 0.13          |
| (1,702)  | 1:89:C:VAL:CG1 | 1:90:C:ARG:CA  | 9        | 0.13          |
| (1,601)  | 1:62:C:LEU:CG  | 1:66:C:LYS:CB  | 8        | 0.13          |
| (1,590)  | 1:62:C:LEU:CG  | 1:85:C:HIS:CB  | 8        | 0.13          |
| (1,480)  | 1:94:C:ILE:CB  | 1:90:C:ARG:CD  | 2        | 0.13          |
| (1,480)  | 1:94:C:ILE:CB  | 1:90:C:ARG:CD  | 6        | 0.13          |
| (1,477)  | 1:71:C:GLY:CA  | 1:82:C:ASP:CB  | 1        | 0.13          |
| (1,444)  | 1:36:C:ILE:CA  | 1:89:C:VAL:CG1 | 1        | 0.13          |
| (1,144)  | 1:70:C:ASP:CA  | 1:68:C:LYS:CD  | 2        | 0.13          |
| (1,72)   | 1:61:C:ILE:CG1 | 1:60:C:VAL:CB  | 1        | 0.13          |
| (1,72)   | 1:61:C:ILE:CG1 | 1:60:C:VAL:CB  | 3        | 0.13          |
| (1,14)   | 1:46:C:TYR:CB  | 1:77:C:LYS:CB  | 2        | 0.13          |
| (1,1)    | 1:26:C:PRO:CG  | 1:28:C:ARG:C   | 1        | 0.13          |
| (2,40)   | 1:84:C:GLY:H   | 1:67:C:GLY:O   | 10       | 0.12          |
| (2,22)   | 1:53:C:ALA:H   | 1:50:C:THR:O   | 1        | 0.12          |
| (2,22)   | 1:53:C:ALA:H   | 1:50:C:THR:O   | 5        | 0.12          |
| (2,22)   | 1:53:C:ALA:H   | 1:50:C:THR:O   | 10       | 0.12          |
| (2,20)   | 1:57:C:TRP:H   | 1:48:C:GLY:O   | 8        | 0.12          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (2,13)   | 1:61:C:ILE:N   | 1:43:C:THR:O   | 4        | 0.12          |
| (1,1433) | 1:72:C:THR:CG2 | 1:73:C:VAL:CG1 | 1        | 0.12          |
| (1,1419) | 1:62:C:LEU:CD1 | 1:67:C:GLY:CA  | 4        | 0.12          |
| (1,1355) | 1:85:C:HIS:CB  | 1:71:C:GLY:CA  | 1        | 0.12          |
| (1,1144) | 1:93:C:GLN:CA  | 1:27:C:LEU:CD1 | 10       | 0.12          |
| (1,913)  | 1:83:C:GLU:CA  | 1:86:C:GLY:C   | 3        | 0.12          |
| (1,794)  | 1:76:C:ARG:CG  | 1:51:C:LEU:CA  | 5        | 0.12          |
| (1,722)  | 1:36:C:ILE:CG2 | 1:92:C:SER:CA  | 9        | 0.12          |
| (1,718)  | 1:72:C:THR:CG2 | 1:78:C:TYR:CA  | 3        | 0.12          |
| (1,718)  | 1:72:C:THR:CG2 | 1:78:C:TYR:CA  | 7        | 0.12          |
| (1,702)  | 1:89:C:VAL:CG1 | 1:90:C:ARG:CA  | 1        | 0.12          |
| (1,702)  | 1:89:C:VAL:CG1 | 1:90:C:ARG:CA  | 3        | 0.12          |
| (1,702)  | 1:89:C:VAL:CG1 | 1:90:C:ARG:CA  | 7        | 0.12          |
| (1,672)  | 1:34:C:GLU:CB  | 1:40:C:HIS:CA  | 8        | 0.12          |
| (1,602)  | 1:90:C:ARG:CG  | 1:58:C:VAL:CB  | 2        | 0.12          |
| (1,601)  | 1:62:C:LEU:CG  | 1:66:C:LYS:CB  | 7        | 0.12          |
| (1,589)  | 1:58:C:VAL:CG1 | 1:57:C:TRP:CB  | 2        | 0.12          |
| (1,144)  | 1:70:C:ASP:CA  | 1:68:C:LYS:CD  | 9        | 0.12          |
| (1,67)   | 1:68:C:LYS:CG  | 1:83:C:GLU:CB  | 10       | 0.12          |
| (1,14)   | 1:46:C:TYR:CB  | 1:77:C:LYS:CB  | 8        | 0.12          |
| (2,20)   | 1:57:C:TRP:H   | 1:48:C:GLY:O   | 5        | 0.11          |
| (1,1419) | 1:62:C:LEU:CD1 | 1:67:C:GLY:CA  | 2        | 0.11          |
| (1,1293) | 1:88:C:PHE:CB  | 1:90:C:ARG:CB  | 3        | 0.11          |
| (1,1291) | 1:90:C:ARG:CD  | 1:94:C:ILE:CB  | 5        | 0.11          |
| (1,1291) | 1:90:C:ARG:CD  | 1:94:C:ILE:CB  | 9        | 0.11          |
| (1,1241) | 1:52:C:PHE:CA  | 1:49:C:ALA:CA  | 4        | 0.11          |
| (1,1240) | 1:52:C:PHE:CA  | 1:49:C:ALA:CA  | 4        | 0.11          |
| (1,1185) | 1:69:C:ASN:CA  | 1:77:C:LYS:CB  | 10       | 0.11          |
| (1,1158) | 1:79:C:PHE:CA  | 1:72:C:THR:CG2 | 4        | 0.11          |
| (1,1119) | 1:43:C:THR:CA  | 1:29:C:VAL:CB  | 2        | 0.11          |
| (1,843)  | 1:73:C:VAL:CB  | 1:52:C:PHE:C   | 6        | 0.11          |
| (1,723)  | 1:72:C:THR:CG2 | 1:79:C:PHE:CA  | 4        | 0.11          |
| (1,702)  | 1:89:C:VAL:CG1 | 1:90:C:ARG:CA  | 6        | 0.11          |
| (1,697)  | 1:74:C:GLN:CB  | 1:77:C:LYS:CA  | 6        | 0.11          |
| (1,697)  | 1:74:C:GLN:CB  | 1:77:C:LYS:CA  | 8        | 0.11          |
| (1,637)  | 1:73:C:VAL:CG1 | 1:69:C:ASN:CB  | 9        | 0.11          |
| (1,589)  | 1:58:C:VAL:CG1 | 1:57:C:TRP:CB  | 7        | 0.11          |
| (1,480)  | 1:94:C:ILE:CB  | 1:90:C:ARG:CD  | 5        | 0.11          |
| (1,480)  | 1:94:C:ILE:CB  | 1:90:C:ARG:CD  | 9        | 0.11          |
| (1,444)  | 1:36:C:ILE:CA  | 1:89:C:VAL:CG1 | 4        | 0.11          |
| (1,444)  | 1:36:C:ILE:CA  | 1:89:C:VAL:CG1 | 8        | 0.11          |
| (1,144)  | 1:70:C:ASP:CA  | 1:68:C:LYS:CD  | 6        | 0.11          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,135)  | 1:32:C:ARG:CB  | 1:34:C:GLU:CA  | 2        | 0.11          |
| (1,106)  | 1:40:C:HIS:C   | 1:33:C:VAL:CB  | 6        | 0.11          |
| (1,89)   | 1:55:C:GLY:C   | 1:50:C:THR:CA  | 5        | 0.11          |
| (1,65)   | 1:41:C:ARG:CB  | 1:32:C:ARG:CG  | 8        | 0.11          |
| (1,58)   | 1:32:C:ARG:CG  | 1:41:C:ARG:CB  | 8        | 0.11          |
| (1,45)   | 1:62:C:LEU:CA  | 1:60:C:VAL:CB  | 5        | 0.11          |
| (2,20)   | 1:57:C:TRP:H   | 1:48:C:GLY:O   | 2        | 0.1           |
| (1,1374) | 1:62:C:LEU:CG  | 1:61:C:ILE:CG1 | 1        | 0.1           |
| (1,1374) | 1:62:C:LEU:CG  | 1:61:C:ILE:CG1 | 3        | 0.1           |
| (1,1368) | 1:61:C:ILE:CG1 | 1:62:C:LEU:CG  | 1        | 0.1           |
| (1,1368) | 1:61:C:ILE:CG1 | 1:62:C:LEU:CG  | 3        | 0.1           |
| (1,1158) | 1:79:C:PHE:CA  | 1:72:C:THR:CG2 | 10       | 0.1           |
| (1,909)  | 1:62:C:LEU:CD1 | 1:63:C:ASP:CG  | 4        | 0.1           |
| (1,892)  | 1:94:C:ILE:CG2 | 1:40:C:HIS:C   | 4        | 0.1           |
| (1,723)  | 1:72:C:THR:CG2 | 1:79:C:PHE:CA  | 10       | 0.1           |
| (1,702)  | 1:89:C:VAL:CG1 | 1:90:C:ARG:CA  | 4        | 0.1           |
| (1,702)  | 1:89:C:VAL:CG1 | 1:90:C:ARG:CA  | 8        | 0.1           |
| (1,672)  | 1:34:C:GLU:CB  | 1:40:C:HIS:CA  | 1        | 0.1           |
| (1,618)  | 1:61:C:ILE:CG1 | 1:60:C:VAL:CB  | 5        | 0.1           |
| (1,599)  | 1:27:C:LEU:CG  | 1:29:C:VAL:CB  | 7        | 0.1           |
| (1,590)  | 1:62:C:LEU:CG  | 1:85:C:HIS:CB  | 4        | 0.1           |
| (1,527)  | 1:29:C:VAL:CB  | 1:27:C:LEU:CG  | 7        | 0.1           |
| (1,116)  | 1:93:C:GLN:CG  | 1:90:C:ARG:CB  | 9        | 0.1           |
| (1,67)   | 1:68:C:LYS:CG  | 1:83:C:GLU:CB  | 7        | 0.1           |
| (1,1)    | 1:26:C:PRO:CG  | 1:28:C:ARG:C   | 8        | 0.1           |

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

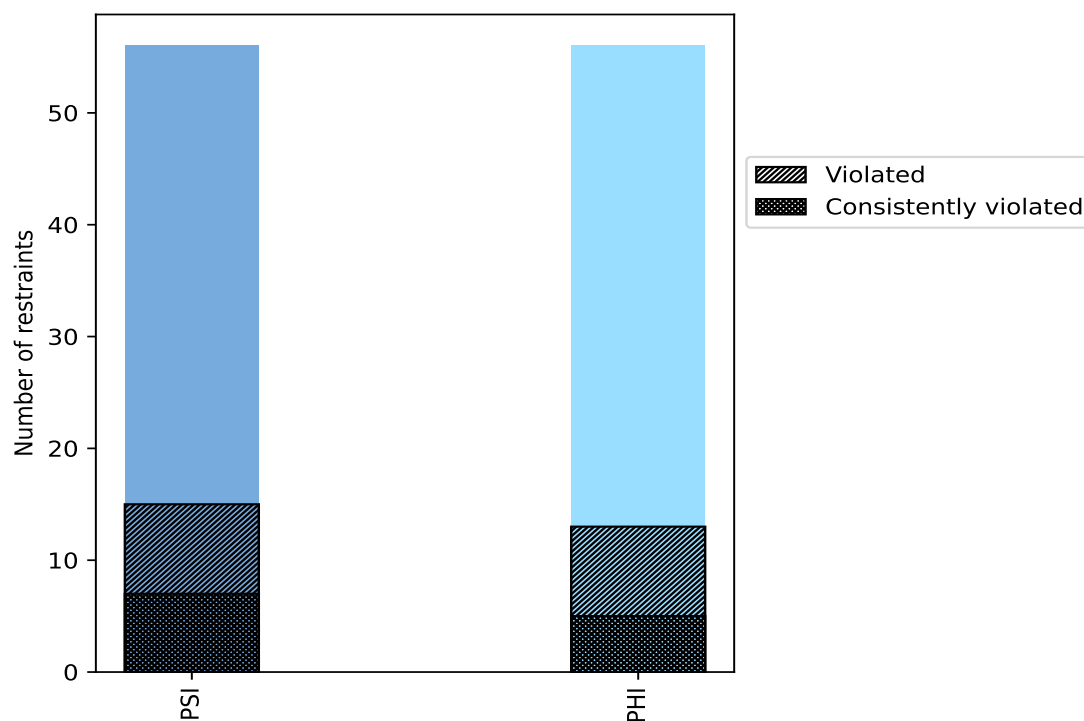
### 10.1 Summary of dihedral-angle violations [i](#)

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

| Angle type | Count | % <sup>1</sup> | Violated <sup>3</sup> |                |                | Consistently Violated <sup>4</sup> |                |                |
|------------|-------|----------------|-----------------------|----------------|----------------|------------------------------------|----------------|----------------|
|            |       |                | Count                 | % <sup>2</sup> | % <sup>1</sup> | Count                              | % <sup>2</sup> | % <sup>1</sup> |
| PSI        | 56    | 50.0           | 15                    | 26.8           | 13.4           | 7                                  | 12.5           | 6.2            |
| PHI        | 56    | 50.0           | 13                    | 23.2           | 11.6           | 5                                  | 8.9            | 4.5            |
| Total      | 112   | 100.0          | 28                    | 25.0           | 25.0           | 12                                 | 10.7           | 10.7           |

<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](#)



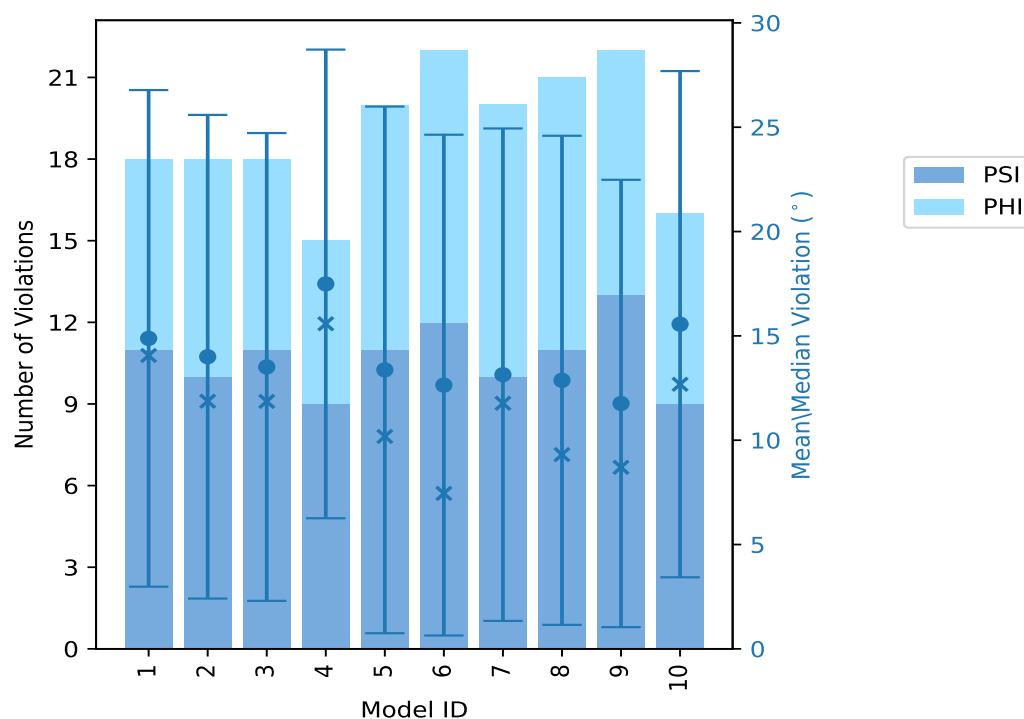
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

## 10.2 Dihedral-angle violation statistics for each model [i](#)

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

| Model ID | Number of violations |     |       | Mean (°) | Max (°) | SD (°) | Median (°) |
|----------|----------------------|-----|-------|----------|---------|--------|------------|
|          | PSI                  | PHI | Total |          |         |        |            |
| 1        | 11                   | 7   | 18    | 14.88    | 38.48   | 11.9   | 14.06      |
| 2        | 10                   | 8   | 18    | 14.0     | 40.72   | 11.59  | 11.87      |
| 3        | 11                   | 7   | 18    | 13.51    | 38.41   | 11.21  | 11.86      |
| 4        | 9                    | 6   | 15    | 17.49    | 39.7    | 11.23  | 15.58      |
| 5        | 11                   | 9   | 20    | 13.37    | 42.89   | 12.62  | 10.18      |
| 6        | 12                   | 10  | 22    | 12.64    | 40.0    | 12.0   | 7.45       |
| 7        | 10                   | 10  | 20    | 13.14    | 38.08   | 11.8   | 11.77      |
| 8        | 11                   | 10  | 21    | 12.87    | 37.6    | 11.72  | 9.31       |
| 9        | 13                   | 9   | 22    | 11.76    | 38.16   | 10.72  | 8.7        |
| 10       | 9                    | 7   | 16    | 15.56    | 40.32   | 12.13  | 12.68      |

### 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

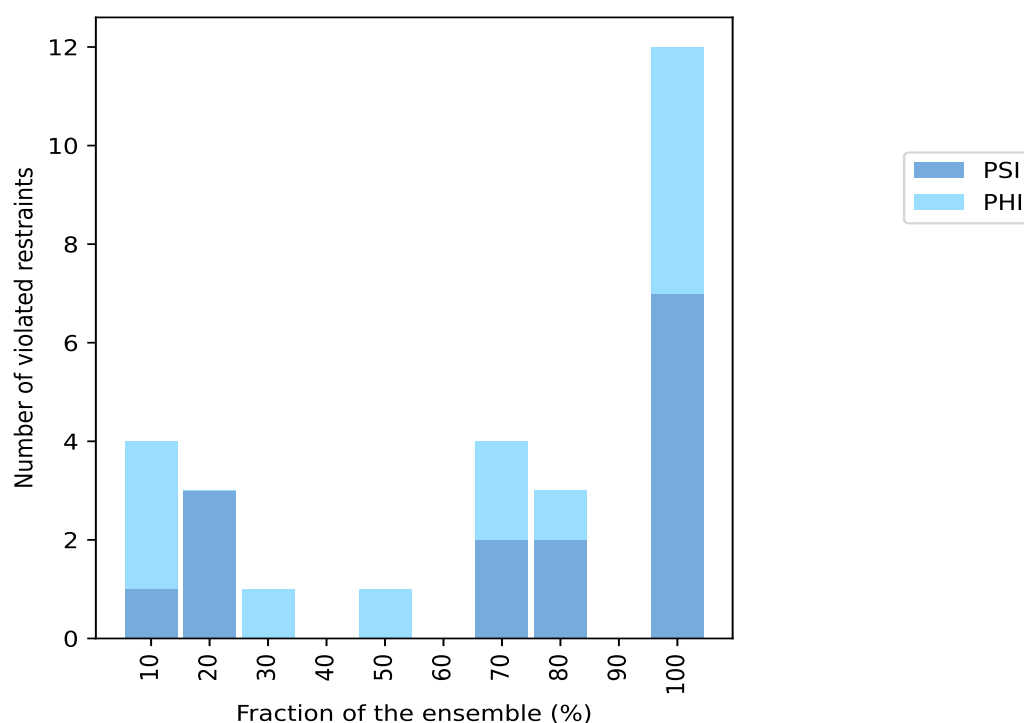
### 10.3 Dihedral-angle violation statistics for the ensemble [i](#)

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 |       |
|-------------------------------|-----|-------|--------------------------|-------|
| PSI                           | PHI | Total | Count <sup>1</sup>       | %     |
| 1                             | 3   | 4     | 1                        | 10.0  |
| 3                             | 0   | 3     | 2                        | 20.0  |
| 0                             | 1   | 1     | 3                        | 30.0  |
| 0                             | 0   | 0     | 4                        | 40.0  |
| 0                             | 1   | 1     | 5                        | 50.0  |
| 0                             | 0   | 0     | 6                        | 60.0  |
| 2                             | 2   | 4     | 7                        | 70.0  |
| 2                             | 1   | 3     | 8                        | 80.0  |
| 0                             | 0   | 0     | 9                        | 90.0  |
| 7                             | 5   | 12    | 10                       | 100.0 |

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

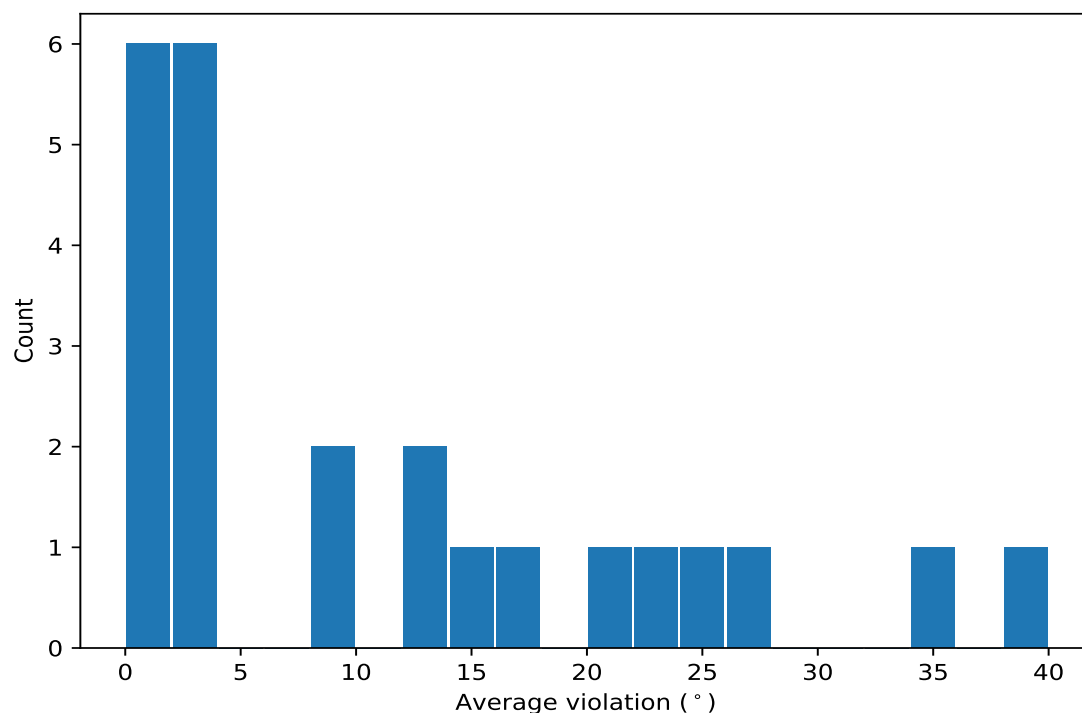
#### 10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



## 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 [i](#)

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

| Key     | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Models <sup>1</sup> | Mean  | SD <sup>2</sup> | Median |
|---------|--------------|---------------|---------------|--------------|---------------------|-------|-----------------|--------|
| (1,32)  | 1:45:C:ALA:N | 1:45:C:ALA:CA | 1:45:C:ALA:C  | 1:46:C:TYR:N | 10                  | 39.44 | 1.53            | 39.09  |
| (1,33)  | 1:45:C:ALA:C | 1:46:C:TYR:N  | 1:46:C:TYR:CA | 1:46:C:TYR:C | 10                  | 35.95 | 0.95            | 36.0   |
| (1,16)  | 1:36:C:ILE:N | 1:36:C:ILE:CA | 1:36:C:ILE:C  | 1:37:C:GLY:N | 10                  | 26.0  | 4.36            | 27.38  |
| (1,17)  | 1:36:C:ILE:C | 1:37:C:GLY:N  | 1:37:C:GLY:CA | 1:37:C:GLY:C | 10                  | 25.32 | 0.61            | 25.4   |
| (1,69)  | 1:71:C:GLY:C | 1:72:C:THR:N  | 1:72:C:THR:CA | 1:72:C:THR:C | 10                  | 23.15 | 1.75            | 23.6   |
| (1,18)  | 1:37:C:GLY:N | 1:37:C:GLY:CA | 1:37:C:GLY:C  | 1:38:C:LYS:N | 10                  | 20.71 | 2.61            | 20.47  |
| (1,66)  | 1:68:C:LYS:N | 1:68:C:LYS:CA | 1:68:C:LYS:C  | 1:69:C:ASN:N | 10                  | 16.78 | 2.61            | 16.46  |
| (1,65)  | 1:67:C:GLY:C | 1:68:C:LYS:N  | 1:68:C:LYS:CA | 1:68:C:LYS:C | 10                  | 14.85 | 1.05            | 14.9   |
| (1,12)  | 1:34:C:GLU:N | 1:34:C:GLU:CA | 1:34:C:GLU:C  | 1:35:C:VAL:N | 10                  | 12.73 | 2.92            | 13.06  |
| (1,86)  | 1:80:C:THR:N | 1:80:C:THR:CA | 1:80:C:THR:C  | 1:81:C:CYS:N | 10                  | 12.67 | 4.37            | 14.78  |
| (1,87)  | 1:80:C:THR:C | 1:81:C:CYS:N  | 1:81:C:CYS:CA | 1:81:C:CYS:C | 10                  | 8.97  | 2.71            | 9.45   |
| (1,68)  | 1:69:C:ASN:N | 1:69:C:ASN:CA | 1:69:C:ASN:C  | 1:70:C:ASP:N | 10                  | 8.42  | 2.98            | 9.23   |
| (1,109) | 1:92:C:SER:C | 1:93:C:GLN:N  | 1:93:C:GLN:CA | 1:93:C:GLN:C | 8                   | 3.67  | 1.24            | 3.98   |

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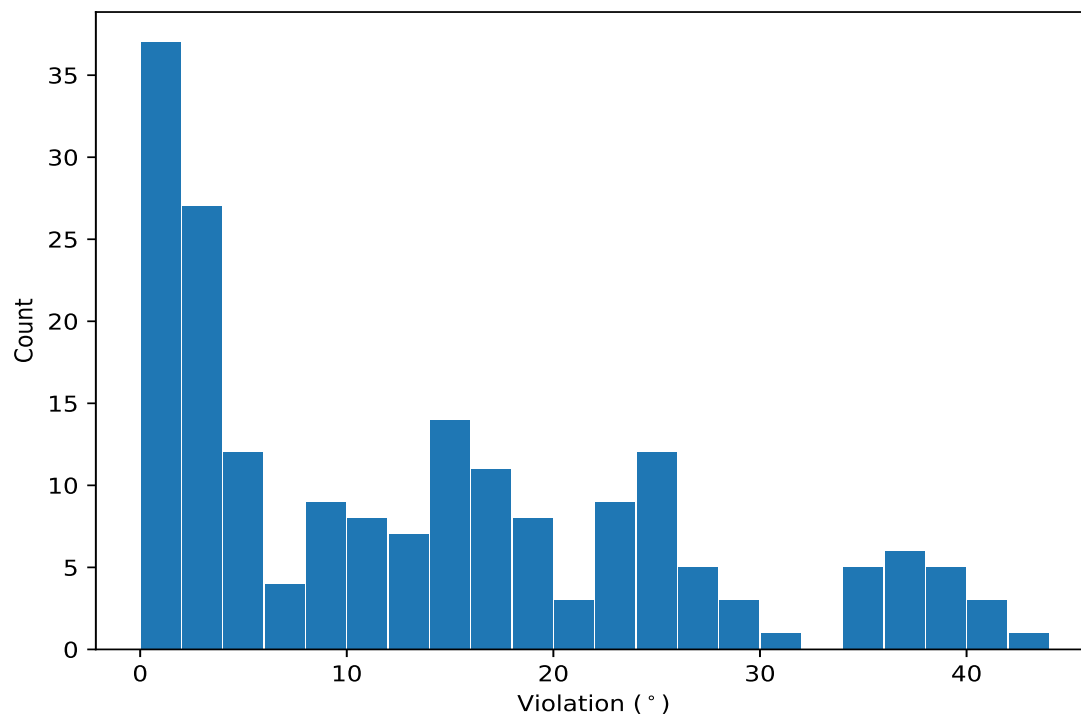
| Key     | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Models <sup>1</sup> | Mean | SD <sup>2</sup> | Median |
|---------|--------------|---------------|---------------|--------------|---------------------|------|-----------------|--------|
| (1,8)   | 1:31:C:SER:N | 1:31:C:SER:CA | 1:31:C:SER:C  | 1:32:C:ARG:N | 8                   | 3.34 | 0.86            | 3.3    |
| (1,100) | 1:88:C:PHE:N | 1:88:C:PHE:CA | 1:88:C:PHE:C  | 1:89:C:VAL:N | 8                   | 2.21 | 0.91            | 2.02   |
| (1,90)  | 1:82:C:ASP:N | 1:82:C:ASP:CA | 1:82:C:ASP:C  | 1:83:C:GLU:N | 7                   | 2.55 | 0.85            | 2.47   |
| (1,80)  | 1:77:C:LYS:N | 1:77:C:LYS:CA | 1:77:C:LYS:C  | 1:78:C:TYR:N | 7                   | 2.44 | 0.7             | 2.57   |
| (1,37)  | 1:48:C:GLY:C | 1:49:C:ALA:N  | 1:49:C:ALA:CA | 1:49:C:ALA:C | 7                   | 1.77 | 0.55            | 1.67   |
| (1,85)  | 1:79:C:PHE:C | 1:80:C:THR:N  | 1:80:C:THR:CA | 1:80:C:THR:C | 7                   | 1.56 | 0.18            | 1.53   |
| (1,21)  | 1:38:C:LYS:C | 1:39:C:GLY:N  | 1:39:C:GLY:CA | 1:39:C:GLY:C | 5                   | 1.87 | 0.29            | 1.84   |
| (1,77)  | 1:75:C:GLY:C | 1:76:C:ARG:N  | 1:76:C:ARG:CA | 1:76:C:ARG:C | 3                   | 1.37 | 0.11            | 1.33   |
| (1,2)   | 1:27:C:LEU:N | 1:27:C:LEU:CA | 1:27:C:LEU:C  | 1:28:C:ARG:N | 2                   | 2.67 | 0.1             | 2.67   |
| (1,22)  | 1:39:C:GLY:N | 1:39:C:GLY:CA | 1:39:C:GLY:C  | 1:40:C:HIS:N | 2                   | 1.56 | 0.28            | 1.56   |
| (1,62)  | 1:63:C:ASP:N | 1:63:C:ASP:CA | 1:63:C:ASP:C  | 1:64:C:GLU:N | 2                   | 1.35 | 0.07            | 1.35   |

<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 (°) |
|--------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,32) | 1:45:C:ALA:N | 1:45:C:ALA:CA | 1:45:C:ALA:C  | 1:46:C:TYR:N | 5        | 42.89         |
| (1,32) | 1:45:C:ALA:N | 1:45:C:ALA:CA | 1:45:C:ALA:C  | 1:46:C:TYR:N | 2        | 40.72         |
| (1,32) | 1:45:C:ALA:N | 1:45:C:ALA:CA | 1:45:C:ALA:C  | 1:46:C:TYR:N | 10       | 40.32         |
| (1,32) | 1:45:C:ALA:N | 1:45:C:ALA:CA | 1:45:C:ALA:C  | 1:46:C:TYR:N | 6        | 40.0          |
| (1,32) | 1:45:C:ALA:N | 1:45:C:ALA:CA | 1:45:C:ALA:C  | 1:46:C:TYR:N | 4        | 39.7          |
| (1,32) | 1:45:C:ALA:N | 1:45:C:ALA:CA | 1:45:C:ALA:C  | 1:46:C:TYR:N | 1        | 38.48         |
| (1,32) | 1:45:C:ALA:N | 1:45:C:ALA:CA | 1:45:C:ALA:C  | 1:46:C:TYR:N | 3        | 38.41         |
| (1,32) | 1:45:C:ALA:N | 1:45:C:ALA:CA | 1:45:C:ALA:C  | 1:46:C:TYR:N | 9        | 38.16         |
| (1,32) | 1:45:C:ALA:N | 1:45:C:ALA:CA | 1:45:C:ALA:C  | 1:46:C:TYR:N | 7        | 38.08         |
| (1,32) | 1:45:C:ALA:N | 1:45:C:ALA:CA | 1:45:C:ALA:C  | 1:46:C:TYR:N | 8        | 37.6          |
| (1,33) | 1:45:C:ALA:C | 1:46:C:TYR:N  | 1:46:C:TYR:CA | 1:46:C:TYR:C | 5        | 37.31         |
| (1,33) | 1:45:C:ALA:C | 1:46:C:TYR:N  | 1:46:C:TYR:CA | 1:46:C:TYR:C | 6        | 37.31         |
| (1,33) | 1:45:C:ALA:C | 1:46:C:TYR:N  | 1:46:C:TYR:CA | 1:46:C:TYR:C | 2        | 36.58         |
| (1,33) | 1:45:C:ALA:C | 1:46:C:TYR:N  | 1:46:C:TYR:CA | 1:46:C:TYR:C | 4        | 36.39         |
| (1,33) | 1:45:C:ALA:C | 1:46:C:TYR:N  | 1:46:C:TYR:CA | 1:46:C:TYR:C | 10       | 36.34         |
| (1,33) | 1:45:C:ALA:C | 1:46:C:TYR:N  | 1:46:C:TYR:CA | 1:46:C:TYR:C | 7        | 35.65         |
| (1,33) | 1:45:C:ALA:C | 1:46:C:TYR:N  | 1:46:C:TYR:CA | 1:46:C:TYR:C | 1        | 35.59         |
| (1,33) | 1:45:C:ALA:C | 1:46:C:TYR:N  | 1:46:C:TYR:CA | 1:46:C:TYR:C | 3        | 35.2          |
| (1,33) | 1:45:C:ALA:C | 1:46:C:TYR:N  | 1:46:C:TYR:CA | 1:46:C:TYR:C | 8        | 34.66         |
| (1,33) | 1:45:C:ALA:C | 1:46:C:TYR:N  | 1:46:C:TYR:CA | 1:46:C:TYR:C | 9        | 34.51         |
| (1,16) | 1:36:C:ILE:N | 1:36:C:ILE:CA | 1:36:C:ILE:C  | 1:37:C:GLY:N | 6        | 30.04         |
| (1,16) | 1:36:C:ILE:N | 1:36:C:ILE:CA | 1:36:C:ILE:C  | 1:37:C:GLY:N | 8        | 29.53         |
| (1,16) | 1:36:C:ILE:N | 1:36:C:ILE:CA | 1:36:C:ILE:C  | 1:37:C:GLY:N | 1        | 29.38         |
| (1,16) | 1:36:C:ILE:N | 1:36:C:ILE:CA | 1:36:C:ILE:C  | 1:37:C:GLY:N | 5        | 28.67         |
| (1,16) | 1:36:C:ILE:N | 1:36:C:ILE:CA | 1:36:C:ILE:C  | 1:37:C:GLY:N | 7        | 27.63         |
| (1,16) | 1:36:C:ILE:N | 1:36:C:ILE:CA | 1:36:C:ILE:C  | 1:37:C:GLY:N | 10       | 27.12         |
| (1,16) | 1:36:C:ILE:N | 1:36:C:ILE:CA | 1:36:C:ILE:C  | 1:37:C:GLY:N | 4        | 27.03         |
| (1,17) | 1:36:C:ILE:C | 1:37:C:GLY:N  | 1:37:C:GLY:CA | 1:37:C:GLY:C | 4        | 26.47         |
| (1,17) | 1:36:C:ILE:C | 1:37:C:GLY:N  | 1:37:C:GLY:CA | 1:37:C:GLY:C | 1        | 26.02         |
| (1,17) | 1:36:C:ILE:C | 1:37:C:GLY:N  | 1:37:C:GLY:CA | 1:37:C:GLY:C | 3        | 25.59         |
| (1,17) | 1:36:C:ILE:C | 1:37:C:GLY:N  | 1:37:C:GLY:CA | 1:37:C:GLY:C | 2        | 25.58         |
| (1,17) | 1:36:C:ILE:C | 1:37:C:GLY:N  | 1:37:C:GLY:CA | 1:37:C:GLY:C | 6        | 25.54         |
| (1,69) | 1:71:C:GLY:C | 1:72:C:THR:N  | 1:72:C:THR:CA | 1:72:C:THR:C | 10       | 25.31         |
| (1,17) | 1:36:C:ILE:C | 1:37:C:GLY:N  | 1:37:C:GLY:CA | 1:37:C:GLY:C | 9        | 25.25         |
| (1,17) | 1:36:C:ILE:C | 1:37:C:GLY:N  | 1:37:C:GLY:CA | 1:37:C:GLY:C | 5        | 25.02         |
| (1,17) | 1:36:C:ILE:C | 1:37:C:GLY:N  | 1:37:C:GLY:CA | 1:37:C:GLY:C | 8        | 24.67         |
| (1,17) | 1:36:C:ILE:C | 1:37:C:GLY:N  | 1:37:C:GLY:CA | 1:37:C:GLY:C | 10       | 24.67         |
| (1,69) | 1:71:C:GLY:C | 1:72:C:THR:N  | 1:72:C:THR:CA | 1:72:C:THR:C | 7        | 24.65         |
| (1,18) | 1:37:C:GLY:N | 1:37:C:GLY:CA | 1:37:C:GLY:C  | 1:38:C:LYS:N | 1        | 24.63         |
| (1,69) | 1:71:C:GLY:C | 1:72:C:THR:N  | 1:72:C:THR:CA | 1:72:C:THR:C | 4        | 24.62         |
| (1,17) | 1:36:C:ILE:C | 1:37:C:GLY:N  | 1:37:C:GLY:CA | 1:37:C:GLY:C | 7        | 24.44         |
| (1,18) | 1:37:C:GLY:N | 1:37:C:GLY:CA | 1:37:C:GLY:C  | 1:38:C:LYS:N | 8        | 23.93         |
| (1,16) | 1:36:C:ILE:N | 1:36:C:ILE:CA | 1:36:C:ILE:C  | 1:37:C:GLY:N | 3        | 23.8          |
| (1,69) | 1:71:C:GLY:C | 1:72:C:THR:N  | 1:72:C:THR:CA | 1:72:C:THR:C | 5        | 23.76         |
| (1,69) | 1:71:C:GLY:C | 1:72:C:THR:N  | 1:72:C:THR:CA | 1:72:C:THR:C | 6        | 23.61         |
| (1,69) | 1:71:C:GLY:C | 1:72:C:THR:N  | 1:72:C:THR:CA | 1:72:C:THR:C | 1        | 23.58         |
| (1,69) | 1:71:C:GLY:C | 1:72:C:THR:N  | 1:72:C:THR:CA | 1:72:C:THR:C | 8        | 23.3          |
| (1,18) | 1:37:C:GLY:N | 1:37:C:GLY:CA | 1:37:C:GLY:C  | 1:38:C:LYS:N | 5        | 23.03         |
| (1,69) | 1:71:C:GLY:C | 1:72:C:THR:N  | 1:72:C:THR:CA | 1:72:C:THR:C | 9        | 22.81         |
| (1,18) | 1:37:C:GLY:N | 1:37:C:GLY:CA | 1:37:C:GLY:C  | 1:38:C:LYS:N | 6        | 22.5          |
| (1,18) | 1:37:C:GLY:N | 1:37:C:GLY:CA | 1:37:C:GLY:C  | 1:38:C:LYS:N | 7        | 21.9          |

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| Key    | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Model ID | Violation (°) |
|--------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,16) | 1:36:C:ILE:N | 1:36:C:ILE:CA | 1:36:C:ILE:C  | 1:37:C:GLY:N | 2        | 21.34         |
| (1,66) | 1:68:C:LYS:N | 1:68:C:LYS:CA | 1:68:C:LYS:C  | 1:69:C:ASN:N | 2        | 20.75         |
| (1,69) | 1:71:C:GLY:C | 1:72:C:THR:N  | 1:72:C:THR:CA | 1:72:C:THR:C | 3        | 19.95         |
| (1,69) | 1:71:C:GLY:C | 1:72:C:THR:N  | 1:72:C:THR:CA | 1:72:C:THR:C | 2        | 19.9          |
| (1,66) | 1:68:C:LYS:N | 1:68:C:LYS:CA | 1:68:C:LYS:C  | 1:69:C:ASN:N | 4        | 19.82         |
| (1,66) | 1:68:C:LYS:N | 1:68:C:LYS:CA | 1:68:C:LYS:C  | 1:69:C:ASN:N | 10       | 19.3          |
| (1,18) | 1:37:C:GLY:N | 1:37:C:GLY:CA | 1:37:C:GLY:C  | 1:38:C:LYS:N | 10       | 19.04         |
| (1,66) | 1:68:C:LYS:N | 1:68:C:LYS:CA | 1:68:C:LYS:C  | 1:69:C:ASN:N | 5        | 18.55         |
| (1,18) | 1:37:C:GLY:N | 1:37:C:GLY:CA | 1:37:C:GLY:C  | 1:38:C:LYS:N | 2        | 18.43         |
| (1,18) | 1:37:C:GLY:N | 1:37:C:GLY:CA | 1:37:C:GLY:C  | 1:38:C:LYS:N | 9        | 18.3          |
| (1,18) | 1:37:C:GLY:N | 1:37:C:GLY:CA | 1:37:C:GLY:C  | 1:38:C:LYS:N | 4        | 17.79         |
| (1,18) | 1:37:C:GLY:N | 1:37:C:GLY:CA | 1:37:C:GLY:C  | 1:38:C:LYS:N | 3        | 17.54         |
| (1,86) | 1:80:C:THR:N | 1:80:C:THR:CA | 1:80:C:THR:C  | 1:81:C:CYS:N | 7        | 17.53         |
| (1,66) | 1:68:C:LYS:N | 1:68:C:LYS:CA | 1:68:C:LYS:C  | 1:69:C:ASN:N | 8        | 17.14         |
| (1,12) | 1:34:C:GLU:N | 1:34:C:GLU:CA | 1:34:C:GLU:C  | 1:35:C:VAL:N | 9        | 16.61         |
| (1,65) | 1:67:C:GLY:C | 1:68:C:LYS:N  | 1:68:C:LYS:CA | 1:68:C:LYS:C | 3        | 16.39         |
| (1,65) | 1:67:C:GLY:C | 1:68:C:LYS:N  | 1:68:C:LYS:CA | 1:68:C:LYS:C | 7        | 16.32         |
| (1,12) | 1:34:C:GLU:N | 1:34:C:GLU:CA | 1:34:C:GLU:C  | 1:35:C:VAL:N | 1        | 16.2          |
| (1,86) | 1:80:C:THR:N | 1:80:C:THR:CA | 1:80:C:THR:C  | 1:81:C:CYS:N | 9        | 16.15         |
| (1,86) | 1:80:C:THR:N | 1:80:C:THR:CA | 1:80:C:THR:C  | 1:81:C:CYS:N | 1        | 16.11         |
| (1,86) | 1:80:C:THR:N | 1:80:C:THR:CA | 1:80:C:THR:C  | 1:81:C:CYS:N | 6        | 16.04         |
| (1,66) | 1:68:C:LYS:N | 1:68:C:LYS:CA | 1:68:C:LYS:C  | 1:69:C:ASN:N | 3        | 15.79         |
| (1,65) | 1:67:C:GLY:C | 1:68:C:LYS:N  | 1:68:C:LYS:CA | 1:68:C:LYS:C | 4        | 15.58         |
| (1,16) | 1:36:C:ILE:N | 1:36:C:ILE:CA | 1:36:C:ILE:C  | 1:37:C:GLY:N | 9        | 15.45         |
| (1,66) | 1:68:C:LYS:N | 1:68:C:LYS:CA | 1:68:C:LYS:C  | 1:69:C:ASN:N | 1        | 15.31         |
| (1,12) | 1:34:C:GLU:N | 1:34:C:GLU:CA | 1:34:C:GLU:C  | 1:35:C:VAL:N | 8        | 15.21         |
| (1,65) | 1:67:C:GLY:C | 1:68:C:LYS:N  | 1:68:C:LYS:CA | 1:68:C:LYS:C | 6        | 15.02         |
| (1,65) | 1:67:C:GLY:C | 1:68:C:LYS:N  | 1:68:C:LYS:CA | 1:68:C:LYS:C | 9        | 15.01         |
| (1,86) | 1:80:C:THR:N | 1:80:C:THR:CA | 1:80:C:THR:C  | 1:81:C:CYS:N | 8        | 14.94         |
| (1,65) | 1:67:C:GLY:C | 1:68:C:LYS:N  | 1:68:C:LYS:CA | 1:68:C:LYS:C | 2        | 14.8          |
| (1,65) | 1:67:C:GLY:C | 1:68:C:LYS:N  | 1:68:C:LYS:CA | 1:68:C:LYS:C | 8        | 14.7          |
| (1,86) | 1:80:C:THR:N | 1:80:C:THR:CA | 1:80:C:THR:C  | 1:81:C:CYS:N | 4        | 14.62         |
| (1,66) | 1:68:C:LYS:N | 1:68:C:LYS:CA | 1:68:C:LYS:C  | 1:69:C:ASN:N | 6        | 14.61         |
| (1,12) | 1:34:C:GLU:N | 1:34:C:GLU:CA | 1:34:C:GLU:C  | 1:35:C:VAL:N | 4        | 14.36         |
| (1,65) | 1:67:C:GLY:C | 1:68:C:LYS:N  | 1:68:C:LYS:CA | 1:68:C:LYS:C | 5        | 14.19         |
| (1,66) | 1:68:C:LYS:N | 1:68:C:LYS:CA | 1:68:C:LYS:C  | 1:69:C:ASN:N | 9        | 13.94         |
| (1,65) | 1:67:C:GLY:C | 1:68:C:LYS:N  | 1:68:C:LYS:CA | 1:68:C:LYS:C | 10       | 13.73         |
| (1,12) | 1:34:C:GLU:N | 1:34:C:GLU:CA | 1:34:C:GLU:C  | 1:35:C:VAL:N | 6        | 13.53         |
| (1,87) | 1:80:C:THR:C | 1:81:C:CYS:N  | 1:81:C:CYS:CA | 1:81:C:CYS:C | 3        | 13.03         |
| (1,65) | 1:67:C:GLY:C | 1:68:C:LYS:N  | 1:68:C:LYS:CA | 1:68:C:LYS:C | 1        | 12.8          |
| (1,12) | 1:34:C:GLU:N | 1:34:C:GLU:CA | 1:34:C:GLU:C  | 1:35:C:VAL:N | 7        | 12.58         |
| (1,66) | 1:68:C:LYS:N | 1:68:C:LYS:CA | 1:68:C:LYS:C  | 1:69:C:ASN:N | 7        | 12.56         |
| (1,12) | 1:34:C:GLU:N | 1:34:C:GLU:CA | 1:34:C:GLU:C  | 1:35:C:VAL:N | 2        | 11.98         |
| (1,68) | 1:69:C:ASN:N | 1:69:C:ASN:CA | 1:69:C:ASN:C  | 1:70:C:ASP:N | 5        | 11.96         |
| (1,68) | 1:69:C:ASN:N | 1:69:C:ASN:CA | 1:69:C:ASN:C  | 1:70:C:ASP:N | 2        | 11.76         |
| (1,87) | 1:80:C:THR:C | 1:81:C:CYS:N  | 1:81:C:CYS:CA | 1:81:C:CYS:C | 5        | 11.7          |
| (1,86) | 1:80:C:THR:N | 1:80:C:THR:CA | 1:80:C:THR:C  | 1:81:C:CYS:N | 10       | 11.62         |
| (1,87) | 1:80:C:THR:C | 1:81:C:CYS:N  | 1:81:C:CYS:CA | 1:81:C:CYS:C | 10       | 11.59         |
| (1,68) | 1:69:C:ASN:N | 1:69:C:ASN:CA | 1:69:C:ASN:C  | 1:70:C:ASP:N | 7        | 10.98         |
| (1,12) | 1:34:C:GLU:N | 1:34:C:GLU:CA | 1:34:C:GLU:C  | 1:35:C:VAL:N | 3        | 10.7          |
| (1,68) | 1:69:C:ASN:N | 1:69:C:ASN:CA | 1:69:C:ASN:C  | 1:70:C:ASP:N | 9        | 9.69          |

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| Key     | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Model ID | Violation (°) |
|---------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,87)  | 1:80:C:THR:C | 1:81:C:CYS:N  | 1:81:C:CYS:CA | 1:81:C:CYS:C | 1        | 9.6           |
| (1,87)  | 1:80:C:THR:C | 1:81:C:CYS:N  | 1:81:C:CYS:CA | 1:81:C:CYS:C | 2        | 9.59          |
| (1,68)  | 1:69:C:ASN:N | 1:69:C:ASN:CA | 1:69:C:ASN:C  | 1:70:C:ASP:N | 6        | 9.48          |
| (1,87)  | 1:80:C:THR:C | 1:81:C:CYS:N  | 1:81:C:CYS:CA | 1:81:C:CYS:C | 8        | 9.31          |
| (1,68)  | 1:69:C:ASN:N | 1:69:C:ASN:CA | 1:69:C:ASN:C  | 1:70:C:ASP:N | 4        | 8.98          |
| (1,86)  | 1:80:C:THR:N | 1:80:C:THR:CA | 1:80:C:THR:C  | 1:81:C:CYS:N | 5        | 8.65          |
| (1,12)  | 1:34:C:GLU:N | 1:34:C:GLU:CA | 1:34:C:GLU:C  | 1:35:C:VAL:N | 10       | 8.59          |
| (1,68)  | 1:69:C:ASN:N | 1:69:C:ASN:CA | 1:69:C:ASN:C  | 1:70:C:ASP:N | 8        | 8.23          |
| (1,87)  | 1:80:C:THR:C | 1:81:C:CYS:N  | 1:81:C:CYS:CA | 1:81:C:CYS:C | 4        | 7.96          |
| (1,87)  | 1:80:C:THR:C | 1:81:C:CYS:N  | 1:81:C:CYS:CA | 1:81:C:CYS:C | 9        | 7.71          |
| (1,12)  | 1:34:C:GLU:N | 1:34:C:GLU:CA | 1:34:C:GLU:C  | 1:35:C:VAL:N | 5        | 7.56          |
| (1,86)  | 1:80:C:THR:N | 1:80:C:THR:CA | 1:80:C:THR:C  | 1:81:C:CYS:N | 2        | 6.8           |
| (1,68)  | 1:69:C:ASN:N | 1:69:C:ASN:CA | 1:69:C:ASN:C  | 1:70:C:ASP:N | 3        | 5.69          |
| (1,87)  | 1:80:C:THR:C | 1:81:C:CYS:N  | 1:81:C:CYS:CA | 1:81:C:CYS:C | 6        | 5.42          |
| (1,109) | 1:92:C:SER:C | 1:93:C:GLN:N  | 1:93:C:GLN:CA | 1:93:C:GLN:C | 9        | 5.3           |
| (1,68)  | 1:69:C:ASN:N | 1:69:C:ASN:CA | 1:69:C:ASN:C  | 1:70:C:ASP:N | 1        | 5.17          |
| (1,109) | 1:92:C:SER:C | 1:93:C:GLN:N  | 1:93:C:GLN:CA | 1:93:C:GLN:C | 6        | 4.64          |
| (1,109) | 1:92:C:SER:C | 1:93:C:GLN:N  | 1:93:C:GLN:CA | 1:93:C:GLN:C | 7        | 4.54          |
| (1,8)   | 1:31:C:SER:N | 1:31:C:SER:CA | 1:31:C:SER:C  | 1:32:C:ARG:N | 10       | 4.48          |
| (1,100) | 1:88:C:PHE:N | 1:88:C:PHE:CA | 1:88:C:PHE:C  | 1:89:C:VAL:N | 9        | 4.42          |
| (1,86)  | 1:80:C:THR:N | 1:80:C:THR:CA | 1:80:C:THR:C  | 1:81:C:CYS:N | 3        | 4.23          |
| (1,8)   | 1:31:C:SER:N | 1:31:C:SER:CA | 1:31:C:SER:C  | 1:32:C:ARG:N | 6        | 4.23          |
| (1,109) | 1:92:C:SER:C | 1:93:C:GLN:N  | 1:93:C:GLN:CA | 1:93:C:GLN:C | 1        | 4.21          |
| (1,8)   | 1:31:C:SER:N | 1:31:C:SER:CA | 1:31:C:SER:C  | 1:32:C:ARG:N | 3        | 4.17          |
| (1,90)  | 1:82:C:ASP:N | 1:82:C:ASP:CA | 1:82:C:ASP:C  | 1:83:C:GLU:N | 1        | 3.96          |
| (1,87)  | 1:80:C:THR:C | 1:81:C:CYS:N  | 1:81:C:CYS:CA | 1:81:C:CYS:C | 7        | 3.83          |
| (1,109) | 1:92:C:SER:C | 1:93:C:GLN:N  | 1:93:C:GLN:CA | 1:93:C:GLN:C | 4        | 3.75          |
| (1,8)   | 1:31:C:SER:N | 1:31:C:SER:CA | 1:31:C:SER:C  | 1:32:C:ARG:N | 9        | 3.73          |
| (1,80)  | 1:77:C:LYS:N | 1:77:C:LYS:CA | 1:77:C:LYS:C  | 1:78:C:TYR:N | 2        | 3.52          |
| (1,109) | 1:92:C:SER:C | 1:93:C:GLN:N  | 1:93:C:GLN:CA | 1:93:C:GLN:C | 3        | 3.48          |
| (1,90)  | 1:82:C:ASP:N | 1:82:C:ASP:CA | 1:82:C:ASP:C  | 1:83:C:GLU:N | 6        | 3.22          |
| (1,37)  | 1:48:C:GLY:C | 1:49:C:ALA:N  | 1:49:C:ALA:CA | 1:49:C:ALA:C | 3        | 3.01          |
| (1,90)  | 1:82:C:ASP:N | 1:82:C:ASP:CA | 1:82:C:ASP:C  | 1:83:C:GLU:N | 2        | 2.94          |
| (1,8)   | 1:31:C:SER:N | 1:31:C:SER:CA | 1:31:C:SER:C  | 1:32:C:ARG:N | 2        | 2.86          |
| (1,8)   | 1:31:C:SER:N | 1:31:C:SER:CA | 1:31:C:SER:C  | 1:32:C:ARG:N | 4        | 2.83          |
| (1,80)  | 1:77:C:LYS:N | 1:77:C:LYS:CA | 1:77:C:LYS:C  | 1:78:C:TYR:N | 6        | 2.8           |
| (1,2)   | 1:27:C:LEU:N | 1:27:C:LEU:CA | 1:27:C:LEU:C  | 1:28:C:ARG:N | 9        | 2.77          |
| (1,100) | 1:88:C:PHE:N | 1:88:C:PHE:CA | 1:88:C:PHE:C  | 1:89:C:VAL:N | 6        | 2.6           |
| (1,80)  | 1:77:C:LYS:N | 1:77:C:LYS:CA | 1:77:C:LYS:C  | 1:78:C:TYR:N | 8        | 2.58          |
| (1,80)  | 1:77:C:LYS:N | 1:77:C:LYS:CA | 1:77:C:LYS:C  | 1:78:C:TYR:N | 7        | 2.57          |
| (1,2)   | 1:27:C:LEU:N | 1:27:C:LEU:CA | 1:27:C:LEU:C  | 1:28:C:ARG:N | 1        | 2.57          |
| (1,80)  | 1:77:C:LYS:N | 1:77:C:LYS:CA | 1:77:C:LYS:C  | 1:78:C:TYR:N | 3        | 2.52          |
| (1,90)  | 1:82:C:ASP:N | 1:82:C:ASP:CA | 1:82:C:ASP:C  | 1:83:C:GLU:N | 4        | 2.47          |
| (1,21)  | 1:38:C:LYS:C | 1:39:C:GLY:N  | 1:39:C:GLY:CA | 1:39:C:GLY:C | 5        | 2.38          |
| (1,90)  | 1:82:C:ASP:N | 1:82:C:ASP:CA | 1:82:C:ASP:C  | 1:83:C:GLU:N | 8        | 2.36          |
| (1,68)  | 1:69:C:ASN:N | 1:69:C:ASN:CA | 1:69:C:ASN:C  | 1:70:C:ASP:N | 10       | 2.28          |
| (1,8)   | 1:31:C:SER:N | 1:31:C:SER:CA | 1:31:C:SER:C  | 1:32:C:ARG:N | 8        | 2.23          |
| (1,8)   | 1:31:C:SER:N | 1:31:C:SER:CA | 1:31:C:SER:C  | 1:32:C:ARG:N | 5        | 2.2           |
| (1,100) | 1:88:C:PHE:N | 1:88:C:PHE:CA | 1:88:C:PHE:C  | 1:89:C:VAL:N | 8        | 2.11          |
| (1,80)  | 1:77:C:LYS:N | 1:77:C:LYS:CA | 1:77:C:LYS:C  | 1:78:C:TYR:N | 5        | 2.07          |
| (1,100) | 1:88:C:PHE:N | 1:88:C:PHE:CA | 1:88:C:PHE:C  | 1:89:C:VAL:N | 7        | 2.04          |

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| Key     | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Model ID | Violation (°) |
|---------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,100) | 1:88:C:PHE:N | 1:88:C:PHE:CA | 1:88:C:PHE:C  | 1:89:C:VAL:N | 3        | 1.99          |
| (1,21)  | 1:38:C:LYS:C | 1:39:C:GLY:N  | 1:39:C:GLY:CA | 1:39:C:GLY:C | 6        | 1.88          |
| (1,85)  | 1:79:C:PHE:C | 1:80:C:THR:N  | 1:80:C:THR:CA | 1:80:C:THR:C | 6        | 1.87          |
| (1,109) | 1:92:C:SER:C | 1:93:C:GLN:N  | 1:93:C:GLN:CA | 1:93:C:GLN:C | 8        | 1.84          |
| (1,22)  | 1:39:C:GLY:N | 1:39:C:GLY:CA | 1:39:C:GLY:C  | 1:40:C:HIS:N | 9        | 1.84          |
| (1,21)  | 1:38:C:LYS:C | 1:39:C:GLY:N  | 1:39:C:GLY:CA | 1:39:C:GLY:C | 8        | 1.84          |
| (1,37)  | 1:48:C:GLY:C | 1:49:C:ALA:N  | 1:49:C:ALA:CA | 1:49:C:ALA:C | 2        | 1.81          |
| (1,37)  | 1:48:C:GLY:C | 1:49:C:ALA:N  | 1:49:C:ALA:CA | 1:49:C:ALA:C | 7        | 1.79          |
| (1,100) | 1:88:C:PHE:N | 1:88:C:PHE:CA | 1:88:C:PHE:C  | 1:89:C:VAL:N | 1        | 1.75          |
| (1,21)  | 1:38:C:LYS:C | 1:39:C:GLY:N  | 1:39:C:GLY:CA | 1:39:C:GLY:C | 9        | 1.74          |
| (1,85)  | 1:79:C:PHE:C | 1:80:C:THR:N  | 1:80:C:THR:CA | 1:80:C:THR:C | 9        | 1.68          |
| (1,90)  | 1:82:C:ASP:N | 1:82:C:ASP:CA | 1:82:C:ASP:C  | 1:83:C:GLU:N | 3        | 1.67          |
| (1,37)  | 1:48:C:GLY:C | 1:49:C:ALA:N  | 1:49:C:ALA:CA | 1:49:C:ALA:C | 10       | 1.67          |
| (1,37)  | 1:48:C:GLY:C | 1:49:C:ALA:N  | 1:49:C:ALA:CA | 1:49:C:ALA:C | 5        | 1.64          |
| (1,85)  | 1:79:C:PHE:C | 1:80:C:THR:N  | 1:80:C:THR:CA | 1:80:C:THR:C | 8        | 1.61          |
| (1,109) | 1:92:C:SER:C | 1:93:C:GLN:N  | 1:93:C:GLN:CA | 1:93:C:GLN:C | 5        | 1.6           |
| (1,85)  | 1:79:C:PHE:C | 1:80:C:THR:N  | 1:80:C:THR:CA | 1:80:C:THR:C | 2        | 1.53          |
| (1,85)  | 1:79:C:PHE:C | 1:80:C:THR:N  | 1:80:C:THR:CA | 1:80:C:THR:C | 5        | 1.51          |
| (1,77)  | 1:75:C:GLY:C | 1:76:C:ARG:N  | 1:76:C:ARG:CA | 1:76:C:ARG:C | 7        | 1.51          |
| (1,85)  | 1:79:C:PHE:C | 1:80:C:THR:N  | 1:80:C:THR:CA | 1:80:C:THR:C | 10       | 1.5           |
| (1,21)  | 1:38:C:LYS:C | 1:39:C:GLY:N  | 1:39:C:GLY:CA | 1:39:C:GLY:C | 7        | 1.5           |
| (1,79)  | 1:76:C:ARG:C | 1:77:C:LYS:N  | 1:77:C:LYS:CA | 1:77:C:LYS:C | 1        | 1.44          |
| (1,62)  | 1:63:C:ASP:N | 1:63:C:ASP:CA | 1:63:C:ASP:C  | 1:64:C:GLU:N | 7        | 1.42          |
| (1,100) | 1:88:C:PHE:N | 1:88:C:PHE:CA | 1:88:C:PHE:C  | 1:89:C:VAL:N | 10       | 1.4           |
| (1,100) | 1:88:C:PHE:N | 1:88:C:PHE:CA | 1:88:C:PHE:C  | 1:89:C:VAL:N | 5        | 1.39          |
| (1,77)  | 1:75:C:GLY:C | 1:76:C:ARG:N  | 1:76:C:ARG:CA | 1:76:C:ARG:C | 6        | 1.33          |
| (1,62)  | 1:63:C:ASP:N | 1:63:C:ASP:CA | 1:63:C:ASP:C  | 1:64:C:GLU:N | 6        | 1.28          |
| (1,22)  | 1:39:C:GLY:N | 1:39:C:GLY:CA | 1:39:C:GLY:C  | 1:40:C:HIS:N | 5        | 1.28          |
| (1,37)  | 1:48:C:GLY:C | 1:49:C:ALA:N  | 1:49:C:ALA:CA | 1:49:C:ALA:C | 8        | 1.27          |
| (1,77)  | 1:75:C:GLY:C | 1:76:C:ARG:N  | 1:76:C:ARG:CA | 1:76:C:ARG:C | 8        | 1.26          |
| (1,90)  | 1:82:C:ASP:N | 1:82:C:ASP:CA | 1:82:C:ASP:C  | 1:83:C:GLU:N | 9        | 1.25          |
| (1,85)  | 1:79:C:PHE:C | 1:80:C:THR:N  | 1:80:C:THR:CA | 1:80:C:THR:C | 7        | 1.22          |
| (1,95)  | 1:85:C:HIS:C | 1:86:C:GLY:N  | 1:86:C:GLY:CA | 1:86:C:GLY:C | 9        | 1.2           |
| (1,37)  | 1:48:C:GLY:C | 1:49:C:ALA:N  | 1:49:C:ALA:CA | 1:49:C:ALA:C | 6        | 1.2           |
| (1,46)  | 1:54:C:THR:N | 1:54:C:THR:CA | 1:54:C:THR:C  | 1:55:C:GLY:N | 9        | 1.17          |
| (1,1)   | 1:26:C:PRO:C | 1:27:C:LEU:N  | 1:27:C:LEU:CA | 1:27:C:LEU:C | 2        | 1.15          |
| (1,80)  | 1:77:C:LYS:N | 1:77:C:LYS:CA | 1:77:C:LYS:C  | 1:78:C:TYR:N | 1        | 1.03          |