



# Full wwPDB NMR Structure Validation Report ⓘ

Mar 26, 2026 – 01:19 PM UTC

PDB ID : 2MR5 / pdb\_00002mr5  
BMRB ID : 25061  
Title : Solution NMR Structure of De novo designed Protein, Northeast Structural Genomics Consortium (NESG) Target OR457  
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Deposited on : 2014-07-01

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

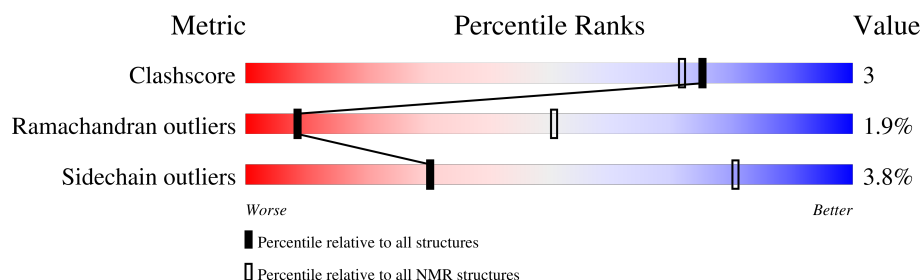
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 88%.

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



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

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 136    |                  |

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 7 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

| Well-defined (core) protein residues |                       |                   |              |
|--------------------------------------|-----------------------|-------------------|--------------|
| Well-defined core                    | Residue range (total) | Backbone RMSD (Å) | Medoid model |
| 1                                    | A:2-A:127 (126)       | 0.91              | 7            |

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

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

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

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

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2276 atoms, of which 1158 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called De novo designed Protein OR457.

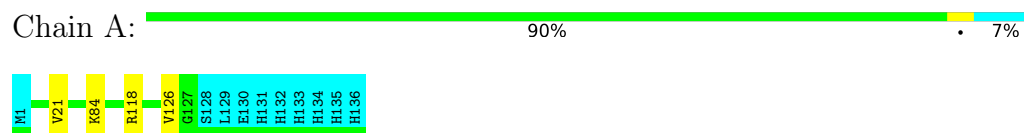
| Mol | Chain | Residues | Atoms |     |      |     |     |   | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|-------|
| 1   | A     | 136      | Total | C   | H    | N   | O   | S | 0     |
|     |       |          | 2276  | 701 | 1158 | 201 | 215 | 1 |       |

## 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: De novo designed Protein OR457

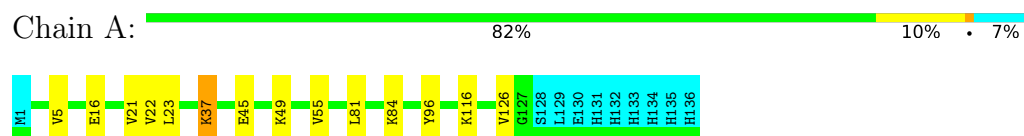


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

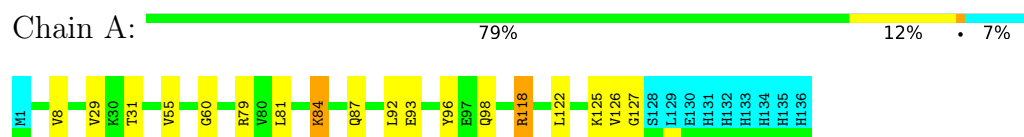
#### 4.2.1 Score per residue for model 1

- Molecule 1: De novo designed Protein OR457



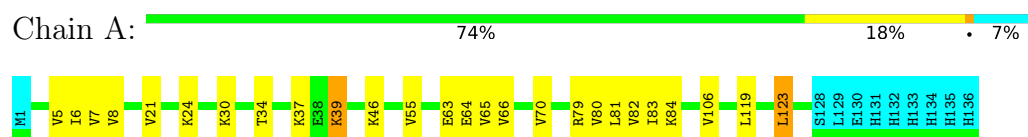
#### 4.2.2 Score per residue for model 2

- Molecule 1: De novo designed Protein OR457



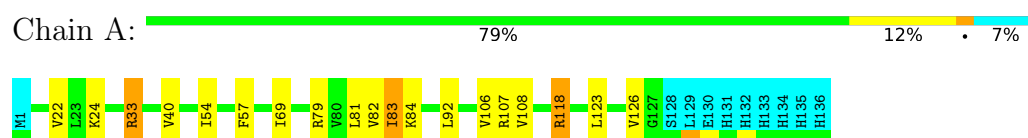
### 4.2.3 Score per residue for model 3

- Molecule 1: De novo designed Protein OR457



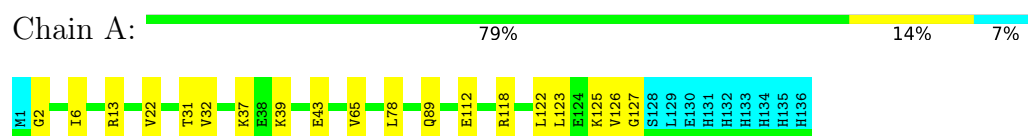
### 4.2.4 Score per residue for model 4

- Molecule 1: De novo designed Protein OR457



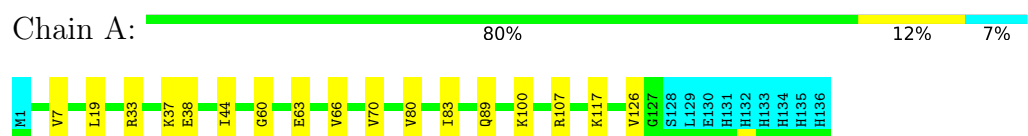
### 4.2.5 Score per residue for model 5

- Molecule 1: De novo designed Protein OR457



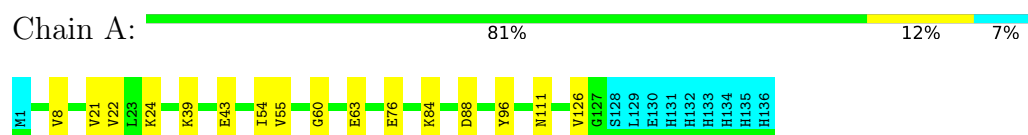
### 4.2.6 Score per residue for model 6

- Molecule 1: De novo designed Protein OR457



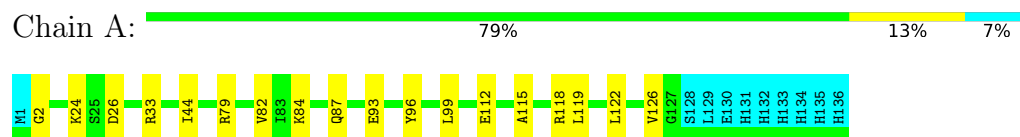
### 4.2.7 Score per residue for model 7 (medoid)

- Molecule 1: De novo designed Protein OR457



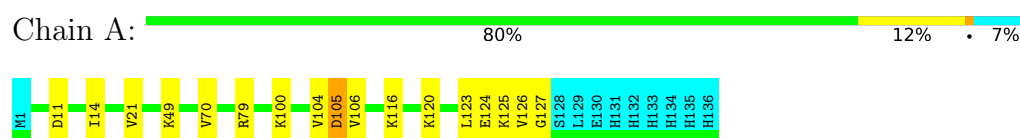
### 4.2.8 Score per residue for model 8

- Molecule 1: De novo designed Protein OR457



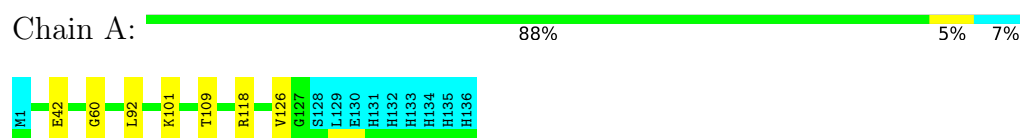
### 4.2.9 Score per residue for model 9

- Molecule 1: De novo designed Protein OR457



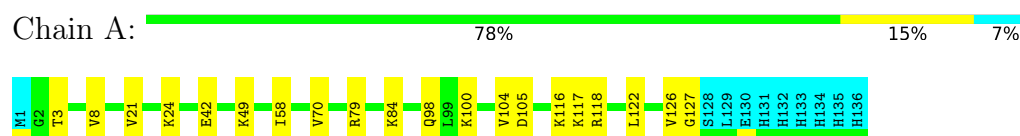
### 4.2.10 Score per residue for model 10

- Molecule 1: De novo designed Protein OR457



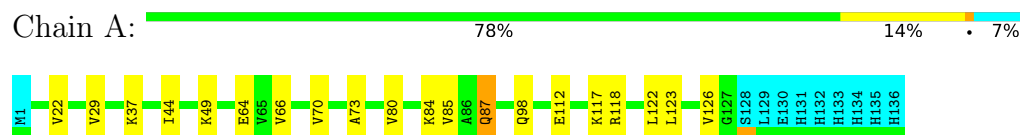
### 4.2.11 Score per residue for model 11

- Molecule 1: De novo designed Protein OR457



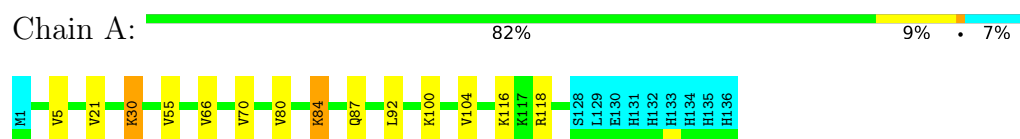
### 4.2.12 Score per residue for model 12

- Molecule 1: De novo designed Protein OR457



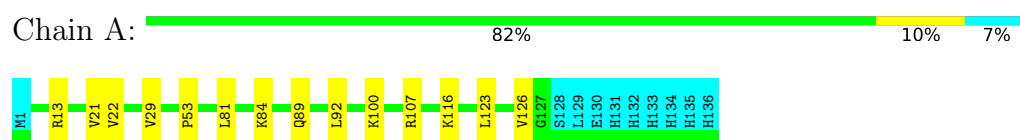
### 4.2.13 Score per residue for model 13

- Molecule 1: De novo designed Protein OR457



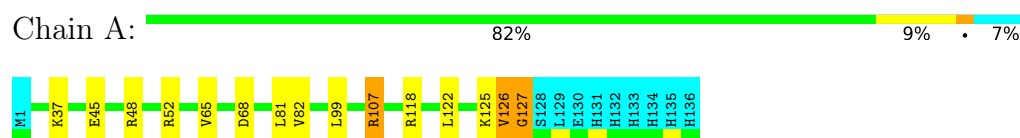
### 4.2.14 Score per residue for model 14

- Molecule 1: De novo designed Protein OR457



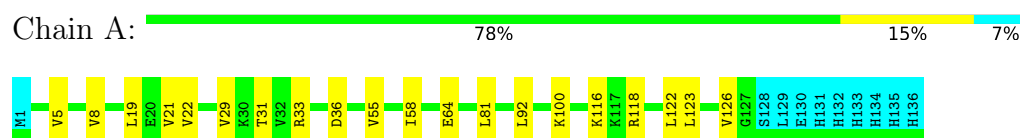
### 4.2.15 Score per residue for model 15

- Molecule 1: De novo designed Protein OR457



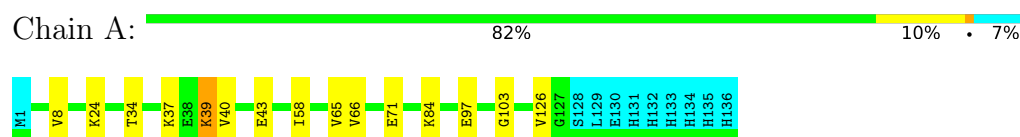
### 4.2.16 Score per residue for model 16

- Molecule 1: De novo designed Protein OR457



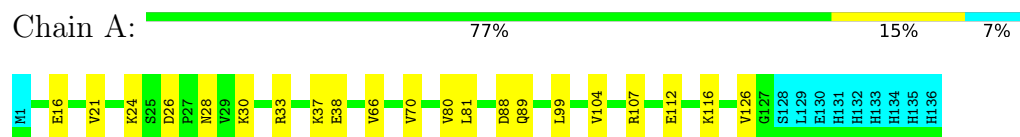
### 4.2.17 Score per residue for model 17

- Molecule 1: De novo designed Protein OR457



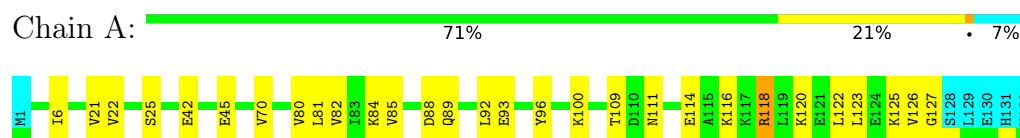
### 4.2.18 Score per residue for model 18

- Molecule 1: De novo designed Protein OR457



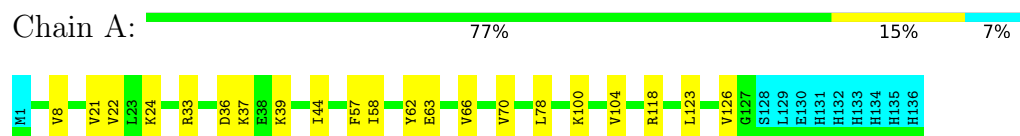
### 4.2.19 Score per residue for model 19

- Molecule 1: De novo designed Protein OR457



### 4.2.20 Score per residue for model 20

- Molecule 1: De novo designed Protein OR457



## 5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

| Software name | Classification        | Version |
|---------------|-----------------------|---------|
| CNS           | refinement            |         |
| CNS           | structure solution    |         |
| CNS           | geometry optimization |         |
| CYANA         | refinement            | 3.0     |
| CYANA         | geometry optimization | 3.0     |
| CYANA         | structure solution    | 3.0     |
| AutoStructure | refinement            | 2.1     |
| TALOS+        | geometry optimization |         |

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                       | 1661           |
| Number of shifts mapped to atoms             | 1661           |
| Number of unparsed shifts                    | 0              |
| Number of shifts with mapping errors         | 0              |
| Number of shifts with mapping warnings       | 0              |
| Assignment completeness (well-defined parts) | 88%            |

## 6 Model quality [i](#)

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

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

| Mol | Chain | Bond lengths |                       | Bond angles |                       |
|-----|-------|--------------|-----------------------|-------------|-----------------------|
|     |       | RMSZ         | #Z>5                  | RMSZ        | #Z>5                  |
| 1   | A     | 1.23±0.03    | 0±1/1033 ( 0.0± 0.1%) | 1.05±0.02   | 0±0/1387 ( 0.0± 0.0%) |
| All | All   | 1.23         | 9/20660 ( 0.0%)       | 1.05        | 0/27740 ( 0.0%)       |

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

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) | Models |       |
|-----|-------|-----|------|-------|------|-------------|----------|--------|-------|
|     |       |     |      |       |      |             |          | Worst  | Total |
| 1   | A     | 125 | LYS  | CA-C  | 7.54 | 1.56        | 1.52     | 15     | 2     |
| 1   | A     | 44  | ILE  | CA-CB | 5.29 | 1.60        | 1.54     | 8      | 1     |
| 1   | A     | 52  | ARG  | C-N   | 5.12 | 1.39        | 1.33     | 15     | 1     |
| 1   | A     | 6   | ILE  | CA-CB | 5.11 | 1.59        | 1.53     | 5      | 1     |
| 1   | A     | 85  | VAL  | CA-CB | 5.08 | 1.58        | 1.53     | 19     | 1     |
| 1   | A     | 26  | ASP  | C-N   | 5.01 | 1.38        | 1.33     | 8      | 2     |
| 1   | A     | 108 | VAL  | CA-CB | 5.00 | 1.59        | 1.53     | 4      | 1     |

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes |
|-----|-------|-------|----------|----------|---------|
| 1   | A     | 1026  | 1077     | 1077     | 7±3     |
| All | All   | 20520 | 21540    | 21540    | 131     |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 3.

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

| Atom-1          | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|-----------------|------------------|----------|-------------|--------|-------|
|                 |                  |          |             | Worst  | Total |
| 1:A:82:VAL:HG11 | 1:A:99:LEU:HD13  | 0.61     | 1.70        | 15     | 1     |
| 1:A:84:LYS:HE2  | 1:A:96:TYR:HB2   | 0.60     | 1.71        | 1      | 1     |
| 1:A:70:VAL:HG22 | 1:A:80:VAL:HG11  | 0.60     | 1.73        | 6      | 6     |
| 1:A:81:LEU:HD11 | 1:A:107:ARG:HG3  | 0.56     | 1.77        | 4      | 1     |
| 1:A:81:LEU:HD11 | 1:A:107:ARG:HG2  | 0.56     | 1.76        | 18     | 2     |
| 1:A:84:LYS:HE3  | 1:A:92:LEU:HD11  | 0.55     | 1.79        | 4      | 1     |
| 1:A:21:VAL:HG21 | 1:A:116:LYS:HG3  | 0.54     | 1.79        | 9      | 5     |
| 1:A:83:ILE:HG21 | 1:A:118:ARG:HD3  | 0.54     | 1.78        | 4      | 1     |
| 1:A:58:ILE:HD13 | 1:A:66:VAL:HG21  | 0.53     | 1.81        | 17     | 1     |
| 1:A:82:VAL:HG21 | 1:A:99:LEU:HD13  | 0.53     | 1.79        | 8      | 1     |
| 1:A:29:VAL:HG22 | 1:A:53:PRO:HG2   | 0.53     | 1.79        | 14     | 1     |
| 1:A:33:ARG:HB3  | 1:A:57:PHE:HB2   | 0.53     | 1.81        | 4      | 1     |
| 1:A:8:VAL:HG22  | 1:A:58:ILE:HD11  | 0.53     | 1.79        | 17     | 1     |
| 1:A:93:GLU:HA   | 1:A:96:TYR:HB3   | 0.52     | 1.80        | 19     | 3     |
| 1:A:33:ARG:HG3  | 1:A:57:PHE:HB2   | 0.52     | 1.80        | 20     | 1     |
| 1:A:6:ILE:HD13  | 1:A:82:VAL:HG22  | 0.52     | 1.82        | 19     | 1     |
| 1:A:70:VAL:HG11 | 1:A:104:VAL:HG21 | 0.51     | 1.82        | 13     | 3     |
| 1:A:22:VAL:HG11 | 1:A:55:VAL:HG21  | 0.51     | 1.81        | 1      | 2     |
| 1:A:37:LYS:HA   | 1:A:65:VAL:HG13  | 0.50     | 1.81        | 15     | 1     |
| 1:A:11:ASP:HB2  | 1:A:14:ILE:HG12  | 0.50     | 1.83        | 9      | 1     |
| 1:A:82:VAL:HB   | 1:A:106:VAL:HG12 | 0.49     | 1.83        | 3      | 2     |
| 1:A:29:VAL:HG11 | 1:A:55:VAL:HG23  | 0.49     | 1.83        | 2      | 1     |
| 1:A:22:VAL:HG13 | 1:A:123:LEU:HD21 | 0.49     | 1.85        | 12     | 7     |
| 1:A:19:LEU:HB2  | 1:A:33:ARG:HH12  | 0.48     | 1.68        | 6      | 1     |
| 1:A:88:ASP:HB2  | 1:A:92:LEU:HB2   | 0.47     | 1.86        | 19     | 1     |
| 1:A:44:ILE:HG23 | 1:A:78:LEU:HD12  | 0.47     | 1.85        | 20     | 1     |
| 1:A:8:VAL:HB    | 1:A:84:LYS:HB3   | 0.47     | 1.86        | 2      | 2     |
| 1:A:83:ILE:HG23 | 1:A:107:ARG:HB2  | 0.46     | 1.87        | 4      | 1     |
| 1:A:21:VAL:HG21 | 1:A:116:LYS:HB2  | 0.46     | 1.87        | 1      | 1     |
| 1:A:5:VAL:O     | 1:A:55:VAL:HA    | 0.46     | 2.11        | 3      | 2     |
| 1:A:81:LEU:HD11 | 1:A:107:ARG:HD2  | 0.46     | 1.86        | 15     | 1     |
| 1:A:29:VAL:HG21 | 1:A:123:LEU:HG   | 0.45     | 1.88        | 16     | 2     |
| 1:A:118:ARG:O   | 1:A:122:LEU:HG   | 0.45     | 2.11        | 16     | 6     |
| 1:A:21:VAL:HG11 | 1:A:116:LYS:O    | 0.45     | 2.11        | 19     | 1     |
| 1:A:32:VAL:HG11 | 1:A:43:GLU:HG3   | 0.45     | 1.89        | 5      | 1     |
| 1:A:5:VAL:HG11  | 1:A:122:LEU:HD13 | 0.45     | 1.88        | 16     | 1     |
| 1:A:8:VAL:HG11  | 1:A:63:GLU:HB2   | 0.45     | 1.88        | 7      | 2     |
| 1:A:21:VAL:HG21 | 1:A:116:LYS:HG2  | 0.44     | 1.89        | 16     | 1     |
| 1:A:58:ILE:HB   | 1:A:62:TYR:HB2   | 0.44     | 1.88        | 20     | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:30:LYS:HE3   | 1:A:46:LYS:HB3   | 0.44     | 1.88        | 3      | 1     |
| 1:A:122:LEU:HB3  | 1:A:127:GLY:HA2  | 0.44     | 1.89        | 11     | 1     |
| 1:A:119:LEU:O    | 1:A:123:LEU:HB2  | 0.44     | 2.13        | 3      | 1     |
| 1:A:40:VAL:HG11  | 1:A:69:ILE:HD13  | 0.44     | 1.88        | 4      | 1     |
| 1:A:100:LYS:HA   | 1:A:100:LYS:HE2  | 0.44     | 1.90        | 19     | 1     |
| 1:A:39:LYS:O     | 1:A:43:GLU:HG2   | 0.44     | 2.13        | 17     | 3     |
| 1:A:100:LYS:HE3  | 1:A:105:ASP:HA   | 0.44     | 1.89        | 11     | 2     |
| 1:A:34:THR:HG21  | 1:A:39:LYS:HG2   | 0.44     | 1.88        | 3      | 1     |
| 1:A:37:LYS:H     | 1:A:37:LYS:HD2   | 0.44     | 1.72        | 1      | 1     |
| 1:A:85:VAL:HG12  | 1:A:87:GLN:HG2   | 0.44     | 1.89        | 12     | 1     |
| 1:A:111:ASN:HB2  | 1:A:114:GLU:HG2  | 0.43     | 1.90        | 19     | 1     |
| 1:A:5:VAL:HA     | 1:A:81:LEU:O     | 0.43     | 2.13        | 16     | 3     |
| 1:A:66:VAL:O     | 1:A:70:VAL:HG23  | 0.43     | 2.14        | 18     | 6     |
| 1:A:70:VAL:HG11  | 1:A:104:VAL:HG22 | 0.43     | 1.91        | 20     | 1     |
| 1:A:19:LEU:HD22  | 1:A:33:ARG:NH2   | 0.43     | 2.29        | 16     | 1     |
| 1:A:6:ILE:HG21   | 1:A:66:VAL:HG21  | 0.43     | 1.91        | 3      | 1     |
| 1:A:3:THR:HG22   | 1:A:79:ARG:HB3   | 0.43     | 1.90        | 11     | 1     |
| 1:A:42:GLU:O     | 1:A:45:GLU:HG2   | 0.43     | 2.14        | 19     | 1     |
| 1:A:36:ASP:HB3   | 1:A:39:LYS:HB3   | 0.43     | 1.91        | 20     | 1     |
| 1:A:21:VAL:HA    | 1:A:24:LYS:HE2   | 0.42     | 1.90        | 11     | 4     |
| 1:A:19:LEU:HD22  | 1:A:33:ARG:HH21  | 0.42     | 1.74        | 16     | 1     |
| 1:A:34:THR:HG23  | 1:A:40:VAL:HG22  | 0.42     | 1.91        | 17     | 1     |
| 1:A:109:THR:HB   | 1:A:114:GLU:HB2  | 0.42     | 1.91        | 19     | 1     |
| 1:A:45:GLU:O     | 1:A:49:LYS:HB2   | 0.42     | 2.15        | 1      | 1     |
| 1:A:84:LYS:HG3   | 1:A:92:LEU:HD11  | 0.42     | 1.90        | 13     | 1     |
| 1:A:7:VAL:HA     | 1:A:83:ILE:O     | 0.42     | 2.14        | 3      | 2     |
| 1:A:122:LEU:HD22 | 1:A:127:GLY:HA2  | 0.42     | 1.91        | 15     | 1     |
| 1:A:79:ARG:NH2   | 1:A:81:LEU:HD22  | 0.42     | 2.30        | 2      | 1     |
| 1:A:2:GLY:HA3    | 1:A:78:LEU:HD22  | 0.41     | 1.92        | 5      | 1     |
| 1:A:37:LYS:HE2   | 1:A:65:VAL:HG13  | 0.41     | 1.92        | 5      | 2     |
| 1:A:8:VAL:HA     | 1:A:58:ILE:O     | 0.41     | 2.15        | 16     | 2     |
| 1:A:89:GLN:HB2   | 1:A:92:LEU:HB2   | 0.41     | 1.93        | 14     | 1     |
| 1:A:8:VAL:HG21   | 1:A:63:GLU:HG3   | 0.41     | 1.92        | 3      | 2     |
| 1:A:120:LYS:O    | 1:A:124:GLU:HG2  | 0.41     | 2.14        | 9      | 1     |
| 1:A:8:VAL:HG22   | 1:A:58:ILE:HB    | 0.41     | 1.92        | 11     | 1     |
| 1:A:99:LEU:HB3   | 1:A:104:VAL:HB   | 0.41     | 1.93        | 18     | 1     |
| 1:A:37:LYS:HE3   | 1:A:65:VAL:HG13  | 0.41     | 1.92        | 3      | 1     |
| 1:A:96:TYR:HA    | 1:A:99:LEU:HD12  | 0.41     | 1.93        | 8      | 1     |
| 1:A:115:ALA:O    | 1:A:119:LEU:HG   | 0.41     | 2.16        | 8      | 1     |
| 1:A:109:THR:HG22 | 1:A:118:ARG:HD2  | 0.41     | 1.93        | 10     | 1     |
| 1:A:31:THR:HG22  | 1:A:55:VAL:HB    | 0.40     | 1.92        | 16     | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:16:GLU:HA   | 1:A:33:ARG:NH2  | 0.40     | 2.31        | 18     | 1     |
| 1:A:44:ILE:HD13 | 1:A:73:ALA:HB2  | 0.40     | 1.93        | 12     | 1     |
| 1:A:25:SER:HB2  | 1:A:120:LYS:HG3 | 0.40     | 1.93        | 19     | 1     |

## 6.3 Torsion angles [i](#)

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

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

| Mol | Chain | Analysed        | Favoured      | Allowed    | Outliers   | Percentiles |    |
|-----|-------|-----------------|---------------|------------|------------|-------------|----|
| 1   | A     | 126/136 (93%)   | 118±3 (93±2%) | 6±2 (5±2%) | 2±1 (2±1%) | 8           | 51 |
| All | All   | 2520/2720 (93%) | 2353 (93%)    | 120 (5%)   | 47 (2%)    | 8           | 51 |

All 13 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 126 | VAL  | 18             |
| 1   | A     | 127 | GLY  | 5              |
| 1   | A     | 60  | GLY  | 4              |
| 1   | A     | 87  | GLN  | 4              |
| 1   | A     | 89  | GLN  | 4              |
| 1   | A     | 37  | LYS  | 3              |
| 1   | A     | 31  | THR  | 2              |
| 1   | A     | 88  | ASP  | 2              |
| 1   | A     | 111 | ASN  | 1              |
| 1   | A     | 2   | GLY  | 1              |
| 1   | A     | 30  | LYS  | 1              |
| 1   | A     | 36  | ASP  | 1              |
| 1   | A     | 103 | GLY  | 1              |

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

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

was analysed and the total number of residues.

| Mol | Chain | Analysed        | Rotameric     | Outliers   | Percentiles |    |
|-----|-------|-----------------|---------------|------------|-------------|----|
| 1   | A     | 115/125 (92%)   | 111±1 (96±1%) | 4±1 (4±1%) | 30          | 81 |
| All | All   | 2300/2500 (92%) | 2213 (96%)    | 87 (4%)    | 30          | 81 |

All 39 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 84  | LYS  | 9              |
| 1   | A     | 118 | ARG  | 7              |
| 1   | A     | 100 | LYS  | 5              |
| 1   | A     | 24  | LYS  | 4              |
| 1   | A     | 112 | GLU  | 4              |
| 1   | A     | 92  | LEU  | 3              |
| 1   | A     | 98  | GLN  | 3              |
| 1   | A     | 125 | LYS  | 3              |
| 1   | A     | 64  | GLU  | 3              |
| 1   | A     | 79  | ARG  | 3              |
| 1   | A     | 117 | LYS  | 3              |
| 1   | A     | 49  | LYS  | 3              |
| 1   | A     | 37  | LYS  | 2              |
| 1   | A     | 39  | LYS  | 2              |
| 1   | A     | 123 | LEU  | 2              |
| 1   | A     | 33  | ARG  | 2              |
| 1   | A     | 54  | ILE  | 2              |
| 1   | A     | 13  | ARG  | 2              |
| 1   | A     | 38  | GLU  | 2              |
| 1   | A     | 107 | ARG  | 2              |
| 1   | A     | 42  | GLU  | 2              |
| 1   | A     | 30  | LYS  | 2              |
| 1   | A     | 16  | GLU  | 1              |
| 1   | A     | 23  | LEU  | 1              |
| 1   | A     | 83  | ILE  | 1              |
| 1   | A     | 44  | ILE  | 1              |
| 1   | A     | 63  | GLU  | 1              |
| 1   | A     | 76  | GLU  | 1              |
| 1   | A     | 96  | TYR  | 1              |
| 1   | A     | 105 | ASP  | 1              |
| 1   | A     | 106 | VAL  | 1              |
| 1   | A     | 101 | LYS  | 1              |
| 1   | A     | 45  | GLU  | 1              |
| 1   | A     | 48  | ARG  | 1              |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 68  | ASP  | 1              |
| 1   | A     | 126 | VAL  | 1              |
| 1   | A     | 71  | GLU  | 1              |
| 1   | A     | 97  | GLU  | 1              |
| 1   | A     | 28  | ASN  | 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 [i](#)

There are no chain breaks in this entry.

## 7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 88% for the well-defined parts and 83% for the entire structure.

### 7.1 Chemical shift list 1

File name: working\_cs.cif

Chemical shift list name: *assigned\_chem\_shift\_list\_2*

#### 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                  | 1661 |
| Number of shifts mapped to atoms        | 1661 |
| Number of unparsed shifts               | 0    |
| Number of shifts with mapping errors    | 0    |
| Number of shifts with mapping warnings  | 0    |
| Number of shift outliers (ShiftChecker) | 0    |

#### 7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

| Nucleus                | # values | Correction $\pm$ precision, ppm | Suggested action           |
|------------------------|----------|---------------------------------|----------------------------|
| $^{13}\text{C}_\alpha$ | 126      | $-0.03 \pm 0.11$                | None needed ( $< 0.5$ ppm) |
| $^{13}\text{C}_\beta$  | 121      | $0.27 \pm 0.04$                 | None needed ( $< 0.5$ ppm) |
| $^{13}\text{C}'$       | 120      | $0.19 \pm 0.13$                 | None needed ( $< 0.5$ ppm) |
| $^{15}\text{N}$        | 112      | $-0.07 \pm 0.17$                | 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 88%, i.e. 1624 atoms were assigned a chemical shift out of a possible 1841. 0 out of 32 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total          | $^1\text{H}$  | $^{13}\text{C}$ | $^{15}\text{N}$ |
|-----------|----------------|---------------|-----------------|-----------------|
| Backbone  | 587/632 (93%)  | 238/256 (93%) | 240/252 (95%)   | 109/124 (88%)   |
| Sidechain | 993/1162 (85%) | 677/745 (91%) | 308/364 (85%)   | 8/53 (15%)      |

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|          | Total           | <sup>1</sup> H | <sup>13</sup> C | <sup>15</sup> N |
|----------|-----------------|----------------|-----------------|-----------------|
| Aromatic | 44/47 (94%)     | 22/22 (100%)   | 22/25 (88%)     | 0/0 (—%)        |
| Overall  | 1624/1841 (88%) | 937/1023 (92%) | 570/641 (89%)   | 117/177 (66%)   |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 83%, i.e. 1661 atoms were assigned a chemical shift out of a possible 1990. 0 out of 33 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total           | <sup>1</sup> H | <sup>13</sup> C | <sup>15</sup> N |
|-----------|-----------------|----------------|-----------------|-----------------|
| Backbone  | 602/682 (88%)   | 244/276 (88%)  | 246/272 (90%)   | 112/134 (84%)   |
| Sidechain | 1015/1213 (84%) | 692/779 (89%)  | 315/381 (83%)   | 8/53 (15%)      |
| Aromatic  | 44/95 (46%)     | 22/46 (48%)    | 22/37 (59%)     | 0/12 (0%)       |
| Overall   | 1661/1990 (83%) | 958/1101 (87%) | 583/690 (84%)   | 120/199 (60%)   |

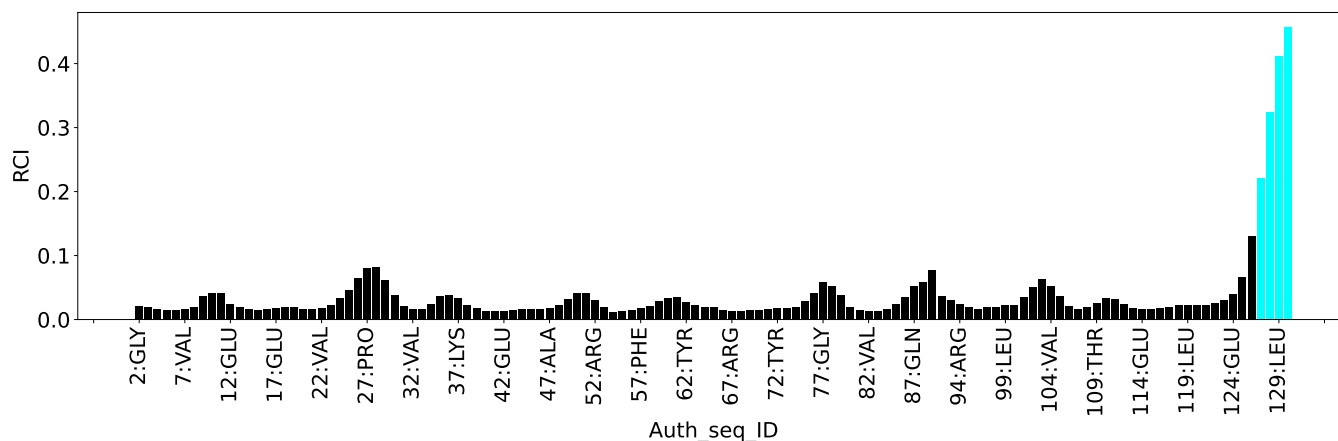
#### 7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

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

Random coil index (RCI) for chain A:



## 8 NMR restraints analysis

### 8.1 Conformationally restricting restraints

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

| Description                                              | Value |
|----------------------------------------------------------|-------|
| Total distance restraints                                | 2416  |
| Intra-residue ( $ i-j =0$ )                              | 404   |
| Sequential ( $ i-j =1$ )                                 | 640   |
| Medium range ( $ i-j >1$ and $ i-j <5$ )                 | 561   |
| Long range ( $ i-j \geq 5$ )                             | 811   |
| Inter-chain                                              | 0     |
| Hydrogen bond restraints                                 | 0     |
| Disulfide bond restraints                                | 0     |
| Total dihedral-angle restraints                          | 158   |
| Number of unmapped restraints                            | 0     |
| Number of restraints per residue                         | 18.9  |
| Number of long range restraints per residue <sup>1</sup> | 6.0   |

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

### 8.2 Residual restraint violations

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

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

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

| Bins (Å)         | Average number of violations per model | Max (Å) |
|------------------|----------------------------------------|---------|
| 0.1-0.2 (Small)  | 16.4                                   | 0.2     |
| 0.2-0.5 (Medium) | 8.0                                    | 0.45    |
| >0.5 (Large)     | None                                   | None    |

### 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)   | 28.4                                   | 9.97    |
| 10.0-20.0 (Medium) | 0.1                                    | 10.86   |
| >20.0 (Large)      | None                                   | None    |

## 9 Distance violation analysis ⓘ

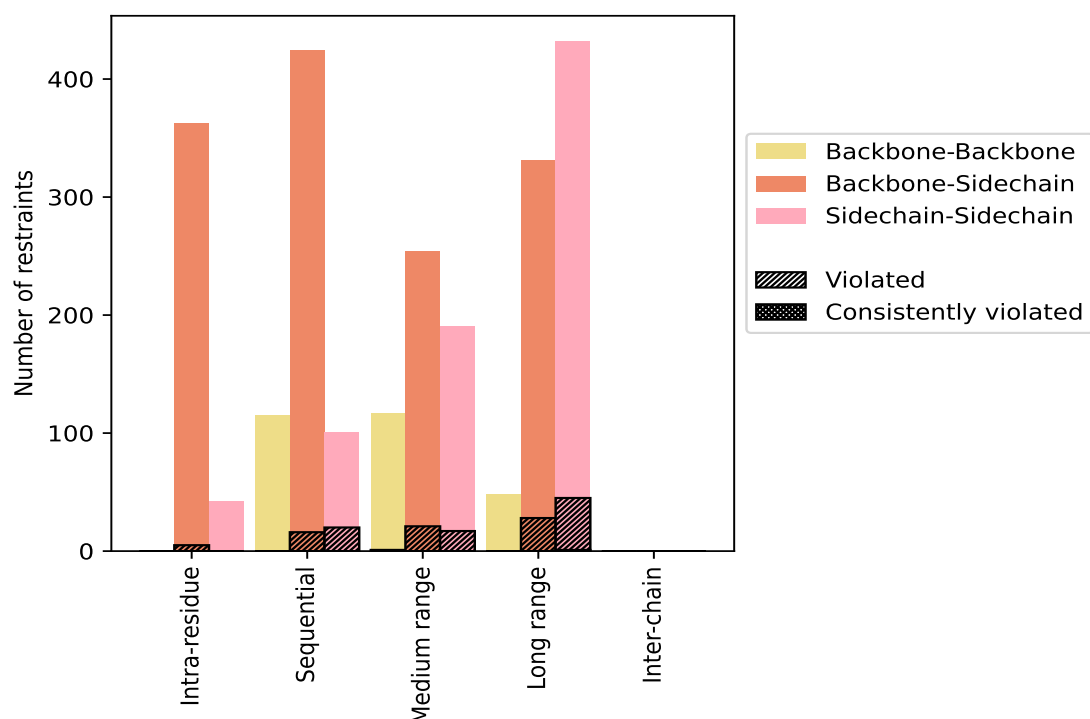
### 9.1 Summary of distance violations ⓘ

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

| Restrains type                                                              | Count       | % <sup>1</sup> | Violated <sup>3</sup> |                |                | Consistently Violated <sup>4</sup> |                |                |
|-----------------------------------------------------------------------------|-------------|----------------|-----------------------|----------------|----------------|------------------------------------|----------------|----------------|
|                                                                             |             |                | Count                 | % <sup>2</sup> | % <sup>1</sup> | Count                              | % <sup>2</sup> | % <sup>1</sup> |
| <b>Intra-residue (<math> i-j =0</math>)</b>                                 | <b>404</b>  | <b>16.7</b>    | <b>5</b>              | <b>1.2</b>     | <b>0.2</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                                                          | 362         | 15.0           | 5                     | 1.4            | 0.2            | 0                                  | 0.0            | 0.0            |
| Sidechain-Sidechain                                                         | 42          | 1.7            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| <b>Sequential (<math> i-j =1</math>)</b>                                    | <b>640</b>  | <b>26.5</b>    | <b>36</b>             | <b>5.6</b>     | <b>1.5</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| Backbone-Backbone                                                           | 115         | 4.8            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 424         | 17.5           | 16                    | 3.8            | 0.7            | 0                                  | 0.0            | 0.0            |
| Sidechain-Sidechain                                                         | 101         | 4.2            | 20                    | 19.8           | 0.8            | 0                                  | 0.0            | 0.0            |
| <b>Medium range (<math> i-j &gt;1</math> &amp; <math> i-j &lt;5</math>)</b> | <b>561</b>  | <b>23.2</b>    | <b>39</b>             | <b>7.0</b>     | <b>1.6</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| Backbone-Backbone                                                           | 117         | 4.8            | 1                     | 0.9            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 254         | 10.5           | 21                    | 8.3            | 0.9            | 0                                  | 0.0            | 0.0            |
| Sidechain-Sidechain                                                         | 190         | 7.9            | 17                    | 8.9            | 0.7            | 0                                  | 0.0            | 0.0            |
| <b>Long range (<math> i-j \geq 5</math>)</b>                                | <b>811</b>  | <b>33.6</b>    | <b>73</b>             | <b>9.0</b>     | <b>3.0</b>     | <b>1</b>                           | <b>0.1</b>     | <b>0.0</b>     |
| Backbone-Backbone                                                           | 48          | 2.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 331         | 13.7           | 28                    | 8.5            | 1.2            | 0                                  | 0.0            | 0.0            |
| Sidechain-Sidechain                                                         | 432         | 17.9           | 45                    | 10.4           | 1.9            | 1                                  | 0.2            | 0.0            |
| <b>Inter-chain</b>                                                          | <b>0</b>    | <b>0.0</b>     | <b>0</b>              | <b>0.0</b>     | <b>0.0</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| Backbone-Backbone                                                           | 0           | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 0           | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Sidechain-Sidechain                                                         | 0           | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| <b>Hydrogen bond</b>                                                        | <b>0</b>    | <b>0.0</b>     | <b>0</b>              | <b>0.0</b>     | <b>0.0</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| <b>Disulfide bond</b>                                                       | <b>0</b>    | <b>0.0</b>     | <b>0</b>              | <b>0.0</b>     | <b>0.0</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| <b>Total</b>                                                                | <b>2416</b> | <b>100.0</b>   | <b>153</b>            | <b>6.3</b>     | <b>6.3</b>     | <b>1</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| Backbone-Backbone                                                           | 280         | 11.6           | 1                     | 0.4            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 1371        | 56.7           | 70                    | 5.1            | 2.9            | 0                                  | 0.0            | 0.0            |
| Sidechain-Sidechain                                                         | 765         | 31.7           | 82                    | 10.7           | 3.4            | 1                                  | 0.1            | 0.0            |

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

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



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

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

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

| Model ID | Number of violations |                 |                 |                 |                 |       | Mean (Å) | Max (Å) | SD <sup>6</sup> (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
|          | IR <sup>1</sup>      | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total |          |         |                     |            |
| 1        | 1                    | 4               | 4               | 15              | 0               | 24    | 0.18     | 0.36    | 0.07                | 0.16       |
| 2        | 0                    | 6               | 7               | 12              | 0               | 25    | 0.17     | 0.25    | 0.05                | 0.15       |
| 3        | 1                    | 7               | 6               | 9               | 0               | 23    | 0.19     | 0.32    | 0.07                | 0.19       |
| 4        | 0                    | 7               | 5               | 14              | 0               | 26    | 0.18     | 0.41    | 0.07                | 0.16       |
| 5        | 1                    | 7               | 4               | 13              | 0               | 25    | 0.18     | 0.32    | 0.07                | 0.15       |
| 6        | 2                    | 9               | 9               | 16              | 0               | 36    | 0.18     | 0.36    | 0.06                | 0.16       |
| 7        | 2                    | 6               | 4               | 10              | 0               | 22    | 0.18     | 0.29    | 0.06                | 0.16       |
| 8        | 1                    | 8               | 7               | 9               | 0               | 25    | 0.17     | 0.3     | 0.05                | 0.16       |
| 9        | 1                    | 6               | 4               | 14              | 0               | 25    | 0.17     | 0.32    | 0.05                | 0.16       |
| 10       | 1                    | 6               | 5               | 17              | 0               | 29    | 0.17     | 0.34    | 0.06                | 0.15       |

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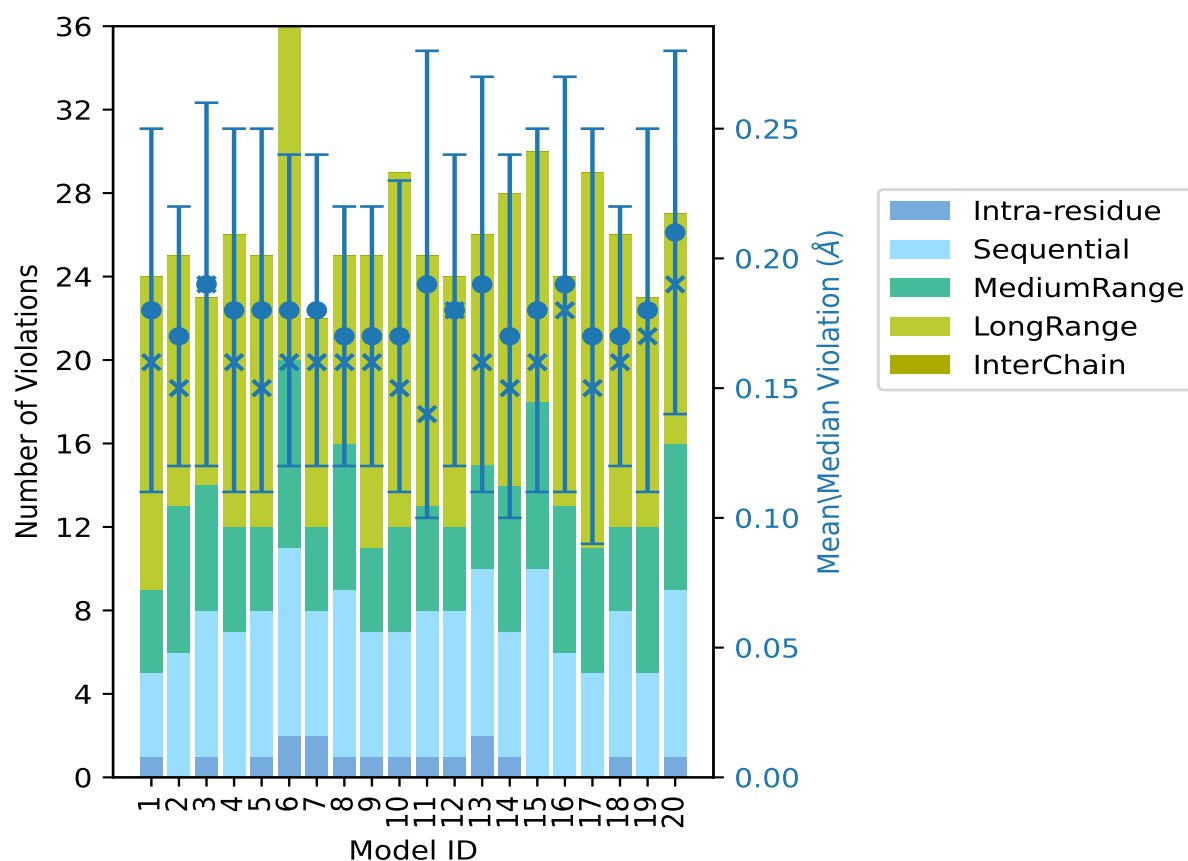
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| Model ID | Number of violations |                 |                 |                 |                 |       | Mean (Å) | Max (Å) | SD <sup>6</sup> (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
|          | IR <sup>1</sup>      | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total |          |         |                     |            |
| 11       | 1                    | 7               | 5               | 12              | 0               | 25    | 0.19     | 0.45    | 0.09                | 0.14       |
| 12       | 1                    | 7               | 4               | 12              | 0               | 24    | 0.18     | 0.33    | 0.06                | 0.18       |
| 13       | 2                    | 8               | 5               | 11              | 0               | 26    | 0.19     | 0.41    | 0.08                | 0.16       |
| 14       | 1                    | 6               | 7               | 14              | 0               | 28    | 0.17     | 0.37    | 0.07                | 0.15       |
| 15       | 0                    | 10              | 8               | 12              | 0               | 30    | 0.18     | 0.36    | 0.07                | 0.16       |
| 16       | 0                    | 6               | 7               | 11              | 0               | 24    | 0.19     | 0.43    | 0.08                | 0.18       |
| 17       | 0                    | 5               | 6               | 18              | 0               | 29    | 0.17     | 0.38    | 0.08                | 0.15       |
| 18       | 1                    | 7               | 4               | 14              | 0               | 26    | 0.17     | 0.3     | 0.05                | 0.16       |
| 19       | 0                    | 5               | 7               | 11              | 0               | 23    | 0.18     | 0.33    | 0.07                | 0.17       |
| 20       | 1                    | 8               | 7               | 11              | 0               | 27    | 0.21     | 0.35    | 0.07                | 0.19       |

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

<sup>5</sup>Inter-chain restraints, <sup>6</sup>Standard deviation

### 9.2.1 Bar graph : Distance Violation statistics for each model ⓘ



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

### 9.3 Distance violation statistics for the ensemble

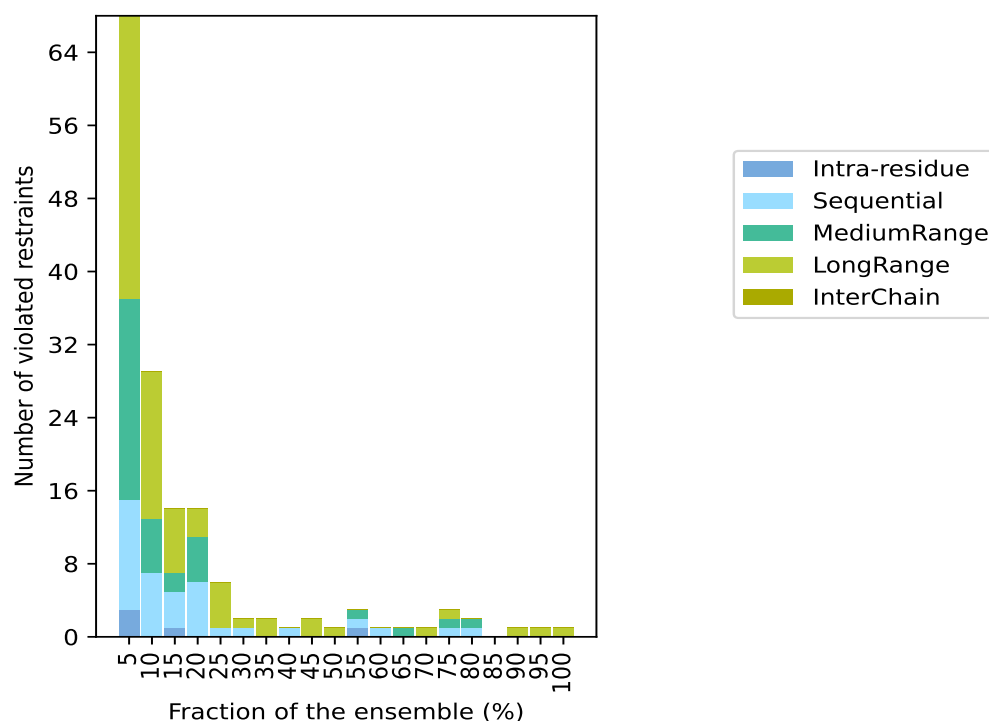
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 2263(IR:399, SQ:604, MR:522, LR:738, IC:0) restraints are 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>       | %     |
| 3                             | 12              | 22              | 31              | 0               | 68    | 1                        | 5.0   |
| 0                             | 7               | 6               | 16              | 0               | 29    | 2                        | 10.0  |
| 1                             | 4               | 2               | 7               | 0               | 14    | 3                        | 15.0  |
| 0                             | 6               | 5               | 3               | 0               | 14    | 4                        | 20.0  |
| 0                             | 1               | 0               | 5               | 0               | 6     | 5                        | 25.0  |
| 0                             | 1               | 0               | 1               | 0               | 2     | 6                        | 30.0  |
| 0                             | 0               | 0               | 2               | 0               | 2     | 7                        | 35.0  |
| 0                             | 1               | 0               | 0               | 0               | 1     | 8                        | 40.0  |
| 0                             | 0               | 0               | 2               | 0               | 2     | 9                        | 45.0  |
| 0                             | 0               | 0               | 1               | 0               | 1     | 10                       | 50.0  |
| 1                             | 1               | 1               | 0               | 0               | 3     | 11                       | 55.0  |
| 0                             | 1               | 0               | 0               | 0               | 1     | 12                       | 60.0  |
| 0                             | 0               | 1               | 0               | 0               | 1     | 13                       | 65.0  |
| 0                             | 0               | 0               | 1               | 0               | 1     | 14                       | 70.0  |
| 0                             | 1               | 1               | 1               | 0               | 3     | 15                       | 75.0  |
| 0                             | 1               | 1               | 0               | 0               | 2     | 16                       | 80.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 17                       | 85.0  |
| 0                             | 0               | 0               | 1               | 0               | 1     | 18                       | 90.0  |
| 0                             | 0               | 0               | 1               | 0               | 1     | 19                       | 95.0  |
| 0                             | 0               | 0               | 1               | 0               | 1     | 20                       | 100.0 |

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

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

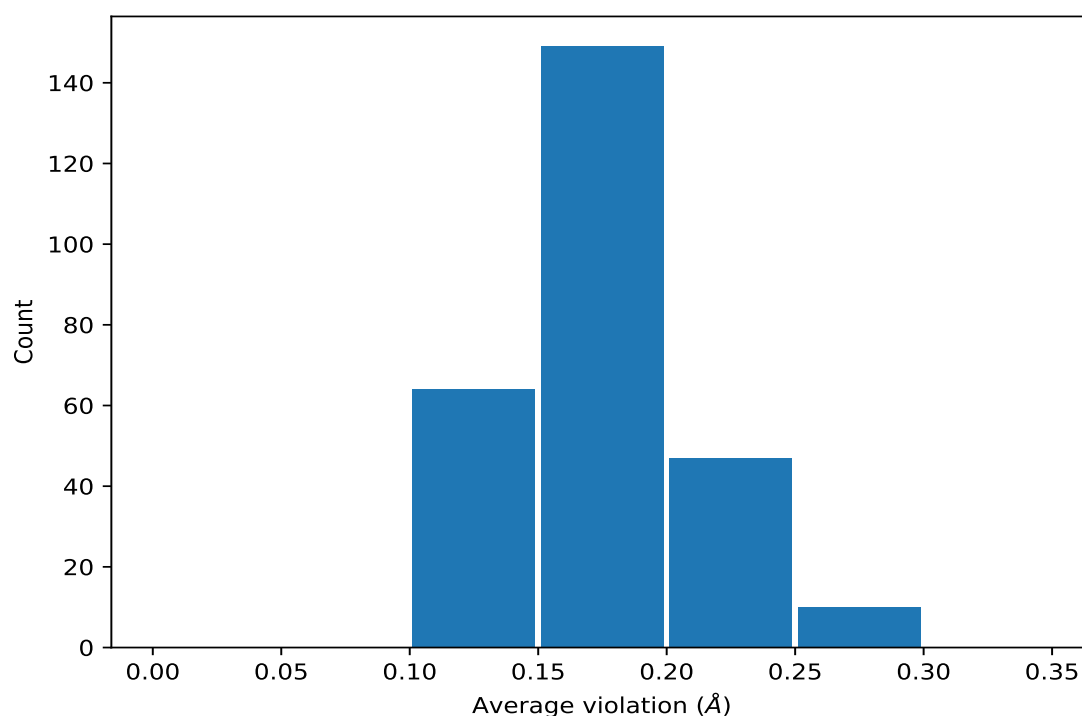
### 9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

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

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



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

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

| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (2,780)  | 1:20:A:GLU:HG2  | 1:57:A:PHE:HE1  | 20                  | 0.28     | 0.07                | 0.29       |
| (2,780)  | 1:20:A:GLU:HG2  | 1:57:A:PHE:HE2  | 20                  | 0.28     | 0.07                | 0.29       |
| (2,780)  | 1:20:A:GLU:HG3  | 1:57:A:PHE:HE1  | 20                  | 0.28     | 0.07                | 0.29       |
| (2,780)  | 1:20:A:GLU:HG3  | 1:57:A:PHE:HE2  | 20                  | 0.28     | 0.07                | 0.29       |
| (2,398)  | 1:4:A:VAL:H     | 1:81:A:LEU:HD11 | 19                  | 0.24     | 0.08                | 0.21       |
| (2,398)  | 1:4:A:VAL:H     | 1:81:A:LEU:HD12 | 19                  | 0.24     | 0.08                | 0.21       |
| (2,398)  | 1:4:A:VAL:H     | 1:81:A:LEU:HD13 | 19                  | 0.24     | 0.08                | 0.21       |
| (1,1078) | 1:15:A:LEU:HD21 | 1:57:A:PHE:HZ   | 18                  | 0.2      | 0.05                | 0.21       |
| (1,1078) | 1:15:A:LEU:HD22 | 1:57:A:PHE:HZ   | 18                  | 0.2      | 0.05                | 0.21       |
| (1,1078) | 1:15:A:LEU:HD23 | 1:57:A:PHE:HZ   | 18                  | 0.2      | 0.05                | 0.21       |
| (2,875)  | 1:84:A:LYS:HE2  | 1:85:A:VAL:HA   | 16                  | 0.23     | 0.1                 | 0.18       |
| (2,875)  | 1:84:A:LYS:HE3  | 1:85:A:VAL:HA   | 16                  | 0.23     | 0.1                 | 0.18       |
| (1,345)  | 1:19:A:LEU:HD21 | 1:23:A:LEU:H    | 16                  | 0.22     | 0.05                | 0.22       |
| (1,345)  | 1:19:A:LEU:HD22 | 1:23:A:LEU:H    | 16                  | 0.22     | 0.05                | 0.22       |
| (1,345)  | 1:19:A:LEU:HD23 | 1:23:A:LEU:H    | 16                  | 0.22     | 0.05                | 0.22       |
| (1,724)  | 1:58:A:ILE:HB   | 1:63:A:GLU:HB2  | 15                  | 0.19     | 0.06                | 0.18       |

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| Key      | Atom-1          | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,724)  | 1:58:A:ILE:HB   | 1:63:A:GLU:HB3   | 15                  | 0.19     | 0.06                | 0.18       |
| (2,402)  | 1:80:A:VAL:H    | 1:81:A:LEU:HD21  | 15                  | 0.18     | 0.06                | 0.16       |
| (2,402)  | 1:80:A:VAL:H    | 1:81:A:LEU:HD22  | 15                  | 0.18     | 0.06                | 0.16       |
| (2,402)  | 1:80:A:VAL:H    | 1:81:A:LEU:HD23  | 15                  | 0.18     | 0.06                | 0.16       |
| (1,1187) | 1:13:A:ARG:HB2  | 1:17:A:GLU:H     | 15                  | 0.15     | 0.03                | 0.14       |
| (1,1187) | 1:13:A:ARG:HB3  | 1:17:A:GLU:H     | 15                  | 0.15     | 0.03                | 0.14       |
| (1,1324) | 1:44:A:ILE:HD11 | 1:76:A:GLU:HB2   | 14                  | 0.18     | 0.05                | 0.18       |
| (1,1324) | 1:44:A:ILE:HD11 | 1:76:A:GLU:HB3   | 14                  | 0.18     | 0.05                | 0.18       |
| (1,1324) | 1:44:A:ILE:HD12 | 1:76:A:GLU:HB2   | 14                  | 0.18     | 0.05                | 0.18       |
| (1,1324) | 1:44:A:ILE:HD12 | 1:76:A:GLU:HB3   | 14                  | 0.18     | 0.05                | 0.18       |
| (1,1324) | 1:44:A:ILE:HD13 | 1:76:A:GLU:HB2   | 14                  | 0.18     | 0.05                | 0.18       |
| (1,1324) | 1:44:A:ILE:HD13 | 1:76:A:GLU:HB3   | 14                  | 0.18     | 0.05                | 0.18       |
| (2,866)  | 1:81:A:LEU:HB2  | 1:83:A:ILE:HA    | 13                  | 0.19     | 0.05                | 0.18       |
| (2,866)  | 1:81:A:LEU:HB3  | 1:83:A:ILE:HA    | 13                  | 0.19     | 0.05                | 0.18       |
| (1,1447) | 1:99:A:LEU:HD11 | 1:100:A:LYS:HG2  | 12                  | 0.2      | 0.08                | 0.18       |
| (1,1447) | 1:99:A:LEU:HD11 | 1:100:A:LYS:HG3  | 12                  | 0.2      | 0.08                | 0.18       |
| (1,1447) | 1:99:A:LEU:HD12 | 1:100:A:LYS:HG2  | 12                  | 0.2      | 0.08                | 0.18       |
| (1,1447) | 1:99:A:LEU:HD12 | 1:100:A:LYS:HG3  | 12                  | 0.2      | 0.08                | 0.18       |
| (1,1447) | 1:99:A:LEU:HD13 | 1:100:A:LYS:HG2  | 12                  | 0.2      | 0.08                | 0.18       |
| (1,1447) | 1:99:A:LEU:HD13 | 1:100:A:LYS:HG3  | 12                  | 0.2      | 0.08                | 0.18       |
| (1,299)  | 1:116:A:LYS:H   | 1:116:A:LYS:HD2  | 11                  | 0.22     | 0.05                | 0.22       |
| (1,299)  | 1:116:A:LYS:H   | 1:116:A:LYS:HD3  | 11                  | 0.22     | 0.05                | 0.22       |
| (1,1487) | 1:120:A:LYS:HG2 | 1:123:A:LEU:HD21 | 11                  | 0.18     | 0.06                | 0.16       |
| (1,1487) | 1:120:A:LYS:HG2 | 1:123:A:LEU:HD22 | 11                  | 0.18     | 0.06                | 0.16       |
| (1,1487) | 1:120:A:LYS:HG2 | 1:123:A:LEU:HD23 | 11                  | 0.18     | 0.06                | 0.16       |
| (1,1487) | 1:120:A:LYS:HG3 | 1:123:A:LEU:HD21 | 11                  | 0.18     | 0.06                | 0.16       |
| (1,1487) | 1:120:A:LYS:HG3 | 1:123:A:LEU:HD22 | 11                  | 0.18     | 0.06                | 0.16       |
| (1,1487) | 1:120:A:LYS:HG3 | 1:123:A:LEU:HD23 | 11                  | 0.18     | 0.06                | 0.16       |
| (1,282)  | 1:97:A:GLU:H    | 1:98:A:GLN:HB2   | 11                  | 0.16     | 0.05                | 0.14       |
| (1,282)  | 1:97:A:GLU:H    | 1:98:A:GLN:HB3   | 11                  | 0.16     | 0.05                | 0.14       |
| (1,845)  | 1:37:A:LYS:HD2  | 1:65:A:VAL:HB    | 10                  | 0.25     | 0.06                | 0.25       |
| (1,845)  | 1:37:A:LYS:HD3  | 1:65:A:VAL:HB    | 10                  | 0.25     | 0.06                | 0.25       |
| (2,315)  | 1:81:A:LEU:HB3  | 1:105:A:ASP:HB2  | 9                   | 0.21     | 0.09                | 0.18       |
| (1,997)  | 1:22:A:VAL:H    | 1:119:A:LEU:HD21 | 9                   | 0.15     | 0.02                | 0.14       |
| (1,997)  | 1:22:A:VAL:H    | 1:119:A:LEU:HD22 | 9                   | 0.15     | 0.02                | 0.14       |
| (1,997)  | 1:22:A:VAL:H    | 1:119:A:LEU:HD23 | 9                   | 0.15     | 0.02                | 0.14       |
| (1,77)   | 1:22:A:VAL:H    | 1:23:A:LEU:HB3   | 8                   | 0.14     | 0.02                | 0.14       |
| (1,453)  | 1:80:A:VAL:H    | 1:104:A:VAL:HG21 | 7                   | 0.19     | 0.08                | 0.2        |
| (1,453)  | 1:80:A:VAL:H    | 1:104:A:VAL:HG22 | 7                   | 0.19     | 0.08                | 0.2        |
| (1,453)  | 1:80:A:VAL:H    | 1:104:A:VAL:HG23 | 7                   | 0.19     | 0.08                | 0.2        |
| (2,765)  | 1:9:A:SER:H     | 1:63:A:GLU:HG2   | 7                   | 0.12     | 0.02                | 0.12       |
| (2,765)  | 1:9:A:SER:H     | 1:63:A:GLU:HG3   | 7                   | 0.12     | 0.02                | 0.12       |

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| Key      | Atom-1          | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,1448) | 1:99:A:LEU:HD21 | 1:100:A:LYS:HG2  | 6                   | 0.23     | 0.09                | 0.28       |
| (1,1448) | 1:99:A:LEU:HD21 | 1:100:A:LYS:HG3  | 6                   | 0.23     | 0.09                | 0.28       |
| (1,1448) | 1:99:A:LEU:HD22 | 1:100:A:LYS:HG2  | 6                   | 0.23     | 0.09                | 0.28       |
| (1,1448) | 1:99:A:LEU:HD22 | 1:100:A:LYS:HG3  | 6                   | 0.23     | 0.09                | 0.28       |
| (1,1448) | 1:99:A:LEU:HD23 | 1:100:A:LYS:HG2  | 6                   | 0.23     | 0.09                | 0.28       |
| (1,1448) | 1:99:A:LEU:HD23 | 1:100:A:LYS:HG3  | 6                   | 0.23     | 0.09                | 0.28       |
| (1,1427) | 1:84:A:LYS:HE2  | 1:96:A:TYR:HE1   | 6                   | 0.2      | 0.08                | 0.16       |
| (1,1427) | 1:84:A:LYS:HE2  | 1:96:A:TYR:HE2   | 6                   | 0.2      | 0.08                | 0.16       |
| (1,1427) | 1:84:A:LYS:HE3  | 1:96:A:TYR:HE1   | 6                   | 0.2      | 0.08                | 0.16       |
| (1,1427) | 1:84:A:LYS:HE3  | 1:96:A:TYR:HE2   | 6                   | 0.2      | 0.08                | 0.16       |
| (1,1411) | 1:83:A:ILE:HG12 | 1:107:A:ARG:HA   | 5                   | 0.18     | 0.1                 | 0.12       |
| (1,1411) | 1:83:A:ILE:HG13 | 1:107:A:ARG:HA   | 5                   | 0.18     | 0.1                 | 0.12       |
| (1,1150) | 1:72:A:TYR:HE1  | 1:78:A:LEU:HD11  | 5                   | 0.16     | 0.02                | 0.16       |
| (1,1150) | 1:72:A:TYR:HE1  | 1:78:A:LEU:HD12  | 5                   | 0.16     | 0.02                | 0.16       |
| (1,1150) | 1:72:A:TYR:HE1  | 1:78:A:LEU:HD13  | 5                   | 0.16     | 0.02                | 0.16       |
| (1,1150) | 1:72:A:TYR:HE2  | 1:78:A:LEU:HD11  | 5                   | 0.16     | 0.02                | 0.16       |
| (1,1150) | 1:72:A:TYR:HE2  | 1:78:A:LEU:HD12  | 5                   | 0.16     | 0.02                | 0.16       |
| (1,1150) | 1:72:A:TYR:HE2  | 1:78:A:LEU:HD13  | 5                   | 0.16     | 0.02                | 0.16       |
| (1,1112) | 1:96:A:TYR:HE1  | 1:97:A:GLU:HB2   | 5                   | 0.15     | 0.02                | 0.15       |
| (1,1112) | 1:96:A:TYR:HE1  | 1:97:A:GLU:HB3   | 5                   | 0.15     | 0.02                | 0.15       |
| (1,1112) | 1:96:A:TYR:HE2  | 1:97:A:GLU:HB2   | 5                   | 0.15     | 0.02                | 0.15       |
| (1,1112) | 1:96:A:TYR:HE2  | 1:97:A:GLU:HB3   | 5                   | 0.15     | 0.02                | 0.15       |
| (1,1114) | 1:96:A:TYR:HE1  | 1:106:A:VAL:HG21 | 5                   | 0.15     | 0.05                | 0.14       |
| (1,1114) | 1:96:A:TYR:HE1  | 1:106:A:VAL:HG22 | 5                   | 0.15     | 0.05                | 0.14       |
| (1,1114) | 1:96:A:TYR:HE1  | 1:106:A:VAL:HG23 | 5                   | 0.15     | 0.05                | 0.14       |
| (1,1114) | 1:96:A:TYR:HE2  | 1:106:A:VAL:HG21 | 5                   | 0.15     | 0.05                | 0.14       |
| (1,1114) | 1:96:A:TYR:HE2  | 1:106:A:VAL:HG22 | 5                   | 0.15     | 0.05                | 0.14       |
| (1,1114) | 1:96:A:TYR:HE2  | 1:106:A:VAL:HG23 | 5                   | 0.15     | 0.05                | 0.14       |
| (2,363)  | 1:81:A:LEU:HG   | 1:105:A:ASP:HB2  | 5                   | 0.15     | 0.04                | 0.15       |
| (2,687)  | 1:9:A:SER:HB2   | 1:84:A:LYS:HA    | 5                   | 0.14     | 0.05                | 0.1        |
| (1,1504) | 1:129:A:LEU:HB2 | 1:130:A:GLU:HB2  | 4                   | 0.28     | 0.11                | 0.25       |
| (1,1504) | 1:129:A:LEU:HB2 | 1:130:A:GLU:HB3  | 4                   | 0.28     | 0.11                | 0.25       |
| (1,1504) | 1:129:A:LEU:HB3 | 1:130:A:GLU:HB2  | 4                   | 0.28     | 0.11                | 0.25       |
| (1,1504) | 1:129:A:LEU:HB3 | 1:130:A:GLU:HB3  | 4                   | 0.28     | 0.11                | 0.25       |
| (1,1429) | 1:86:A:ALA:HB1  | 1:87:A:GLN:HB2   | 4                   | 0.24     | 0.06                | 0.25       |
| (1,1429) | 1:86:A:ALA:HB1  | 1:87:A:GLN:HB3   | 4                   | 0.24     | 0.06                | 0.25       |
| (1,1429) | 1:86:A:ALA:HB2  | 1:87:A:GLN:HB2   | 4                   | 0.24     | 0.06                | 0.25       |
| (1,1429) | 1:86:A:ALA:HB2  | 1:87:A:GLN:HB3   | 4                   | 0.24     | 0.06                | 0.25       |
| (1,1429) | 1:86:A:ALA:HB3  | 1:87:A:GLN:HB2   | 4                   | 0.24     | 0.06                | 0.25       |
| (1,1429) | 1:86:A:ALA:HB3  | 1:87:A:GLN:HB3   | 4                   | 0.24     | 0.06                | 0.25       |
| (1,1422) | 1:84:A:LYS:HG2  | 1:95:A:PHE:HD1   | 4                   | 0.19     | 0.07                | 0.18       |
| (1,1422) | 1:84:A:LYS:HG2  | 1:95:A:PHE:HD2   | 4                   | 0.19     | 0.07                | 0.18       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1422) | 1:84:A:LYS:HG3  | 1:95:A:PHE:HD1  | 4                   | 0.19     | 0.07                | 0.18       |
| (1,1422) | 1:84:A:LYS:HG3  | 1:95:A:PHE:HD2  | 4                   | 0.19     | 0.07                | 0.18       |
| (1,1198) | 1:16:A:GLU:HG2  | 1:19:A:LEU:HD11 | 4                   | 0.19     | 0.02                | 0.18       |
| (1,1198) | 1:16:A:GLU:HG2  | 1:19:A:LEU:HD12 | 4                   | 0.19     | 0.02                | 0.18       |
| (1,1198) | 1:16:A:GLU:HG2  | 1:19:A:LEU:HD13 | 4                   | 0.19     | 0.02                | 0.18       |
| (1,1198) | 1:16:A:GLU:HG3  | 1:19:A:LEU:HD11 | 4                   | 0.19     | 0.02                | 0.18       |
| (1,1198) | 1:16:A:GLU:HG3  | 1:19:A:LEU:HD12 | 4                   | 0.19     | 0.02                | 0.18       |
| (1,1198) | 1:16:A:GLU:HG3  | 1:19:A:LEU:HD13 | 4                   | 0.19     | 0.02                | 0.18       |
| (1,977)  | 1:64:A:GLU:HG2  | 1:65:A:VAL:HG11 | 4                   | 0.18     | 0.04                | 0.2        |
| (1,977)  | 1:64:A:GLU:HG2  | 1:65:A:VAL:HG12 | 4                   | 0.18     | 0.04                | 0.2        |
| (1,977)  | 1:64:A:GLU:HG2  | 1:65:A:VAL:HG13 | 4                   | 0.18     | 0.04                | 0.2        |
| (1,977)  | 1:64:A:GLU:HG3  | 1:65:A:VAL:HG11 | 4                   | 0.18     | 0.04                | 0.2        |
| (1,977)  | 1:64:A:GLU:HG3  | 1:65:A:VAL:HG12 | 4                   | 0.18     | 0.04                | 0.2        |
| (1,977)  | 1:64:A:GLU:HG3  | 1:65:A:VAL:HG13 | 4                   | 0.18     | 0.04                | 0.2        |
| (1,1458) | 1:111:A:ASN:HB2 | 1:112:A:GLU:HG2 | 4                   | 0.16     | 0.09                | 0.12       |
| (1,1458) | 1:111:A:ASN:HB2 | 1:112:A:GLU:HG3 | 4                   | 0.16     | 0.09                | 0.12       |
| (1,1458) | 1:111:A:ASN:HB3 | 1:112:A:GLU:HG2 | 4                   | 0.16     | 0.09                | 0.12       |
| (1,1458) | 1:111:A:ASN:HB3 | 1:112:A:GLU:HG3 | 4                   | 0.16     | 0.09                | 0.12       |
| (1,1188) | 1:13:A:ARG:HG2  | 1:16:A:GLU:HB2  | 4                   | 0.15     | 0.03                | 0.15       |
| (1,1188) | 1:13:A:ARG:HG2  | 1:16:A:GLU:HB3  | 4                   | 0.15     | 0.03                | 0.15       |
| (1,1188) | 1:13:A:ARG:HG3  | 1:16:A:GLU:HB2  | 4                   | 0.15     | 0.03                | 0.15       |
| (1,1188) | 1:13:A:ARG:HG3  | 1:16:A:GLU:HB3  | 4                   | 0.15     | 0.03                | 0.15       |
| (2,720)  | 1:6:A:ILE:HB    | 1:55:A:VAL:HG11 | 4                   | 0.15     | 0.04                | 0.15       |
| (2,720)  | 1:6:A:ILE:HB    | 1:55:A:VAL:HG12 | 4                   | 0.15     | 0.04                | 0.15       |
| (2,720)  | 1:6:A:ILE:HB    | 1:55:A:VAL:HG13 | 4                   | 0.15     | 0.04                | 0.15       |
| (1,658)  | 1:129:A:LEU:HG  | 1:130:A:GLU:HG2 | 4                   | 0.15     | 0.05                | 0.13       |
| (1,658)  | 1:129:A:LEU:HG  | 1:130:A:GLU:HG3 | 4                   | 0.15     | 0.05                | 0.13       |
| (1,902)  | 1:95:A:PHE:HA   | 1:97:A:GLU:HB2  | 4                   | 0.14     | 0.02                | 0.15       |
| (1,902)  | 1:95:A:PHE:HA   | 1:97:A:GLU:HB3  | 4                   | 0.14     | 0.02                | 0.15       |
| (1,1269) | 1:36:A:ASP:HB2  | 1:39:A:LYS:HA   | 4                   | 0.13     | 0.02                | 0.13       |
| (1,1269) | 1:36:A:ASP:HB3  | 1:39:A:LYS:HA   | 4                   | 0.13     | 0.02                | 0.13       |
| (2,892)  | 1:97:A:GLU:HB2  | 1:98:A:GLN:HE21 | 4                   | 0.13     | 0.01                | 0.12       |
| (2,892)  | 1:97:A:GLU:HB2  | 1:98:A:GLN:HE22 | 4                   | 0.13     | 0.01                | 0.12       |
| (2,892)  | 1:97:A:GLU:HB3  | 1:98:A:GLN:HE21 | 4                   | 0.13     | 0.01                | 0.12       |
| (2,892)  | 1:97:A:GLU:HB3  | 1:98:A:GLN:HE22 | 4                   | 0.13     | 0.01                | 0.12       |
| (1,154)  | 1:36:A:ASP:H    | 1:40:A:VAL:H    | 4                   | 0.12     | 0.03                | 0.12       |
| (1,1113) | 1:96:A:TYR:HE1  | 1:106:A:VAL:HB  | 4                   | 0.12     | 0.01                | 0.12       |
| (1,1113) | 1:96:A:TYR:HE2  | 1:106:A:VAL:HB  | 4                   | 0.12     | 0.01                | 0.12       |
| (2,78)   | 1:33:A:ARG:HD2  | 1:34:A:THR:H    | 3                   | 0.23     | 0.04                | 0.23       |
| (1,873)  | 1:87:A:GLN:H    | 1:88:A:ASP:HB2  | 3                   | 0.2      | 0.07                | 0.18       |
| (1,873)  | 1:87:A:GLN:H    | 1:88:A:ASP:HB3  | 3                   | 0.2      | 0.07                | 0.18       |
| (2,523)  | 1:27:A:PRO:HB3  | 1:28:A:ASN:HB2  | 3                   | 0.19     | 0.03                | 0.18       |

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| Key      | Atom-1          | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (2,523)  | 1:27:A:PRO:HB3  | 1:28:A:ASN:HB3   | 3                   | 0.19     | 0.03                | 0.18       |
| (1,880)  | 1:83:A:ILE:HD11 | 1:115:A:ALA:HA   | 3                   | 0.16     | 0.04                | 0.13       |
| (1,880)  | 1:83:A:ILE:HD12 | 1:115:A:ALA:HA   | 3                   | 0.16     | 0.04                | 0.13       |
| (1,880)  | 1:83:A:ILE:HD13 | 1:115:A:ALA:HA   | 3                   | 0.16     | 0.04                | 0.13       |
| (1,1117) | 1:96:A:TYR:HD1  | 1:106:A:VAL:HB   | 3                   | 0.15     | 0.02                | 0.14       |
| (1,1117) | 1:96:A:TYR:HD2  | 1:106:A:VAL:HB   | 3                   | 0.15     | 0.02                | 0.14       |
| (1,767)  | 1:37:A:LYS:HE2  | 1:65:A:VAL:HB    | 3                   | 0.14     | 0.0                 | 0.14       |
| (1,767)  | 1:37:A:LYS:HE3  | 1:65:A:VAL:HB    | 3                   | 0.14     | 0.0                 | 0.14       |
| (1,836)  | 1:62:A:TYR:HA   | 1:64:A:GLU:HG2   | 3                   | 0.14     | 0.0                 | 0.14       |
| (1,836)  | 1:62:A:TYR:HA   | 1:64:A:GLU:HG3   | 3                   | 0.14     | 0.0                 | 0.14       |
| (2,792)  | 1:28:A:ASN:HD21 | 1:52:A:ARG:HG2   | 3                   | 0.14     | 0.03                | 0.14       |
| (2,792)  | 1:28:A:ASN:HD21 | 1:52:A:ARG:HG3   | 3                   | 0.14     | 0.03                | 0.14       |
| (2,792)  | 1:28:A:ASN:HD22 | 1:52:A:ARG:HG2   | 3                   | 0.14     | 0.03                | 0.14       |
| (2,792)  | 1:28:A:ASN:HD22 | 1:52:A:ARG:HG3   | 3                   | 0.14     | 0.03                | 0.14       |
| (1,1428) | 1:85:A:VAL:HG21 | 1:111:A:ASN:HB2  | 3                   | 0.14     | 0.01                | 0.14       |
| (1,1428) | 1:85:A:VAL:HG21 | 1:111:A:ASN:HB3  | 3                   | 0.14     | 0.01                | 0.14       |
| (1,1428) | 1:85:A:VAL:HG22 | 1:111:A:ASN:HB2  | 3                   | 0.14     | 0.01                | 0.14       |
| (1,1428) | 1:85:A:VAL:HG22 | 1:111:A:ASN:HB3  | 3                   | 0.14     | 0.01                | 0.14       |
| (1,1428) | 1:85:A:VAL:HG23 | 1:111:A:ASN:HB2  | 3                   | 0.14     | 0.01                | 0.14       |
| (1,1428) | 1:85:A:VAL:HG23 | 1:111:A:ASN:HB3  | 3                   | 0.14     | 0.01                | 0.14       |
| (2,630)  | 1:74:A:GLN:HG2  | 1:104:A:VAL:HG11 | 3                   | 0.14     | 0.02                | 0.14       |
| (2,630)  | 1:74:A:GLN:HG2  | 1:104:A:VAL:HG12 | 3                   | 0.14     | 0.02                | 0.14       |
| (2,630)  | 1:74:A:GLN:HG2  | 1:104:A:VAL:HG13 | 3                   | 0.14     | 0.02                | 0.14       |
| (1,1129) | 1:61:A:ALA:H    | 1:62:A:TYR:HD1   | 3                   | 0.12     | 0.02                | 0.11       |
| (1,1129) | 1:61:A:ALA:H    | 1:62:A:TYR:HD2   | 3                   | 0.12     | 0.02                | 0.11       |
| (2,335)  | 1:59:A:ARG:HB2  | 1:61:A:ALA:HB1   | 3                   | 0.11     | 0.01                | 0.11       |
| (2,335)  | 1:59:A:ARG:HB2  | 1:61:A:ALA:HB2   | 3                   | 0.11     | 0.01                | 0.11       |
| (2,335)  | 1:59:A:ARG:HB2  | 1:61:A:ALA:HB3   | 3                   | 0.11     | 0.01                | 0.11       |
| (1,1196) | 1:16:A:GLU:H    | 1:16:A:GLU:HG2   | 3                   | 0.11     | 0.01                | 0.1        |
| (1,1196) | 1:16:A:GLU:H    | 1:16:A:GLU:HG3   | 3                   | 0.11     | 0.01                | 0.1        |
| (2,318)  | 1:87:A:GLN:HA   | 1:110:A:ASP:HB3  | 3                   | 0.11     | 0.01                | 0.11       |
| (2,316)  | 1:107:A:ARG:HD2 | 1:108:A:VAL:H    | 2                   | 0.24     | 0.06                | 0.24       |
| (1,601)  | 1:114:A:GLU:HB2 | 1:117:A:LYS:HD2  | 2                   | 0.24     | 0.08                | 0.24       |
| (1,601)  | 1:114:A:GLU:HB2 | 1:117:A:LYS:HD3  | 2                   | 0.24     | 0.08                | 0.24       |
| (1,601)  | 1:114:A:GLU:HB3 | 1:117:A:LYS:HD2  | 2                   | 0.24     | 0.08                | 0.24       |
| (1,601)  | 1:114:A:GLU:HB3 | 1:117:A:LYS:HD3  | 2                   | 0.24     | 0.08                | 0.24       |
| (2,438)  | 1:106:A:VAL:HA  | 1:107:A:ARG:HG2  | 2                   | 0.22     | 0.01                | 0.22       |
| (1,1455) | 1:106:A:VAL:H   | 1:107:A:ARG:HG2  | 2                   | 0.22     | 0.08                | 0.22       |
| (1,1455) | 1:106:A:VAL:H   | 1:107:A:ARG:HG3  | 2                   | 0.22     | 0.08                | 0.22       |
| (1,1119) | 1:96:A:TYR:HD1  | 1:106:A:VAL:HG11 | 2                   | 0.19     | 0.01                | 0.19       |
| (1,1119) | 1:96:A:TYR:HD1  | 1:106:A:VAL:HG12 | 2                   | 0.19     | 0.01                | 0.19       |
| (1,1119) | 1:96:A:TYR:HD1  | 1:106:A:VAL:HG13 | 2                   | 0.19     | 0.01                | 0.19       |

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| Key      | Atom-1          | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,1119) | 1:96:A:TYR:HD2  | 1:106:A:VAL:HG11 | 2                   | 0.19     | 0.01                | 0.19       |
| (1,1119) | 1:96:A:TYR:HD2  | 1:106:A:VAL:HG12 | 2                   | 0.19     | 0.01                | 0.19       |
| (1,1119) | 1:96:A:TYR:HD2  | 1:106:A:VAL:HG13 | 2                   | 0.19     | 0.01                | 0.19       |
| (1,322)  | 1:6:A:ILE:H     | 1:83:A:ILE:HD11  | 2                   | 0.18     | 0.03                | 0.18       |
| (1,322)  | 1:6:A:ILE:H     | 1:83:A:ILE:HD12  | 2                   | 0.18     | 0.03                | 0.18       |
| (1,322)  | 1:6:A:ILE:H     | 1:83:A:ILE:HD13  | 2                   | 0.18     | 0.03                | 0.18       |
| (1,1265) | 1:36:A:ASP:H    | 1:39:A:LYS:HD2   | 2                   | 0.18     | 0.02                | 0.18       |
| (1,1265) | 1:36:A:ASP:H    | 1:39:A:LYS:HD3   | 2                   | 0.18     | 0.02                | 0.18       |
| (1,1346) | 1:53:A:PRO:HB2  | 1:126:A:VAL:HG11 | 2                   | 0.18     | 0.03                | 0.18       |
| (1,1346) | 1:53:A:PRO:HB2  | 1:126:A:VAL:HG12 | 2                   | 0.18     | 0.03                | 0.18       |
| (1,1346) | 1:53:A:PRO:HB2  | 1:126:A:VAL:HG13 | 2                   | 0.18     | 0.03                | 0.18       |
| (1,1346) | 1:53:A:PRO:HB2  | 1:126:A:VAL:HG21 | 2                   | 0.18     | 0.03                | 0.18       |
| (1,1346) | 1:53:A:PRO:HB2  | 1:126:A:VAL:HG22 | 2                   | 0.18     | 0.03                | 0.18       |
| (1,1346) | 1:53:A:PRO:HB2  | 1:126:A:VAL:HG23 | 2                   | 0.18     | 0.03                | 0.18       |
| (2,478)  | 1:100:A:LYS:HA  | 1:106:A:VAL:HG21 | 2                   | 0.18     | 0.02                | 0.18       |
| (2,478)  | 1:100:A:LYS:HA  | 1:106:A:VAL:HG22 | 2                   | 0.18     | 0.02                | 0.18       |
| (2,478)  | 1:100:A:LYS:HA  | 1:106:A:VAL:HG23 | 2                   | 0.18     | 0.02                | 0.18       |
| (2,889)  | 1:92:A:LEU:HD21 | 1:110:A:ASP:HB2  | 2                   | 0.18     | 0.03                | 0.18       |
| (2,889)  | 1:92:A:LEU:HD21 | 1:110:A:ASP:HB3  | 2                   | 0.18     | 0.03                | 0.18       |
| (2,889)  | 1:92:A:LEU:HD22 | 1:110:A:ASP:HB2  | 2                   | 0.18     | 0.03                | 0.18       |
| (2,889)  | 1:92:A:LEU:HD22 | 1:110:A:ASP:HB3  | 2                   | 0.18     | 0.03                | 0.18       |
| (2,889)  | 1:92:A:LEU:HD23 | 1:110:A:ASP:HB2  | 2                   | 0.18     | 0.03                | 0.18       |
| (2,889)  | 1:92:A:LEU:HD23 | 1:110:A:ASP:HB3  | 2                   | 0.18     | 0.03                | 0.18       |
| (2,711)  | 1:8:A:VAL:HB    | 1:66:A:VAL:HG21  | 2                   | 0.17     | 0.01                | 0.17       |
| (2,711)  | 1:8:A:VAL:HB    | 1:66:A:VAL:HG22  | 2                   | 0.17     | 0.01                | 0.17       |
| (2,711)  | 1:8:A:VAL:HB    | 1:66:A:VAL:HG23  | 2                   | 0.17     | 0.01                | 0.17       |
| (1,389)  | 1:70:A:VAL:HB   | 1:72:A:TYR:H     | 2                   | 0.16     | 0.01                | 0.16       |
| (1,500)  | 1:23:A:LEU:HG   | 1:31:A:THR:HG21  | 2                   | 0.16     | 0.06                | 0.16       |
| (1,500)  | 1:23:A:LEU:HG   | 1:31:A:THR:HG22  | 2                   | 0.16     | 0.06                | 0.16       |
| (1,500)  | 1:23:A:LEU:HG   | 1:31:A:THR:HG23  | 2                   | 0.16     | 0.06                | 0.16       |
| (2,886)  | 1:87:A:GLN:HB2  | 1:92:A:LEU:HD11  | 2                   | 0.16     | 0.06                | 0.16       |
| (2,886)  | 1:87:A:GLN:HB2  | 1:92:A:LEU:HD12  | 2                   | 0.16     | 0.06                | 0.16       |
| (2,886)  | 1:87:A:GLN:HB2  | 1:92:A:LEU:HD13  | 2                   | 0.16     | 0.06                | 0.16       |
| (2,886)  | 1:87:A:GLN:HB3  | 1:92:A:LEU:HD11  | 2                   | 0.16     | 0.06                | 0.16       |
| (2,886)  | 1:87:A:GLN:HB3  | 1:92:A:LEU:HD12  | 2                   | 0.16     | 0.06                | 0.16       |
| (2,886)  | 1:87:A:GLN:HB3  | 1:92:A:LEU:HD13  | 2                   | 0.16     | 0.06                | 0.16       |
| (1,556)  | 1:19:A:LEU:HD11 | 1:23:A:LEU:HD21  | 2                   | 0.16     | 0.05                | 0.16       |
| (1,556)  | 1:19:A:LEU:HD11 | 1:23:A:LEU:HD22  | 2                   | 0.16     | 0.05                | 0.16       |
| (1,556)  | 1:19:A:LEU:HD11 | 1:23:A:LEU:HD23  | 2                   | 0.16     | 0.05                | 0.16       |
| (1,556)  | 1:19:A:LEU:HD12 | 1:23:A:LEU:HD21  | 2                   | 0.16     | 0.05                | 0.16       |
| (1,556)  | 1:19:A:LEU:HD12 | 1:23:A:LEU:HD22  | 2                   | 0.16     | 0.05                | 0.16       |
| (1,556)  | 1:19:A:LEU:HD12 | 1:23:A:LEU:HD23  | 2                   | 0.16     | 0.05                | 0.16       |

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| Key      | Atom-1          | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,556)  | 1:19:A:LEU:HD13 | 1:23:A:LEU:HD21  | 2                   | 0.16     | 0.05                | 0.16       |
| (1,556)  | 1:19:A:LEU:HD13 | 1:23:A:LEU:HD22  | 2                   | 0.16     | 0.05                | 0.16       |
| (1,556)  | 1:19:A:LEU:HD13 | 1:23:A:LEU:HD23  | 2                   | 0.16     | 0.05                | 0.16       |
| (1,1226) | 1:24:A:LYS:HG2  | 1:26:A:ASP:H     | 2                   | 0.16     | 0.02                | 0.16       |
| (1,1226) | 1:24:A:LYS:HG3  | 1:26:A:ASP:H     | 2                   | 0.16     | 0.02                | 0.16       |
| (2,473)  | 1:124:A:GLU:HG2 | 1:125:A:LYS:HE2  | 2                   | 0.16     | 0.02                | 0.16       |
| (2,473)  | 1:124:A:GLU:HG2 | 1:125:A:LYS:HE3  | 2                   | 0.16     | 0.02                | 0.16       |
| (2,473)  | 1:124:A:GLU:HG3 | 1:125:A:LYS:HE2  | 2                   | 0.16     | 0.02                | 0.16       |
| (2,473)  | 1:124:A:GLU:HG3 | 1:125:A:LYS:HE3  | 2                   | 0.16     | 0.02                | 0.16       |
| (2,528)  | 1:31:A:THR:HB   | 1:32:A:VAL:HB    | 2                   | 0.16     | 0.01                | 0.16       |
| (1,1419) | 1:84:A:LYS:HB2  | 1:96:A:TYR:HB2   | 2                   | 0.16     | 0.05                | 0.16       |
| (1,1419) | 1:84:A:LYS:HB2  | 1:96:A:TYR:HB3   | 2                   | 0.16     | 0.05                | 0.16       |
| (1,1419) | 1:84:A:LYS:HB3  | 1:96:A:TYR:HB2   | 2                   | 0.16     | 0.05                | 0.16       |
| (1,1419) | 1:84:A:LYS:HB3  | 1:96:A:TYR:HB3   | 2                   | 0.16     | 0.05                | 0.16       |
| (1,1221) | 1:21:A:VAL:HG21 | 1:120:A:LYS:HB2  | 2                   | 0.15     | 0.03                | 0.15       |
| (1,1221) | 1:21:A:VAL:HG21 | 1:120:A:LYS:HB3  | 2                   | 0.15     | 0.03                | 0.15       |
| (1,1221) | 1:21:A:VAL:HG22 | 1:120:A:LYS:HB2  | 2                   | 0.15     | 0.03                | 0.15       |
| (1,1221) | 1:21:A:VAL:HG22 | 1:120:A:LYS:HB3  | 2                   | 0.15     | 0.03                | 0.15       |
| (1,1221) | 1:21:A:VAL:HG23 | 1:120:A:LYS:HB2  | 2                   | 0.15     | 0.03                | 0.15       |
| (1,1221) | 1:21:A:VAL:HG23 | 1:120:A:LYS:HB3  | 2                   | 0.15     | 0.03                | 0.15       |
| (2,440)  | 1:72:A:TYR:HE1  | 1:78:A:LEU:HG    | 2                   | 0.14     | 0.03                | 0.14       |
| (2,440)  | 1:72:A:TYR:HE2  | 1:78:A:LEU:HG    | 2                   | 0.14     | 0.03                | 0.14       |
| (2,709)  | 1:99:A:LEU:HD11 | 1:100:A:LYS:HD2  | 2                   | 0.14     | 0.01                | 0.14       |
| (2,709)  | 1:99:A:LEU:HD11 | 1:100:A:LYS:HD3  | 2                   | 0.14     | 0.01                | 0.14       |
| (2,709)  | 1:99:A:LEU:HD12 | 1:100:A:LYS:HD2  | 2                   | 0.14     | 0.01                | 0.14       |
| (2,709)  | 1:99:A:LEU:HD12 | 1:100:A:LYS:HD3  | 2                   | 0.14     | 0.01                | 0.14       |
| (2,709)  | 1:99:A:LEU:HD13 | 1:100:A:LYS:HD2  | 2                   | 0.14     | 0.01                | 0.14       |
| (2,709)  | 1:99:A:LEU:HD13 | 1:100:A:LYS:HD3  | 2                   | 0.14     | 0.01                | 0.14       |
| (2,348)  | 1:129:A:LEU:HG  | 1:130:A:GLU:HA   | 2                   | 0.13     | 0.01                | 0.13       |
| (2,163)  | 1:74:A:GLN:HE21 | 1:103:A:GLY:H    | 2                   | 0.12     | 0.01                | 0.12       |
| (2,237)  | 1:97:A:GLU:HB2  | 1:101:A:LYS:HE2  | 2                   | 0.12     | 0.02                | 0.12       |
| (2,237)  | 1:97:A:GLU:HB2  | 1:101:A:LYS:HE3  | 2                   | 0.12     | 0.02                | 0.12       |
| (2,237)  | 1:97:A:GLU:HB3  | 1:101:A:LYS:HE2  | 2                   | 0.12     | 0.02                | 0.12       |
| (2,237)  | 1:97:A:GLU:HB3  | 1:101:A:LYS:HE3  | 2                   | 0.12     | 0.02                | 0.12       |
| (2,544)  | 1:40:A:VAL:HB   | 1:66:A:VAL:HA    | 2                   | 0.12     | 0.01                | 0.12       |
| (2,584)  | 1:8:A:VAL:H     | 1:55:A:VAL:HG11  | 2                   | 0.12     | 0.0                 | 0.12       |
| (2,584)  | 1:8:A:VAL:H     | 1:55:A:VAL:HG12  | 2                   | 0.12     | 0.0                 | 0.12       |
| (2,584)  | 1:8:A:VAL:H     | 1:55:A:VAL:HG13  | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,968)  | 1:29:A:VAL:HG21 | 1:54:A:ILE:HA    | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,968)  | 1:29:A:VAL:HG22 | 1:54:A:ILE:HA    | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,968)  | 1:29:A:VAL:HG23 | 1:54:A:ILE:HA    | 2                   | 0.11     | 0.0                 | 0.11       |
| (2,384)  | 1:97:A:GLU:H    | 1:106:A:VAL:HG11 | 2                   | 0.11     | 0.0                 | 0.11       |

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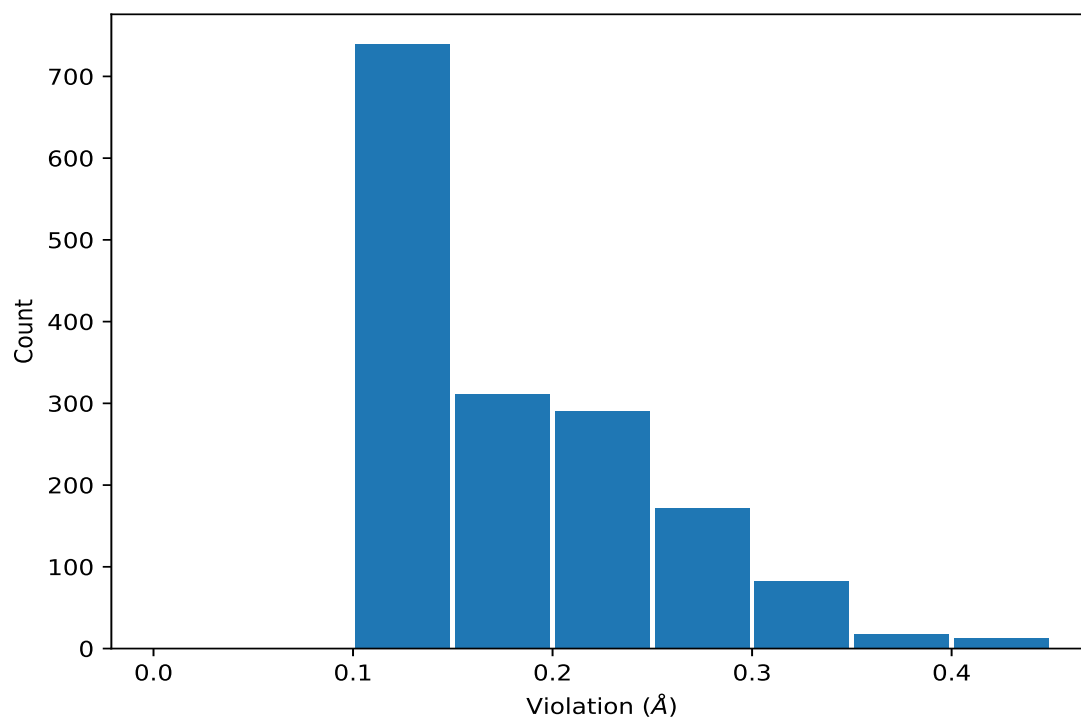
| Key     | Atom-1       | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|--------------|------------------|---------------------|----------|---------------------|------------|
| (2,384) | 1:97:A:GLU:H | 1:106:A:VAL:HG12 | 2                   | 0.11     | 0.0                 | 0.11       |
| (2,384) | 1:97:A:GLU:H | 1:106:A:VAL:HG13 | 2                   | 0.11     | 0.0                 | 0.11       |

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

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

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

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



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

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

| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1504) | 1:129:A:LEU:HB2 | 1:130:A:GLU:HB2 | 11       | 0.45          |
| (1,1504) | 1:129:A:LEU:HB2 | 1:130:A:GLU:HB3 | 11       | 0.45          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1504) | 1:129:A:LEU:HB3 | 1:130:A:GLU:HB2  | 11       | 0.45          |
| (1,1504) | 1:129:A:LEU:HB3 | 1:130:A:GLU:HB3  | 11       | 0.45          |
| (2,398)  | 1:4:A:VAL:H     | 1:81:A:LEU:HD11  | 16       | 0.43          |
| (2,398)  | 1:4:A:VAL:H     | 1:81:A:LEU:HD12  | 16       | 0.43          |
| (2,398)  | 1:4:A:VAL:H     | 1:81:A:LEU:HD13  | 16       | 0.43          |
| (2,875)  | 1:84:A:LYS:HE2  | 1:85:A:VAL:HA    | 13       | 0.41          |
| (2,875)  | 1:84:A:LYS:HE3  | 1:85:A:VAL:HA    | 13       | 0.41          |
| (2,780)  | 1:20:A:GLU:HG2  | 1:57:A:PHE:HE1   | 4        | 0.41          |
| (2,780)  | 1:20:A:GLU:HG2  | 1:57:A:PHE:HE2   | 4        | 0.41          |
| (2,780)  | 1:20:A:GLU:HG3  | 1:57:A:PHE:HE1   | 4        | 0.41          |
| (2,780)  | 1:20:A:GLU:HG3  | 1:57:A:PHE:HE2   | 4        | 0.41          |
| (2,315)  | 1:81:A:LEU:HB3  | 1:105:A:ASP:HB2  | 17       | 0.38          |
| (1,845)  | 1:37:A:LYS:HD2  | 1:65:A:VAL:HB    | 17       | 0.38          |
| (1,845)  | 1:37:A:LYS:HD3  | 1:65:A:VAL:HB    | 17       | 0.38          |
| (2,398)  | 1:4:A:VAL:H     | 1:81:A:LEU:HD11  | 14       | 0.37          |
| (2,398)  | 1:4:A:VAL:H     | 1:81:A:LEU:HD12  | 14       | 0.37          |
| (2,398)  | 1:4:A:VAL:H     | 1:81:A:LEU:HD13  | 14       | 0.37          |
| (1,1411) | 1:83:A:ILE:HG12 | 1:107:A:ARG:HA   | 11       | 0.37          |
| (1,1411) | 1:83:A:ILE:HG13 | 1:107:A:ARG:HA   | 11       | 0.37          |
| (2,875)  | 1:84:A:LYS:HE2  | 1:85:A:VAL:HA    | 6        | 0.36          |
| (2,875)  | 1:84:A:LYS:HE3  | 1:85:A:VAL:HA    | 6        | 0.36          |
| (2,875)  | 1:84:A:LYS:HE2  | 1:85:A:VAL:HA    | 15       | 0.36          |
| (2,875)  | 1:84:A:LYS:HE3  | 1:85:A:VAL:HA    | 15       | 0.36          |
| (2,875)  | 1:84:A:LYS:HE2  | 1:85:A:VAL:HA    | 16       | 0.36          |
| (2,875)  | 1:84:A:LYS:HE3  | 1:85:A:VAL:HA    | 16       | 0.36          |
| (2,780)  | 1:20:A:GLU:HG2  | 1:57:A:PHE:HE1   | 1        | 0.36          |
| (2,780)  | 1:20:A:GLU:HG2  | 1:57:A:PHE:HE2   | 1        | 0.36          |
| (2,780)  | 1:20:A:GLU:HG3  | 1:57:A:PHE:HE1   | 1        | 0.36          |
| (2,780)  | 1:20:A:GLU:HG3  | 1:57:A:PHE:HE2   | 1        | 0.36          |
| (2,875)  | 1:84:A:LYS:HE2  | 1:85:A:VAL:HA    | 11       | 0.35          |
| (2,875)  | 1:84:A:LYS:HE3  | 1:85:A:VAL:HA    | 11       | 0.35          |
| (2,780)  | 1:20:A:GLU:HG2  | 1:57:A:PHE:HE1   | 20       | 0.35          |
| (2,780)  | 1:20:A:GLU:HG2  | 1:57:A:PHE:HE2   | 20       | 0.35          |
| (2,780)  | 1:20:A:GLU:HG3  | 1:57:A:PHE:HE1   | 20       | 0.35          |
| (2,780)  | 1:20:A:GLU:HG3  | 1:57:A:PHE:HE2   | 20       | 0.35          |
| (1,453)  | 1:80:A:VAL:H    | 1:104:A:VAL:HG21 | 20       | 0.35          |
| (1,453)  | 1:80:A:VAL:H    | 1:104:A:VAL:HG22 | 20       | 0.35          |
| (1,453)  | 1:80:A:VAL:H    | 1:104:A:VAL:HG23 | 20       | 0.35          |
| (2,780)  | 1:20:A:GLU:HG2  | 1:57:A:PHE:HE1   | 13       | 0.34          |
| (2,780)  | 1:20:A:GLU:HG2  | 1:57:A:PHE:HE2   | 13       | 0.34          |
| (2,780)  | 1:20:A:GLU:HG3  | 1:57:A:PHE:HE1   | 13       | 0.34          |
| (2,780)  | 1:20:A:GLU:HG3  | 1:57:A:PHE:HE2   | 13       | 0.34          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (2,315)  | 1:81:A:LEU:HB3  | 1:105:A:ASP:HB2  | 10       | 0.34          |
| (1,1447) | 1:99:A:LEU:HD11 | 1:100:A:LYS:HG2  | 16       | 0.34          |
| (1,1447) | 1:99:A:LEU:HD11 | 1:100:A:LYS:HG3  | 16       | 0.34          |
| (1,1447) | 1:99:A:LEU:HD12 | 1:100:A:LYS:HG2  | 16       | 0.34          |
| (1,1447) | 1:99:A:LEU:HD12 | 1:100:A:LYS:HG3  | 16       | 0.34          |
| (1,1447) | 1:99:A:LEU:HD13 | 1:100:A:LYS:HG2  | 16       | 0.34          |
| (1,1447) | 1:99:A:LEU:HD13 | 1:100:A:LYS:HG3  | 16       | 0.34          |
| (1,1427) | 1:84:A:LYS:HE2  | 1:96:A:TYR:HE1   | 14       | 0.34          |
| (1,1427) | 1:84:A:LYS:HE2  | 1:96:A:TYR:HE2   | 14       | 0.34          |
| (1,1427) | 1:84:A:LYS:HE3  | 1:96:A:TYR:HE1   | 14       | 0.34          |
| (1,1427) | 1:84:A:LYS:HE3  | 1:96:A:TYR:HE2   | 14       | 0.34          |
| (2,398)  | 1:4:A:VAL:H     | 1:81:A:LEU:HD11  | 1        | 0.33          |
| (2,398)  | 1:4:A:VAL:H     | 1:81:A:LEU:HD12  | 1        | 0.33          |
| (2,398)  | 1:4:A:VAL:H     | 1:81:A:LEU:HD13  | 1        | 0.33          |
| (1,1487) | 1:120:A:LYS:HG2 | 1:123:A:LEU:HD21 | 19       | 0.33          |
| (1,1487) | 1:120:A:LYS:HG2 | 1:123:A:LEU:HD22 | 19       | 0.33          |
| (1,1487) | 1:120:A:LYS:HG2 | 1:123:A:LEU:HD23 | 19       | 0.33          |
| (1,1487) | 1:120:A:LYS:HG3 | 1:123:A:LEU:HD21 | 19       | 0.33          |
| (1,1487) | 1:120:A:LYS:HG3 | 1:123:A:LEU:HD22 | 19       | 0.33          |
| (1,1487) | 1:120:A:LYS:HG3 | 1:123:A:LEU:HD23 | 19       | 0.33          |
| (1,299)  | 1:116:A:LYS:H   | 1:116:A:LYS:HD2  | 12       | 0.33          |
| (1,299)  | 1:116:A:LYS:H   | 1:116:A:LYS:HD3  | 12       | 0.33          |
| (2,780)  | 1:20:A:GLU:HG2  | 1:57:A:PHE:HE1   | 3        | 0.32          |
| (2,780)  | 1:20:A:GLU:HG2  | 1:57:A:PHE:HE2   | 3        | 0.32          |
| (2,780)  | 1:20:A:GLU:HG3  | 1:57:A:PHE:HE1   | 3        | 0.32          |
| (2,780)  | 1:20:A:GLU:HG3  | 1:57:A:PHE:HE2   | 3        | 0.32          |
| (2,780)  | 1:20:A:GLU:HG2  | 1:57:A:PHE:HE1   | 5        | 0.32          |
| (2,780)  | 1:20:A:GLU:HG2  | 1:57:A:PHE:HE2   | 5        | 0.32          |
| (2,780)  | 1:20:A:GLU:HG3  | 1:57:A:PHE:HE1   | 5        | 0.32          |
| (2,780)  | 1:20:A:GLU:HG3  | 1:57:A:PHE:HE2   | 5        | 0.32          |
| (2,780)  | 1:20:A:GLU:HG2  | 1:57:A:PHE:HE1   | 15       | 0.32          |
| (2,780)  | 1:20:A:GLU:HG2  | 1:57:A:PHE:HE2   | 15       | 0.32          |
| (2,780)  | 1:20:A:GLU:HG3  | 1:57:A:PHE:HE1   | 15       | 0.32          |
| (2,780)  | 1:20:A:GLU:HG3  | 1:57:A:PHE:HE2   | 15       | 0.32          |
| (1,1458) | 1:111:A:ASN:HB2 | 1:112:A:GLU:HG2  | 3        | 0.32          |
| (1,1458) | 1:111:A:ASN:HB2 | 1:112:A:GLU:HG3  | 3        | 0.32          |
| (1,1458) | 1:111:A:ASN:HB3 | 1:112:A:GLU:HG2  | 3        | 0.32          |
| (1,1458) | 1:111:A:ASN:HB3 | 1:112:A:GLU:HG3  | 3        | 0.32          |
| (1,1447) | 1:99:A:LEU:HD11 | 1:100:A:LYS:HG2  | 3        | 0.32          |
| (1,1447) | 1:99:A:LEU:HD11 | 1:100:A:LYS:HG3  | 3        | 0.32          |
| (1,1447) | 1:99:A:LEU:HD12 | 1:100:A:LYS:HG2  | 3        | 0.32          |
| (1,1447) | 1:99:A:LEU:HD12 | 1:100:A:LYS:HG3  | 3        | 0.32          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1447) | 1:99:A:LEU:HD13 | 1:100:A:LYS:HG2 | 3        | 0.32          |
| (1,1447) | 1:99:A:LEU:HD13 | 1:100:A:LYS:HG3 | 3        | 0.32          |
| (1,1429) | 1:86:A:ALA:HB1  | 1:87:A:GLN:HB2  | 9        | 0.32          |
| (1,1429) | 1:86:A:ALA:HB1  | 1:87:A:GLN:HB3  | 9        | 0.32          |
| (1,1429) | 1:86:A:ALA:HB2  | 1:87:A:GLN:HB2  | 9        | 0.32          |
| (1,1429) | 1:86:A:ALA:HB2  | 1:87:A:GLN:HB3  | 9        | 0.32          |
| (1,1429) | 1:86:A:ALA:HB3  | 1:87:A:GLN:HB2  | 9        | 0.32          |
| (1,1429) | 1:86:A:ALA:HB3  | 1:87:A:GLN:HB3  | 9        | 0.32          |
| (1,345)  | 1:19:A:LEU:HD21 | 1:23:A:LEU:H    | 20       | 0.32          |
| (1,345)  | 1:19:A:LEU:HD22 | 1:23:A:LEU:H    | 20       | 0.32          |
| (1,345)  | 1:19:A:LEU:HD23 | 1:23:A:LEU:H    | 20       | 0.32          |
| (2,780)  | 1:20:A:GLU:HG2  | 1:57:A:PHE:HE1  | 11       | 0.31          |
| (2,780)  | 1:20:A:GLU:HG2  | 1:57:A:PHE:HE2  | 11       | 0.31          |
| (2,780)  | 1:20:A:GLU:HG3  | 1:57:A:PHE:HE1  | 11       | 0.31          |
| (2,780)  | 1:20:A:GLU:HG3  | 1:57:A:PHE:HE2  | 11       | 0.31          |
| (2,398)  | 1:4:A:VAL:H     | 1:81:A:LEU:HD11 | 6        | 0.31          |
| (2,398)  | 1:4:A:VAL:H     | 1:81:A:LEU:HD12 | 6        | 0.31          |
| (2,398)  | 1:4:A:VAL:H     | 1:81:A:LEU:HD13 | 6        | 0.31          |
| (2,398)  | 1:4:A:VAL:H     | 1:81:A:LEU:HD11 | 13       | 0.31          |
| (2,398)  | 1:4:A:VAL:H     | 1:81:A:LEU:HD12 | 13       | 0.31          |
| (2,398)  | 1:4:A:VAL:H     | 1:81:A:LEU:HD13 | 13       | 0.31          |
| (2,316)  | 1:107:A:ARG:HD2 | 1:108:A:VAL:H   | 4        | 0.31          |
| (1,724)  | 1:58:A:ILE:HB   | 1:63:A:GLU:HB2  | 20       | 0.31          |
| (1,724)  | 1:58:A:ILE:HB   | 1:63:A:GLU:HB3  | 20       | 0.31          |
| (1,601)  | 1:114:A:GLU:HB2 | 1:117:A:LYS:HD2 | 19       | 0.31          |
| (1,601)  | 1:114:A:GLU:HB2 | 1:117:A:LYS:HD3 | 19       | 0.31          |
| (1,601)  | 1:114:A:GLU:HB3 | 1:117:A:LYS:HD2 | 19       | 0.31          |
| (1,601)  | 1:114:A:GLU:HB3 | 1:117:A:LYS:HD3 | 19       | 0.31          |
| (2,866)  | 1:81:A:LEU:HB2  | 1:83:A:ILE:HA   | 17       | 0.3           |
| (2,866)  | 1:81:A:LEU:HB3  | 1:83:A:ILE:HA   | 17       | 0.3           |
| (2,780)  | 1:20:A:GLU:HG2  | 1:57:A:PHE:HE1  | 8        | 0.3           |
| (2,780)  | 1:20:A:GLU:HG2  | 1:57:A:PHE:HE2  | 8        | 0.3           |
| (2,780)  | 1:20:A:GLU:HG3  | 1:57:A:PHE:HE1  | 8        | 0.3           |
| (2,780)  | 1:20:A:GLU:HG3  | 1:57:A:PHE:HE2  | 8        | 0.3           |
| (2,780)  | 1:20:A:GLU:HG2  | 1:57:A:PHE:HE1  | 12       | 0.3           |
| (2,780)  | 1:20:A:GLU:HG2  | 1:57:A:PHE:HE2  | 12       | 0.3           |
| (2,780)  | 1:20:A:GLU:HG3  | 1:57:A:PHE:HE1  | 12       | 0.3           |
| (2,780)  | 1:20:A:GLU:HG3  | 1:57:A:PHE:HE2  | 12       | 0.3           |
| (1,1504) | 1:129:A:LEU:HB2 | 1:130:A:GLU:HB2 | 18       | 0.3           |
| (1,1504) | 1:129:A:LEU:HB2 | 1:130:A:GLU:HB3 | 18       | 0.3           |
| (1,1504) | 1:129:A:LEU:HB3 | 1:130:A:GLU:HB2 | 18       | 0.3           |
| (1,1504) | 1:129:A:LEU:HB3 | 1:130:A:GLU:HB3 | 18       | 0.3           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1455) | 1:106:A:VAL:H   | 1:107:A:ARG:HG2 | 6        | 0.3           |
| (1,1455) | 1:106:A:VAL:H   | 1:107:A:ARG:HG3 | 6        | 0.3           |
| (1,1448) | 1:99:A:LEU:HD21 | 1:100:A:LYS:HG2 | 12       | 0.3           |
| (1,1448) | 1:99:A:LEU:HD21 | 1:100:A:LYS:HG3 | 12       | 0.3           |
| (1,1448) | 1:99:A:LEU:HD22 | 1:100:A:LYS:HG2 | 12       | 0.3           |
| (1,1448) | 1:99:A:LEU:HD22 | 1:100:A:LYS:HG3 | 12       | 0.3           |
| (1,1448) | 1:99:A:LEU:HD23 | 1:100:A:LYS:HG2 | 12       | 0.3           |
| (1,1448) | 1:99:A:LEU:HD23 | 1:100:A:LYS:HG3 | 12       | 0.3           |
| (1,1448) | 1:99:A:LEU:HD21 | 1:100:A:LYS:HG2 | 15       | 0.3           |
| (1,1448) | 1:99:A:LEU:HD21 | 1:100:A:LYS:HG3 | 15       | 0.3           |
| (1,1448) | 1:99:A:LEU:HD22 | 1:100:A:LYS:HG2 | 15       | 0.3           |
| (1,1448) | 1:99:A:LEU:HD22 | 1:100:A:LYS:HG3 | 15       | 0.3           |
| (1,1448) | 1:99:A:LEU:HD23 | 1:100:A:LYS:HG2 | 15       | 0.3           |
| (1,1448) | 1:99:A:LEU:HD23 | 1:100:A:LYS:HG3 | 15       | 0.3           |
| (1,873)  | 1:87:A:GLN:H    | 1:88:A:ASP:HB2  | 20       | 0.3           |
| (1,873)  | 1:87:A:GLN:H    | 1:88:A:ASP:HB3  | 20       | 0.3           |
| (2,666)  | 1:85:A:VAL:HG11 | 1:109:A:THR:HB  | 7        | 0.29          |
| (2,666)  | 1:85:A:VAL:HG12 | 1:109:A:THR:HB  | 7        | 0.29          |
| (2,666)  | 1:85:A:VAL:HG13 | 1:109:A:THR:HB  | 7        | 0.29          |
| (1,845)  | 1:37:A:LYS:HD2  | 1:65:A:VAL:HB   | 11       | 0.29          |
| (1,845)  | 1:37:A:LYS:HD3  | 1:65:A:VAL:HB   | 11       | 0.29          |
| (1,345)  | 1:19:A:LEU:HD21 | 1:23:A:LEU:H    | 1        | 0.29          |
| (1,345)  | 1:19:A:LEU:HD22 | 1:23:A:LEU:H    | 1        | 0.29          |
| (1,345)  | 1:19:A:LEU:HD23 | 1:23:A:LEU:H    | 1        | 0.29          |
| (1,345)  | 1:19:A:LEU:HD21 | 1:23:A:LEU:H    | 14       | 0.29          |
| (1,345)  | 1:19:A:LEU:HD22 | 1:23:A:LEU:H    | 14       | 0.29          |
| (1,345)  | 1:19:A:LEU:HD23 | 1:23:A:LEU:H    | 14       | 0.29          |
| (1,299)  | 1:116:A:LYS:H   | 1:116:A:LYS:HD2 | 8        | 0.29          |
| (1,299)  | 1:116:A:LYS:H   | 1:116:A:LYS:HD3 | 8        | 0.29          |
| (2,780)  | 1:20:A:GLU:HG2  | 1:57:A:PHE:HE1  | 17       | 0.28          |
| (2,780)  | 1:20:A:GLU:HG2  | 1:57:A:PHE:HE2  | 17       | 0.28          |
| (2,780)  | 1:20:A:GLU:HG3  | 1:57:A:PHE:HE1  | 17       | 0.28          |
| (2,780)  | 1:20:A:GLU:HG3  | 1:57:A:PHE:HE2  | 17       | 0.28          |
| (2,780)  | 1:20:A:GLU:HG2  | 1:57:A:PHE:HE1  | 18       | 0.28          |
| (2,780)  | 1:20:A:GLU:HG2  | 1:57:A:PHE:HE2  | 18       | 0.28          |
| (2,780)  | 1:20:A:GLU:HG3  | 1:57:A:PHE:HE1  | 18       | 0.28          |
| (2,780)  | 1:20:A:GLU:HG3  | 1:57:A:PHE:HE2  | 18       | 0.28          |
| (2,780)  | 1:20:A:GLU:HG2  | 1:57:A:PHE:HE1  | 19       | 0.28          |
| (2,780)  | 1:20:A:GLU:HG2  | 1:57:A:PHE:HE2  | 19       | 0.28          |
| (2,780)  | 1:20:A:GLU:HG3  | 1:57:A:PHE:HE1  | 19       | 0.28          |
| (2,780)  | 1:20:A:GLU:HG3  | 1:57:A:PHE:HE2  | 19       | 0.28          |
| (2,402)  | 1:80:A:VAL:H    | 1:81:A:LEU:HD21 | 7        | 0.28          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,402)  | 1:80:A:VAL:H    | 1:81:A:LEU:HD22 | 7        | 0.28          |
| (2,402)  | 1:80:A:VAL:H    | 1:81:A:LEU:HD23 | 7        | 0.28          |
| (2,78)   | 1:33:A:ARG:HD2  | 1:34:A:THR:H    | 10       | 0.28          |
| (1,1448) | 1:99:A:LEU:HD21 | 1:100:A:LYS:HG2 | 5        | 0.28          |
| (1,1448) | 1:99:A:LEU:HD21 | 1:100:A:LYS:HG3 | 5        | 0.28          |
| (1,1448) | 1:99:A:LEU:HD22 | 1:100:A:LYS:HG2 | 5        | 0.28          |
| (1,1448) | 1:99:A:LEU:HD22 | 1:100:A:LYS:HG3 | 5        | 0.28          |
| (1,1448) | 1:99:A:LEU:HD23 | 1:100:A:LYS:HG2 | 5        | 0.28          |
| (1,1448) | 1:99:A:LEU:HD23 | 1:100:A:LYS:HG3 | 5        | 0.28          |
| (1,1447) | 1:99:A:LEU:HD11 | 1:100:A:LYS:HG2 | 13       | 0.28          |
| (1,1447) | 1:99:A:LEU:HD11 | 1:100:A:LYS:HG3 | 13       | 0.28          |
| (1,1447) | 1:99:A:LEU:HD12 | 1:100:A:LYS:HG2 | 13       | 0.28          |
| (1,1447) | 1:99:A:LEU:HD12 | 1:100:A:LYS:HG3 | 13       | 0.28          |
| (1,1447) | 1:99:A:LEU:HD13 | 1:100:A:LYS:HG2 | 13       | 0.28          |
| (1,1447) | 1:99:A:LEU:HD13 | 1:100:A:LYS:HG3 | 13       | 0.28          |
| (1,1078) | 1:15:A:LEU:HD21 | 1:57:A:PHE:HZ   | 4        | 0.28          |
| (1,1078) | 1:15:A:LEU:HD22 | 1:57:A:PHE:HZ   | 4        | 0.28          |
| (1,1078) | 1:15:A:LEU:HD23 | 1:57:A:PHE:HZ   | 4        | 0.28          |
| (1,1078) | 1:15:A:LEU:HD21 | 1:57:A:PHE:HZ   | 19       | 0.28          |
| (1,1078) | 1:15:A:LEU:HD22 | 1:57:A:PHE:HZ   | 19       | 0.28          |
| (1,1078) | 1:15:A:LEU:HD23 | 1:57:A:PHE:HZ   | 19       | 0.28          |
| (1,966)  | 1:45:A:GLU:HA   | 1:46:A:LYS:HG2  | 3        | 0.28          |
| (1,966)  | 1:45:A:GLU:HA   | 1:46:A:LYS:HG3  | 3        | 0.28          |
| (1,845)  | 1:37:A:LYS:HD2  | 1:65:A:VAL:HB   | 3        | 0.28          |
| (1,845)  | 1:37:A:LYS:HD3  | 1:65:A:VAL:HB   | 3        | 0.28          |
| (1,845)  | 1:37:A:LYS:HD2  | 1:65:A:VAL:HB   | 5        | 0.28          |
| (1,845)  | 1:37:A:LYS:HD3  | 1:65:A:VAL:HB   | 5        | 0.28          |
| (1,724)  | 1:58:A:ILE:HB   | 1:63:A:GLU:HB2  | 15       | 0.28          |
| (1,724)  | 1:58:A:ILE:HB   | 1:63:A:GLU:HB3  | 15       | 0.28          |
| (2,402)  | 1:80:A:VAL:H    | 1:81:A:LEU:HD21 | 6        | 0.27          |
| (2,402)  | 1:80:A:VAL:H    | 1:81:A:LEU:HD22 | 6        | 0.27          |
| (2,402)  | 1:80:A:VAL:H    | 1:81:A:LEU:HD23 | 6        | 0.27          |
| (2,402)  | 1:80:A:VAL:H    | 1:81:A:LEU:HD21 | 11       | 0.27          |
| (2,402)  | 1:80:A:VAL:H    | 1:81:A:LEU:HD22 | 11       | 0.27          |
| (2,402)  | 1:80:A:VAL:H    | 1:81:A:LEU:HD23 | 11       | 0.27          |
| (2,398)  | 1:4:A:VAL:H     | 1:81:A:LEU:HD11 | 10       | 0.27          |
| (2,398)  | 1:4:A:VAL:H     | 1:81:A:LEU:HD12 | 10       | 0.27          |
| (2,398)  | 1:4:A:VAL:H     | 1:81:A:LEU:HD13 | 10       | 0.27          |
| (2,301)  | 1:83:A:ILE:HD11 | 1:118:A:ARG:HD2 | 13       | 0.27          |
| (2,301)  | 1:83:A:ILE:HD11 | 1:118:A:ARG:HD3 | 13       | 0.27          |
| (2,301)  | 1:83:A:ILE:HD12 | 1:118:A:ARG:HD2 | 13       | 0.27          |
| (2,301)  | 1:83:A:ILE:HD12 | 1:118:A:ARG:HD3 | 13       | 0.27          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,301)  | 1:83:A:ILE:HD13 | 1:118:A:ARG:HD2 | 13       | 0.27          |
| (2,301)  | 1:83:A:ILE:HD13 | 1:118:A:ARG:HD3 | 13       | 0.27          |
| (1,1448) | 1:99:A:LEU:HD21 | 1:100:A:LYS:HG2 | 8        | 0.27          |
| (1,1448) | 1:99:A:LEU:HD21 | 1:100:A:LYS:HG3 | 8        | 0.27          |
| (1,1448) | 1:99:A:LEU:HD22 | 1:100:A:LYS:HG2 | 8        | 0.27          |
| (1,1448) | 1:99:A:LEU:HD22 | 1:100:A:LYS:HG3 | 8        | 0.27          |
| (1,1448) | 1:99:A:LEU:HD23 | 1:100:A:LYS:HG2 | 8        | 0.27          |
| (1,1448) | 1:99:A:LEU:HD23 | 1:100:A:LYS:HG3 | 8        | 0.27          |
| (1,1422) | 1:84:A:LYS:HG2  | 1:95:A:PHE:HD1  | 9        | 0.27          |
| (1,1422) | 1:84:A:LYS:HG2  | 1:95:A:PHE:HD2  | 9        | 0.27          |
| (1,1422) | 1:84:A:LYS:HG3  | 1:95:A:PHE:HD1  | 9        | 0.27          |
| (1,1422) | 1:84:A:LYS:HG3  | 1:95:A:PHE:HD2  | 9        | 0.27          |
| (1,1331) | 1:47:A:ALA:HA   | 1:50:A:GLN:HB2  | 20       | 0.27          |
| (1,1331) | 1:47:A:ALA:HA   | 1:50:A:GLN:HB3  | 20       | 0.27          |
| (1,1324) | 1:44:A:ILE:HD11 | 1:76:A:GLU:HB2  | 15       | 0.27          |
| (1,1324) | 1:44:A:ILE:HD11 | 1:76:A:GLU:HB3  | 15       | 0.27          |
| (1,1324) | 1:44:A:ILE:HD12 | 1:76:A:GLU:HB2  | 15       | 0.27          |
| (1,1324) | 1:44:A:ILE:HD12 | 1:76:A:GLU:HB3  | 15       | 0.27          |
| (1,1324) | 1:44:A:ILE:HD13 | 1:76:A:GLU:HB2  | 15       | 0.27          |
| (1,1324) | 1:44:A:ILE:HD13 | 1:76:A:GLU:HB3  | 15       | 0.27          |
| (1,1078) | 1:15:A:LEU:HD21 | 1:57:A:PHE:HZ   | 5        | 0.27          |
| (1,1078) | 1:15:A:LEU:HD22 | 1:57:A:PHE:HZ   | 5        | 0.27          |
| (1,1078) | 1:15:A:LEU:HD23 | 1:57:A:PHE:HZ   | 5        | 0.27          |
| (2,815)  | 1:37:A:LYS:HG2  | 1:65:A:VAL:HB   | 1        | 0.26          |
| (2,815)  | 1:37:A:LYS:HG3  | 1:65:A:VAL:HB   | 1        | 0.26          |
| (2,780)  | 1:20:A:GLU:HG2  | 1:57:A:PHE:HE1  | 7        | 0.26          |
| (2,780)  | 1:20:A:GLU:HG2  | 1:57:A:PHE:HE2  | 7        | 0.26          |
| (2,780)  | 1:20:A:GLU:HG3  | 1:57:A:PHE:HE1  | 7        | 0.26          |
| (2,780)  | 1:20:A:GLU:HG3  | 1:57:A:PHE:HE2  | 7        | 0.26          |
| (2,402)  | 1:80:A:VAL:H    | 1:81:A:LEU:HD21 | 20       | 0.26          |
| (2,402)  | 1:80:A:VAL:H    | 1:81:A:LEU:HD22 | 20       | 0.26          |
| (2,402)  | 1:80:A:VAL:H    | 1:81:A:LEU:HD23 | 20       | 0.26          |
| (1,1429) | 1:86:A:ALA:HB1  | 1:87:A:GLN:HB2  | 6        | 0.26          |
| (1,1429) | 1:86:A:ALA:HB1  | 1:87:A:GLN:HB3  | 6        | 0.26          |
| (1,1429) | 1:86:A:ALA:HB2  | 1:87:A:GLN:HB2  | 6        | 0.26          |
| (1,1429) | 1:86:A:ALA:HB2  | 1:87:A:GLN:HB3  | 6        | 0.26          |
| (1,1429) | 1:86:A:ALA:HB3  | 1:87:A:GLN:HB2  | 6        | 0.26          |
| (1,1429) | 1:86:A:ALA:HB3  | 1:87:A:GLN:HB3  | 6        | 0.26          |
| (1,1427) | 1:84:A:LYS:HE2  | 1:96:A:TYR:HE1  | 17       | 0.26          |
| (1,1427) | 1:84:A:LYS:HE2  | 1:96:A:TYR:HE2  | 17       | 0.26          |
| (1,1427) | 1:84:A:LYS:HE3  | 1:96:A:TYR:HE1  | 17       | 0.26          |
| (1,1427) | 1:84:A:LYS:HE3  | 1:96:A:TYR:HE2  | 17       | 0.26          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,345)  | 1:19:A:LEU:HD21 | 1:23:A:LEU:H    | 9        | 0.26          |
| (1,345)  | 1:19:A:LEU:HD22 | 1:23:A:LEU:H    | 9        | 0.26          |
| (1,345)  | 1:19:A:LEU:HD23 | 1:23:A:LEU:H    | 9        | 0.26          |
| (2,875)  | 1:84:A:LYS:HE2  | 1:85:A:VAL:HA   | 20       | 0.25          |
| (2,875)  | 1:84:A:LYS:HE3  | 1:85:A:VAL:HA   | 20       | 0.25          |
| (2,866)  | 1:81:A:LEU:HB2  | 1:83:A:ILE:HA   | 10       | 0.25          |
| (2,866)  | 1:81:A:LEU:HB3  | 1:83:A:ILE:HA   | 10       | 0.25          |
| (2,691)  | 1:94:A:ARG:HB2  | 1:98:A:GLN:H    | 20       | 0.25          |
| (2,691)  | 1:94:A:ARG:HB3  | 1:98:A:GLN:H    | 20       | 0.25          |
| (2,398)  | 1:4:A:VAL:H     | 1:81:A:LEU:HD11 | 2        | 0.25          |
| (2,398)  | 1:4:A:VAL:H     | 1:81:A:LEU:HD12 | 2        | 0.25          |
| (2,398)  | 1:4:A:VAL:H     | 1:81:A:LEU:HD13 | 2        | 0.25          |
| (1,1422) | 1:84:A:LYS:HG2  | 1:95:A:PHE:HD1  | 20       | 0.25          |
| (1,1422) | 1:84:A:LYS:HG2  | 1:95:A:PHE:HD2  | 20       | 0.25          |
| (1,1422) | 1:84:A:LYS:HG3  | 1:95:A:PHE:HD1  | 20       | 0.25          |
| (1,1422) | 1:84:A:LYS:HG3  | 1:95:A:PHE:HD2  | 20       | 0.25          |
| (1,1078) | 1:15:A:LEU:HD21 | 1:57:A:PHE:HZ   | 12       | 0.25          |
| (1,1078) | 1:15:A:LEU:HD22 | 1:57:A:PHE:HZ   | 12       | 0.25          |
| (1,1078) | 1:15:A:LEU:HD23 | 1:57:A:PHE:HZ   | 12       | 0.25          |
| (1,845)  | 1:37:A:LYS:HD2  | 1:65:A:VAL:HB   | 4        | 0.25          |
| (1,845)  | 1:37:A:LYS:HD3  | 1:65:A:VAL:HB   | 4        | 0.25          |
| (1,845)  | 1:37:A:LYS:HD2  | 1:65:A:VAL:HB   | 7        | 0.25          |
| (1,845)  | 1:37:A:LYS:HD3  | 1:65:A:VAL:HB   | 7        | 0.25          |
| (1,724)  | 1:58:A:ILE:HB   | 1:63:A:GLU:HB2  | 7        | 0.25          |
| (1,724)  | 1:58:A:ILE:HB   | 1:63:A:GLU:HB3  | 7        | 0.25          |
| (1,345)  | 1:19:A:LEU:HD21 | 1:23:A:LEU:H    | 13       | 0.25          |
| (1,345)  | 1:19:A:LEU:HD22 | 1:23:A:LEU:H    | 13       | 0.25          |
| (1,345)  | 1:19:A:LEU:HD23 | 1:23:A:LEU:H    | 13       | 0.25          |
| (1,299)  | 1:116:A:LYS:H   | 1:116:A:LYS:HD2 | 3        | 0.25          |
| (1,299)  | 1:116:A:LYS:H   | 1:116:A:LYS:HD3 | 3        | 0.25          |
| (1,282)  | 1:97:A:GLU:H    | 1:98:A:GLN:HB2  | 4        | 0.25          |
| (1,282)  | 1:97:A:GLU:H    | 1:98:A:GLN:HB3  | 4        | 0.25          |
| (2,878)  | 1:85:A:VAL:HG11 | 1:110:A:ASP:HB2 | 7        | 0.24          |
| (2,878)  | 1:85:A:VAL:HG11 | 1:110:A:ASP:HB3 | 7        | 0.24          |
| (2,878)  | 1:85:A:VAL:HG12 | 1:110:A:ASP:HB2 | 7        | 0.24          |
| (2,878)  | 1:85:A:VAL:HG12 | 1:110:A:ASP:HB3 | 7        | 0.24          |
| (2,878)  | 1:85:A:VAL:HG13 | 1:110:A:ASP:HB2 | 7        | 0.24          |
| (2,878)  | 1:85:A:VAL:HG13 | 1:110:A:ASP:HB3 | 7        | 0.24          |
| (1,1447) | 1:99:A:LEU:HD11 | 1:100:A:LYS:HG2 | 18       | 0.24          |
| (1,1447) | 1:99:A:LEU:HD11 | 1:100:A:LYS:HG3 | 18       | 0.24          |
| (1,1447) | 1:99:A:LEU:HD12 | 1:100:A:LYS:HG2 | 18       | 0.24          |
| (1,1447) | 1:99:A:LEU:HD12 | 1:100:A:LYS:HG3 | 18       | 0.24          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1447) | 1:99:A:LEU:HD13 | 1:100:A:LYS:HG2 | 18       | 0.24          |
| (1,1447) | 1:99:A:LEU:HD13 | 1:100:A:LYS:HG3 | 18       | 0.24          |
| (1,1429) | 1:86:A:ALA:HB1  | 1:87:A:GLN:HB2  | 16       | 0.24          |
| (1,1429) | 1:86:A:ALA:HB1  | 1:87:A:GLN:HB3  | 16       | 0.24          |
| (1,1429) | 1:86:A:ALA:HB2  | 1:87:A:GLN:HB2  | 16       | 0.24          |
| (1,1429) | 1:86:A:ALA:HB2  | 1:87:A:GLN:HB3  | 16       | 0.24          |
| (1,1429) | 1:86:A:ALA:HB3  | 1:87:A:GLN:HB2  | 16       | 0.24          |
| (1,1429) | 1:86:A:ALA:HB3  | 1:87:A:GLN:HB3  | 16       | 0.24          |
| (1,1324) | 1:44:A:ILE:HD11 | 1:76:A:GLU:HB2  | 13       | 0.24          |
| (1,1324) | 1:44:A:ILE:HD11 | 1:76:A:GLU:HB3  | 13       | 0.24          |
| (1,1324) | 1:44:A:ILE:HD12 | 1:76:A:GLU:HB2  | 13       | 0.24          |
| (1,1324) | 1:44:A:ILE:HD12 | 1:76:A:GLU:HB3  | 13       | 0.24          |
| (1,1324) | 1:44:A:ILE:HD13 | 1:76:A:GLU:HB2  | 13       | 0.24          |
| (1,1324) | 1:44:A:ILE:HD13 | 1:76:A:GLU:HB3  | 13       | 0.24          |
| (1,1237) | 1:27:A:PRO:HG2  | 1:28:A:ASN:HD21 | 13       | 0.24          |
| (1,1237) | 1:27:A:PRO:HG2  | 1:28:A:ASN:HD22 | 13       | 0.24          |
| (1,1237) | 1:27:A:PRO:HG3  | 1:28:A:ASN:HD21 | 13       | 0.24          |
| (1,1237) | 1:27:A:PRO:HG3  | 1:28:A:ASN:HD22 | 13       | 0.24          |
| (1,1078) | 1:15:A:LEU:HD21 | 1:57:A:PHE:HZ   | 2        | 0.24          |
| (1,1078) | 1:15:A:LEU:HD22 | 1:57:A:PHE:HZ   | 2        | 0.24          |
| (1,1078) | 1:15:A:LEU:HD23 | 1:57:A:PHE:HZ   | 2        | 0.24          |
| (1,1078) | 1:15:A:LEU:HD21 | 1:57:A:PHE:HZ   | 15       | 0.24          |
| (1,1078) | 1:15:A:LEU:HD22 | 1:57:A:PHE:HZ   | 15       | 0.24          |
| (1,1078) | 1:15:A:LEU:HD23 | 1:57:A:PHE:HZ   | 15       | 0.24          |
| (1,1078) | 1:15:A:LEU:HD21 | 1:57:A:PHE:HZ   | 20       | 0.24          |
| (1,1078) | 1:15:A:LEU:HD22 | 1:57:A:PHE:HZ   | 20       | 0.24          |
| (1,1078) | 1:15:A:LEU:HD23 | 1:57:A:PHE:HZ   | 20       | 0.24          |
| (1,658)  | 1:129:A:LEU:HG  | 1:130:A:GLU:HG2 | 6        | 0.24          |
| (1,658)  | 1:129:A:LEU:HG  | 1:130:A:GLU:HG3 | 6        | 0.24          |
| (1,345)  | 1:19:A:LEU:HD21 | 1:23:A:LEU:H    | 2        | 0.24          |
| (1,345)  | 1:19:A:LEU:HD22 | 1:23:A:LEU:H    | 2        | 0.24          |
| (1,345)  | 1:19:A:LEU:HD23 | 1:23:A:LEU:H    | 2        | 0.24          |
| (2,866)  | 1:81:A:LEU:HB2  | 1:83:A:ILE:HA   | 7        | 0.23          |
| (2,866)  | 1:81:A:LEU:HB3  | 1:83:A:ILE:HA   | 7        | 0.23          |
| (2,780)  | 1:20:A:GLU:HG2  | 1:57:A:PHE:HE1  | 2        | 0.23          |
| (2,780)  | 1:20:A:GLU:HG2  | 1:57:A:PHE:HE2  | 2        | 0.23          |
| (2,780)  | 1:20:A:GLU:HG3  | 1:57:A:PHE:HE1  | 2        | 0.23          |
| (2,780)  | 1:20:A:GLU:HG3  | 1:57:A:PHE:HE2  | 2        | 0.23          |
| (2,523)  | 1:27:A:PRO:HB3  | 1:28:A:ASN:HB2  | 12       | 0.23          |
| (2,523)  | 1:27:A:PRO:HB3  | 1:28:A:ASN:HB3  | 12       | 0.23          |
| (2,438)  | 1:106:A:VAL:HA  | 1:107:A:ARG:HG2 | 6        | 0.23          |
| (2,398)  | 1:4:A:VAL:H     | 1:81:A:LEU:HD11 | 15       | 0.23          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (2,398)  | 1:4:A:VAL:H     | 1:81:A:LEU:HD12  | 15       | 0.23          |
| (2,398)  | 1:4:A:VAL:H     | 1:81:A:LEU:HD13  | 15       | 0.23          |
| (2,78)   | 1:33:A:ARG:HD2  | 1:34:A:THR:H     | 16       | 0.23          |
| (1,1324) | 1:44:A:ILE:HD11 | 1:76:A:GLU:HB2   | 14       | 0.23          |
| (1,1324) | 1:44:A:ILE:HD11 | 1:76:A:GLU:HB3   | 14       | 0.23          |
| (1,1324) | 1:44:A:ILE:HD12 | 1:76:A:GLU:HB2   | 14       | 0.23          |
| (1,1324) | 1:44:A:ILE:HD12 | 1:76:A:GLU:HB3   | 14       | 0.23          |
| (1,1324) | 1:44:A:ILE:HD13 | 1:76:A:GLU:HB2   | 14       | 0.23          |
| (1,1324) | 1:44:A:ILE:HD13 | 1:76:A:GLU:HB3   | 14       | 0.23          |
| (1,1324) | 1:44:A:ILE:HD11 | 1:76:A:GLU:HB2   | 16       | 0.23          |
| (1,1324) | 1:44:A:ILE:HD11 | 1:76:A:GLU:HB3   | 16       | 0.23          |
| (1,1324) | 1:44:A:ILE:HD12 | 1:76:A:GLU:HB2   | 16       | 0.23          |
| (1,1324) | 1:44:A:ILE:HD12 | 1:76:A:GLU:HB3   | 16       | 0.23          |
| (1,1324) | 1:44:A:ILE:HD13 | 1:76:A:GLU:HB2   | 16       | 0.23          |
| (1,1324) | 1:44:A:ILE:HD13 | 1:76:A:GLU:HB3   | 16       | 0.23          |
| (1,1187) | 1:13:A:ARG:HB2  | 1:17:A:GLU:H     | 5        | 0.23          |
| (1,1187) | 1:13:A:ARG:HB3  | 1:17:A:GLU:H     | 5        | 0.23          |
| (1,1114) | 1:96:A:TYR:HE1  | 1:106:A:VAL:HG21 | 10       | 0.23          |
| (1,1114) | 1:96:A:TYR:HE1  | 1:106:A:VAL:HG22 | 10       | 0.23          |
| (1,1114) | 1:96:A:TYR:HE1  | 1:106:A:VAL:HG23 | 10       | 0.23          |
| (1,1114) | 1:96:A:TYR:HE2  | 1:106:A:VAL:HG21 | 10       | 0.23          |
| (1,1114) | 1:96:A:TYR:HE2  | 1:106:A:VAL:HG22 | 10       | 0.23          |
| (1,1114) | 1:96:A:TYR:HE2  | 1:106:A:VAL:HG23 | 10       | 0.23          |
| (1,977)  | 1:64:A:GLU:HG2  | 1:65:A:VAL:HG11  | 4        | 0.23          |
| (1,977)  | 1:64:A:GLU:HG2  | 1:65:A:VAL:HG12  | 4        | 0.23          |
| (1,977)  | 1:64:A:GLU:HG2  | 1:65:A:VAL:HG13  | 4        | 0.23          |
| (1,977)  | 1:64:A:GLU:HG3  | 1:65:A:VAL:HG11  | 4        | 0.23          |
| (1,977)  | 1:64:A:GLU:HG3  | 1:65:A:VAL:HG12  | 4        | 0.23          |
| (1,977)  | 1:64:A:GLU:HG3  | 1:65:A:VAL:HG13  | 4        | 0.23          |
| (1,724)  | 1:58:A:ILE:HB   | 1:63:A:GLU:HB2   | 6        | 0.23          |
| (1,724)  | 1:58:A:ILE:HB   | 1:63:A:GLU:HB3   | 6        | 0.23          |
| (1,724)  | 1:58:A:ILE:HB   | 1:63:A:GLU:HB2   | 13       | 0.23          |
| (1,724)  | 1:58:A:ILE:HB   | 1:63:A:GLU:HB3   | 13       | 0.23          |
| (1,500)  | 1:23:A:LEU:HG   | 1:31:A:THR:HG21  | 6        | 0.23          |
| (1,500)  | 1:23:A:LEU:HG   | 1:31:A:THR:HG22  | 6        | 0.23          |
| (1,500)  | 1:23:A:LEU:HG   | 1:31:A:THR:HG23  | 6        | 0.23          |
| (1,453)  | 1:80:A:VAL:H    | 1:104:A:VAL:HG21 | 6        | 0.23          |
| (1,453)  | 1:80:A:VAL:H    | 1:104:A:VAL:HG22 | 6        | 0.23          |
| (1,453)  | 1:80:A:VAL:H    | 1:104:A:VAL:HG23 | 6        | 0.23          |
| (1,453)  | 1:80:A:VAL:H    | 1:104:A:VAL:HG21 | 14       | 0.23          |
| (1,453)  | 1:80:A:VAL:H    | 1:104:A:VAL:HG22 | 14       | 0.23          |
| (1,453)  | 1:80:A:VAL:H    | 1:104:A:VAL:HG23 | 14       | 0.23          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,345)  | 1:19:A:LEU:HD21 | 1:23:A:LEU:H     | 19       | 0.23          |
| (1,345)  | 1:19:A:LEU:HD22 | 1:23:A:LEU:H     | 19       | 0.23          |
| (1,345)  | 1:19:A:LEU:HD23 | 1:23:A:LEU:H     | 19       | 0.23          |
| (1,299)  | 1:116:A:LYS:H   | 1:116:A:LYS:HD2  | 9        | 0.23          |
| (1,299)  | 1:116:A:LYS:H   | 1:116:A:LYS:HD3  | 9        | 0.23          |
| (1,282)  | 1:97:A:GLU:H    | 1:98:A:GLN:HB2   | 19       | 0.23          |
| (1,282)  | 1:97:A:GLU:H    | 1:98:A:GLN:HB3   | 19       | 0.23          |
| (2,886)  | 1:87:A:GLN:HB2  | 1:92:A:LEU:HD11  | 14       | 0.22          |
| (2,886)  | 1:87:A:GLN:HB2  | 1:92:A:LEU:HD12  | 14       | 0.22          |
| (2,886)  | 1:87:A:GLN:HB2  | 1:92:A:LEU:HD13  | 14       | 0.22          |
| (2,886)  | 1:87:A:GLN:HB3  | 1:92:A:LEU:HD11  | 14       | 0.22          |
| (2,886)  | 1:87:A:GLN:HB3  | 1:92:A:LEU:HD12  | 14       | 0.22          |
| (2,886)  | 1:87:A:GLN:HB3  | 1:92:A:LEU:HD13  | 14       | 0.22          |
| (2,866)  | 1:81:A:LEU:HB2  | 1:83:A:ILE:HA    | 5        | 0.22          |
| (2,866)  | 1:81:A:LEU:HB3  | 1:83:A:ILE:HA    | 5        | 0.22          |
| (2,866)  | 1:81:A:LEU:HB2  | 1:83:A:ILE:HA    | 16       | 0.22          |
| (2,866)  | 1:81:A:LEU:HB3  | 1:83:A:ILE:HA    | 16       | 0.22          |
| (2,780)  | 1:20:A:GLU:HG2  | 1:57:A:PHE:HE1   | 9        | 0.22          |
| (2,780)  | 1:20:A:GLU:HG2  | 1:57:A:PHE:HE2   | 9        | 0.22          |
| (2,780)  | 1:20:A:GLU:HG3  | 1:57:A:PHE:HE1   | 9        | 0.22          |
| (2,780)  | 1:20:A:GLU:HG3  | 1:57:A:PHE:HE2   | 9        | 0.22          |
| (2,687)  | 1:9:A:SER:HB2   | 1:84:A:LYS:HA    | 10       | 0.22          |
| (2,679)  | 1:92:A:LEU:HD11 | 1:108:A:VAL:HA   | 1        | 0.22          |
| (2,679)  | 1:92:A:LEU:HD12 | 1:108:A:VAL:HA   | 1        | 0.22          |
| (2,679)  | 1:92:A:LEU:HD13 | 1:108:A:VAL:HA   | 1        | 0.22          |
| (2,438)  | 1:106:A:VAL:HA  | 1:107:A:ARG:HG2  | 15       | 0.22          |
| (2,315)  | 1:81:A:LEU:HB3  | 1:105:A:ASP:HB2  | 5        | 0.22          |
| (2,149)  | 1:85:A:VAL:HG11 | 1:87:A:GLN:HE22  | 20       | 0.22          |
| (2,149)  | 1:85:A:VAL:HG12 | 1:87:A:GLN:HE22  | 20       | 0.22          |
| (2,149)  | 1:85:A:VAL:HG13 | 1:87:A:GLN:HE22  | 20       | 0.22          |
| (1,1487) | 1:120:A:LYS:HG2 | 1:123:A:LEU:HD21 | 2        | 0.22          |
| (1,1487) | 1:120:A:LYS:HG2 | 1:123:A:LEU:HD22 | 2        | 0.22          |
| (1,1487) | 1:120:A:LYS:HG2 | 1:123:A:LEU:HD23 | 2        | 0.22          |
| (1,1487) | 1:120:A:LYS:HG3 | 1:123:A:LEU:HD21 | 2        | 0.22          |
| (1,1487) | 1:120:A:LYS:HG3 | 1:123:A:LEU:HD22 | 2        | 0.22          |
| (1,1487) | 1:120:A:LYS:HG3 | 1:123:A:LEU:HD23 | 2        | 0.22          |
| (1,1487) | 1:120:A:LYS:HG2 | 1:123:A:LEU:HD21 | 15       | 0.22          |
| (1,1487) | 1:120:A:LYS:HG2 | 1:123:A:LEU:HD22 | 15       | 0.22          |
| (1,1487) | 1:120:A:LYS:HG2 | 1:123:A:LEU:HD23 | 15       | 0.22          |
| (1,1487) | 1:120:A:LYS:HG3 | 1:123:A:LEU:HD21 | 15       | 0.22          |
| (1,1487) | 1:120:A:LYS:HG3 | 1:123:A:LEU:HD22 | 15       | 0.22          |
| (1,1487) | 1:120:A:LYS:HG3 | 1:123:A:LEU:HD23 | 15       | 0.22          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1411) | 1:83:A:ILE:HG12 | 1:107:A:ARG:HA  | 5        | 0.22          |
| (1,1411) | 1:83:A:ILE:HG13 | 1:107:A:ARG:HA  | 5        | 0.22          |
| (1,1198) | 1:16:A:GLU:HG2  | 1:19:A:LEU:HD11 | 2        | 0.22          |
| (1,1198) | 1:16:A:GLU:HG2  | 1:19:A:LEU:HD12 | 2        | 0.22          |
| (1,1198) | 1:16:A:GLU:HG2  | 1:19:A:LEU:HD13 | 2        | 0.22          |
| (1,1198) | 1:16:A:GLU:HG3  | 1:19:A:LEU:HD11 | 2        | 0.22          |
| (1,1198) | 1:16:A:GLU:HG3  | 1:19:A:LEU:HD12 | 2        | 0.22          |
| (1,1198) | 1:16:A:GLU:HG3  | 1:19:A:LEU:HD13 | 2        | 0.22          |
| (1,1078) | 1:15:A:LEU:HD21 | 1:57:A:PHE:HZ   | 6        | 0.22          |
| (1,1078) | 1:15:A:LEU:HD22 | 1:57:A:PHE:HZ   | 6        | 0.22          |
| (1,1078) | 1:15:A:LEU:HD23 | 1:57:A:PHE:HZ   | 6        | 0.22          |
| (1,880)  | 1:83:A:ILE:HD11 | 1:115:A:ALA:HA  | 10       | 0.22          |
| (1,880)  | 1:83:A:ILE:HD12 | 1:115:A:ALA:HA  | 10       | 0.22          |
| (1,880)  | 1:83:A:ILE:HD13 | 1:115:A:ALA:HA  | 10       | 0.22          |
| (1,845)  | 1:37:A:LYS:HD2  | 1:65:A:VAL:HB   | 15       | 0.22          |
| (1,845)  | 1:37:A:LYS:HD3  | 1:65:A:VAL:HB   | 15       | 0.22          |
| (1,723)  | 1:8:A:VAL:HG11  | 1:60:A:GLY:HA3  | 10       | 0.22          |
| (1,723)  | 1:8:A:VAL:HG12  | 1:60:A:GLY:HA3  | 10       | 0.22          |
| (1,723)  | 1:8:A:VAL:HG13  | 1:60:A:GLY:HA3  | 10       | 0.22          |
| (1,661)  | 1:32:A:VAL:HG21 | 1:43:A:GLU:HA   | 13       | 0.22          |
| (1,661)  | 1:32:A:VAL:HG22 | 1:43:A:GLU:HA   | 13       | 0.22          |
| (1,661)  | 1:32:A:VAL:HG23 | 1:43:A:GLU:HA   | 13       | 0.22          |
| (1,345)  | 1:19:A:LEU:HD21 | 1:23:A:LEU:H    | 5        | 0.22          |
| (1,345)  | 1:19:A:LEU:HD22 | 1:23:A:LEU:H    | 5        | 0.22          |
| (1,345)  | 1:19:A:LEU:HD23 | 1:23:A:LEU:H    | 5        | 0.22          |
| (1,345)  | 1:19:A:LEU:HD21 | 1:23:A:LEU:H    | 15       | 0.22          |
| (1,345)  | 1:19:A:LEU:HD22 | 1:23:A:LEU:H    | 15       | 0.22          |
| (1,345)  | 1:19:A:LEU:HD23 | 1:23:A:LEU:H    | 15       | 0.22          |
| (1,299)  | 1:116:A:LYS:H   | 1:116:A:LYS:HD2 | 5        | 0.22          |
| (1,299)  | 1:116:A:LYS:H   | 1:116:A:LYS:HD3 | 5        | 0.22          |
| (1,299)  | 1:116:A:LYS:H   | 1:116:A:LYS:HD2 | 13       | 0.22          |
| (1,299)  | 1:116:A:LYS:H   | 1:116:A:LYS:HD3 | 13       | 0.22          |
| (2,889)  | 1:92:A:LEU:HD21 | 1:110:A:ASP:HB2 | 15       | 0.21          |
| (2,889)  | 1:92:A:LEU:HD21 | 1:110:A:ASP:HB3 | 15       | 0.21          |
| (2,889)  | 1:92:A:LEU:HD22 | 1:110:A:ASP:HB2 | 15       | 0.21          |
| (2,889)  | 1:92:A:LEU:HD22 | 1:110:A:ASP:HB3 | 15       | 0.21          |
| (2,889)  | 1:92:A:LEU:HD23 | 1:110:A:ASP:HB2 | 15       | 0.21          |
| (2,889)  | 1:92:A:LEU:HD23 | 1:110:A:ASP:HB3 | 15       | 0.21          |
| (2,780)  | 1:20:A:GLU:HG2  | 1:57:A:PHE:HE1  | 14       | 0.21          |
| (2,780)  | 1:20:A:GLU:HG2  | 1:57:A:PHE:HE2  | 14       | 0.21          |
| (2,780)  | 1:20:A:GLU:HG3  | 1:57:A:PHE:HE1  | 14       | 0.21          |
| (2,780)  | 1:20:A:GLU:HG3  | 1:57:A:PHE:HE2  | 14       | 0.21          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,780)  | 1:20:A:GLU:HG2  | 1:57:A:PHE:HE1  | 16       | 0.21          |
| (2,780)  | 1:20:A:GLU:HG2  | 1:57:A:PHE:HE2  | 16       | 0.21          |
| (2,780)  | 1:20:A:GLU:HG3  | 1:57:A:PHE:HE1  | 16       | 0.21          |
| (2,780)  | 1:20:A:GLU:HG3  | 1:57:A:PHE:HE2  | 16       | 0.21          |
| (2,720)  | 1:6:A:ILE:HB    | 1:55:A:VAL:HG11 | 18       | 0.21          |
| (2,720)  | 1:6:A:ILE:HB    | 1:55:A:VAL:HG12 | 18       | 0.21          |
| (2,720)  | 1:6:A:ILE:HB    | 1:55:A:VAL:HG13 | 18       | 0.21          |
| (2,402)  | 1:80:A:VAL:H    | 1:81:A:LEU:HD21 | 12       | 0.21          |
| (2,402)  | 1:80:A:VAL:H    | 1:81:A:LEU:HD22 | 12       | 0.21          |
| (2,402)  | 1:80:A:VAL:H    | 1:81:A:LEU:HD23 | 12       | 0.21          |
| (2,398)  | 1:4:A:VAL:H     | 1:81:A:LEU:HD11 | 9        | 0.21          |
| (2,398)  | 1:4:A:VAL:H     | 1:81:A:LEU:HD12 | 9        | 0.21          |
| (2,398)  | 1:4:A:VAL:H     | 1:81:A:LEU:HD13 | 9        | 0.21          |
| (2,398)  | 1:4:A:VAL:H     | 1:81:A:LEU:HD11 | 12       | 0.21          |
| (2,398)  | 1:4:A:VAL:H     | 1:81:A:LEU:HD12 | 12       | 0.21          |
| (2,398)  | 1:4:A:VAL:H     | 1:81:A:LEU:HD13 | 12       | 0.21          |
| (2,363)  | 1:81:A:LEU:HG   | 1:105:A:ASP:HB2 | 16       | 0.21          |
| (1,1078) | 1:15:A:LEU:HD21 | 1:57:A:PHE:HZ   | 3        | 0.21          |
| (1,1078) | 1:15:A:LEU:HD22 | 1:57:A:PHE:HZ   | 3        | 0.21          |
| (1,1078) | 1:15:A:LEU:HD23 | 1:57:A:PHE:HZ   | 3        | 0.21          |
| (1,1078) | 1:15:A:LEU:HD21 | 1:57:A:PHE:HZ   | 17       | 0.21          |
| (1,1078) | 1:15:A:LEU:HD22 | 1:57:A:PHE:HZ   | 17       | 0.21          |
| (1,1078) | 1:15:A:LEU:HD23 | 1:57:A:PHE:HZ   | 17       | 0.21          |
| (1,1078) | 1:15:A:LEU:HD21 | 1:57:A:PHE:HZ   | 18       | 0.21          |
| (1,1078) | 1:15:A:LEU:HD22 | 1:57:A:PHE:HZ   | 18       | 0.21          |
| (1,1078) | 1:15:A:LEU:HD23 | 1:57:A:PHE:HZ   | 18       | 0.21          |
| (1,977)  | 1:64:A:GLU:HG2  | 1:65:A:VAL:HG11 | 6        | 0.21          |
| (1,977)  | 1:64:A:GLU:HG2  | 1:65:A:VAL:HG12 | 6        | 0.21          |
| (1,977)  | 1:64:A:GLU:HG2  | 1:65:A:VAL:HG13 | 6        | 0.21          |
| (1,977)  | 1:64:A:GLU:HG3  | 1:65:A:VAL:HG11 | 6        | 0.21          |
| (1,977)  | 1:64:A:GLU:HG3  | 1:65:A:VAL:HG12 | 6        | 0.21          |
| (1,977)  | 1:64:A:GLU:HG3  | 1:65:A:VAL:HG13 | 6        | 0.21          |
| (1,724)  | 1:58:A:ILE:HB   | 1:63:A:GLU:HB2  | 18       | 0.21          |
| (1,724)  | 1:58:A:ILE:HB   | 1:63:A:GLU:HB3  | 18       | 0.21          |
| (1,556)  | 1:19:A:LEU:HD11 | 1:23:A:LEU:HD21 | 1        | 0.21          |
| (1,556)  | 1:19:A:LEU:HD11 | 1:23:A:LEU:HD22 | 1        | 0.21          |
| (1,556)  | 1:19:A:LEU:HD11 | 1:23:A:LEU:HD23 | 1        | 0.21          |
| (1,556)  | 1:19:A:LEU:HD12 | 1:23:A:LEU:HD21 | 1        | 0.21          |
| (1,556)  | 1:19:A:LEU:HD12 | 1:23:A:LEU:HD22 | 1        | 0.21          |
| (1,556)  | 1:19:A:LEU:HD12 | 1:23:A:LEU:HD23 | 1        | 0.21          |
| (1,556)  | 1:19:A:LEU:HD13 | 1:23:A:LEU:HD21 | 1        | 0.21          |
| (1,556)  | 1:19:A:LEU:HD13 | 1:23:A:LEU:HD22 | 1        | 0.21          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,556)  | 1:19:A:LEU:HD13 | 1:23:A:LEU:HD23 | 1        | 0.21          |
| (1,345)  | 1:19:A:LEU:HD21 | 1:23:A:LEU:H    | 3        | 0.21          |
| (1,345)  | 1:19:A:LEU:HD22 | 1:23:A:LEU:H    | 3        | 0.21          |
| (1,345)  | 1:19:A:LEU:HD23 | 1:23:A:LEU:H    | 3        | 0.21          |
| (1,345)  | 1:19:A:LEU:HD21 | 1:23:A:LEU:H    | 8        | 0.21          |
| (1,345)  | 1:19:A:LEU:HD22 | 1:23:A:LEU:H    | 8        | 0.21          |
| (1,345)  | 1:19:A:LEU:HD23 | 1:23:A:LEU:H    | 8        | 0.21          |
| (1,345)  | 1:19:A:LEU:HD21 | 1:23:A:LEU:H    | 12       | 0.21          |
| (1,345)  | 1:19:A:LEU:HD22 | 1:23:A:LEU:H    | 12       | 0.21          |
| (1,345)  | 1:19:A:LEU:HD23 | 1:23:A:LEU:H    | 12       | 0.21          |
| (1,345)  | 1:19:A:LEU:HD21 | 1:23:A:LEU:H    | 17       | 0.21          |
| (1,345)  | 1:19:A:LEU:HD22 | 1:23:A:LEU:H    | 17       | 0.21          |
| (1,345)  | 1:19:A:LEU:HD23 | 1:23:A:LEU:H    | 17       | 0.21          |
| (1,322)  | 1:6:A:ILE:H     | 1:83:A:ILE:HD11 | 16       | 0.21          |
| (1,322)  | 1:6:A:ILE:H     | 1:83:A:ILE:HD12 | 16       | 0.21          |
| (1,322)  | 1:6:A:ILE:H     | 1:83:A:ILE:HD13 | 16       | 0.21          |
| (1,299)  | 1:116:A:LYS:H   | 1:116:A:LYS:HD2 | 7        | 0.21          |
| (1,299)  | 1:116:A:LYS:H   | 1:116:A:LYS:HD3 | 7        | 0.21          |
| (1,282)  | 1:97:A:GLU:H    | 1:98:A:GLN:HB2  | 9        | 0.21          |
| (1,282)  | 1:97:A:GLU:H    | 1:98:A:GLN:HB3  | 9        | 0.21          |
| (2,875)  | 1:84:A:LYS:HE2  | 1:85:A:VAL:HA   | 4        | 0.2           |
| (2,875)  | 1:84:A:LYS:HE3  | 1:85:A:VAL:HA   | 4        | 0.2           |
| (2,402)  | 1:80:A:VAL:H    | 1:81:A:LEU:HD21 | 19       | 0.2           |
| (2,402)  | 1:80:A:VAL:H    | 1:81:A:LEU:HD22 | 19       | 0.2           |
| (2,402)  | 1:80:A:VAL:H    | 1:81:A:LEU:HD23 | 19       | 0.2           |
| (2,398)  | 1:4:A:VAL:H     | 1:81:A:LEU:HD11 | 3        | 0.2           |
| (2,398)  | 1:4:A:VAL:H     | 1:81:A:LEU:HD12 | 3        | 0.2           |
| (2,398)  | 1:4:A:VAL:H     | 1:81:A:LEU:HD13 | 3        | 0.2           |
| (1,1504) | 1:129:A:LEU:HB2 | 1:130:A:GLU:HB2 | 2        | 0.2           |
| (1,1504) | 1:129:A:LEU:HB2 | 1:130:A:GLU:HB3 | 2        | 0.2           |
| (1,1504) | 1:129:A:LEU:HB3 | 1:130:A:GLU:HB2 | 2        | 0.2           |
| (1,1504) | 1:129:A:LEU:HB3 | 1:130:A:GLU:HB3 | 2        | 0.2           |
| (1,1485) | 1:120:A:LYS:HG2 | 1:123:A:LEU:H   | 9        | 0.2           |
| (1,1485) | 1:120:A:LYS:HG3 | 1:123:A:LEU:H   | 9        | 0.2           |
| (1,1447) | 1:99:A:LEU:HD11 | 1:100:A:LYS:HG2 | 2        | 0.2           |
| (1,1447) | 1:99:A:LEU:HD11 | 1:100:A:LYS:HG3 | 2        | 0.2           |
| (1,1447) | 1:99:A:LEU:HD12 | 1:100:A:LYS:HG2 | 2        | 0.2           |
| (1,1447) | 1:99:A:LEU:HD12 | 1:100:A:LYS:HG3 | 2        | 0.2           |
| (1,1447) | 1:99:A:LEU:HD13 | 1:100:A:LYS:HG2 | 2        | 0.2           |
| (1,1447) | 1:99:A:LEU:HD13 | 1:100:A:LYS:HG3 | 2        | 0.2           |
| (1,1419) | 1:84:A:LYS:HB2  | 1:96:A:TYR:HB2  | 20       | 0.2           |
| (1,1419) | 1:84:A:LYS:HB2  | 1:96:A:TYR:HB3  | 20       | 0.2           |

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| Key      | Atom-1         | Atom-2           | Model ID | Violation (Å) |
|----------|----------------|------------------|----------|---------------|
| (1,1419) | 1:84:A:LYS:HB3 | 1:96:A:TYR:HB2   | 20       | 0.2           |
| (1,1419) | 1:84:A:LYS:HB3 | 1:96:A:TYR:HB3   | 20       | 0.2           |
| (1,1346) | 1:53:A:PRO:HB2 | 1:126:A:VAL:HG11 | 17       | 0.2           |
| (1,1346) | 1:53:A:PRO:HB2 | 1:126:A:VAL:HG12 | 17       | 0.2           |
| (1,1346) | 1:53:A:PRO:HB2 | 1:126:A:VAL:HG13 | 17       | 0.2           |
| (1,1346) | 1:53:A:PRO:HB2 | 1:126:A:VAL:HG21 | 17       | 0.2           |
| (1,1346) | 1:53:A:PRO:HB2 | 1:126:A:VAL:HG22 | 17       | 0.2           |
| (1,1346) | 1:53:A:PRO:HB2 | 1:126:A:VAL:HG23 | 17       | 0.2           |
| (1,1198) | 1:16:A:GLU:HG2 | 1:19:A:LEU:HD11  | 18       | 0.2           |
| (1,1198) | 1:16:A:GLU:HG2 | 1:19:A:LEU:HD12  | 18       | 0.2           |
| (1,1198) | 1:16:A:GLU:HG2 | 1:19:A:LEU:HD13  | 18       | 0.2           |
| (1,1198) | 1:16:A:GLU:HG3 | 1:19:A:LEU:HD11  | 18       | 0.2           |
| (1,1198) | 1:16:A:GLU:HG3 | 1:19:A:LEU:HD12  | 18       | 0.2           |
| (1,1198) | 1:16:A:GLU:HG3 | 1:19:A:LEU:HD13  | 18       | 0.2           |
| (1,1119) | 1:96:A:TYR:HD1 | 1:106:A:VAL:HG11 | 3        | 0.2           |
| (1,1119) | 1:96:A:TYR:HD1 | 1:106:A:VAL:HG12 | 3        | 0.2           |
| (1,1119) | 1:96:A:TYR:HD1 | 1:106:A:VAL:HG13 | 3        | 0.2           |
| (1,1119) | 1:96:A:TYR:HD2 | 1:106:A:VAL:HG11 | 3        | 0.2           |
| (1,1119) | 1:96:A:TYR:HD2 | 1:106:A:VAL:HG12 | 3        | 0.2           |
| (1,1119) | 1:96:A:TYR:HD2 | 1:106:A:VAL:HG13 | 3        | 0.2           |
| (1,845)  | 1:37:A:LYS:HD2 | 1:65:A:VAL:HB    | 6        | 0.2           |
| (1,845)  | 1:37:A:LYS:HD3 | 1:65:A:VAL:HB    | 6        | 0.2           |
| (1,453)  | 1:80:A:VAL:H   | 1:104:A:VAL:HG21 | 8        | 0.2           |
| (1,453)  | 1:80:A:VAL:H   | 1:104:A:VAL:HG22 | 8        | 0.2           |
| (1,453)  | 1:80:A:VAL:H   | 1:104:A:VAL:HG23 | 8        | 0.2           |
| (1,299)  | 1:116:A:LYS:H  | 1:116:A:LYS:HD2  | 11       | 0.2           |
| (1,299)  | 1:116:A:LYS:H  | 1:116:A:LYS:HD3  | 11       | 0.2           |
| (1,299)  | 1:116:A:LYS:H  | 1:116:A:LYS:HD2  | 14       | 0.2           |
| (1,299)  | 1:116:A:LYS:H  | 1:116:A:LYS:HD3  | 14       | 0.2           |
| (2,875)  | 1:84:A:LYS:HE2 | 1:85:A:VAL:HA    | 8        | 0.19          |
| (2,875)  | 1:84:A:LYS:HE3 | 1:85:A:VAL:HA    | 8        | 0.19          |
| (2,866)  | 1:81:A:LEU:HB2 | 1:83:A:ILE:HA    | 2        | 0.19          |
| (2,866)  | 1:81:A:LEU:HB3 | 1:83:A:ILE:HA    | 2        | 0.19          |
| (2,478)  | 1:100:A:LYS:HA | 1:106:A:VAL:HG21 | 19       | 0.19          |
| (2,478)  | 1:100:A:LYS:HA | 1:106:A:VAL:HG22 | 19       | 0.19          |
| (2,478)  | 1:100:A:LYS:HA | 1:106:A:VAL:HG23 | 19       | 0.19          |
| (2,402)  | 1:80:A:VAL:H   | 1:81:A:LEU:HD21  | 13       | 0.19          |
| (2,402)  | 1:80:A:VAL:H   | 1:81:A:LEU:HD22  | 13       | 0.19          |
| (2,402)  | 1:80:A:VAL:H   | 1:81:A:LEU:HD23  | 13       | 0.19          |
| (2,398)  | 1:4:A:VAL:H    | 1:81:A:LEU:HD11  | 8        | 0.19          |
| (2,398)  | 1:4:A:VAL:H    | 1:81:A:LEU:HD12  | 8        | 0.19          |
| (2,398)  | 1:4:A:VAL:H    | 1:81:A:LEU:HD13  | 8        | 0.19          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (2,398)  | 1:4:A:VAL:H     | 1:81:A:LEU:HD11  | 18       | 0.19          |
| (2,398)  | 1:4:A:VAL:H     | 1:81:A:LEU:HD12  | 18       | 0.19          |
| (2,398)  | 1:4:A:VAL:H     | 1:81:A:LEU:HD13  | 18       | 0.19          |
| (1,1487) | 1:120:A:LYS:HG2 | 1:123:A:LEU:HD21 | 16       | 0.19          |
| (1,1487) | 1:120:A:LYS:HG2 | 1:123:A:LEU:HD22 | 16       | 0.19          |
| (1,1487) | 1:120:A:LYS:HG2 | 1:123:A:LEU:HD23 | 16       | 0.19          |
| (1,1487) | 1:120:A:LYS:HG3 | 1:123:A:LEU:HD21 | 16       | 0.19          |
| (1,1487) | 1:120:A:LYS:HG3 | 1:123:A:LEU:HD22 | 16       | 0.19          |
| (1,1487) | 1:120:A:LYS:HG3 | 1:123:A:LEU:HD23 | 16       | 0.19          |
| (1,1447) | 1:99:A:LEU:HD11 | 1:100:A:LYS:HG2  | 7        | 0.19          |
| (1,1447) | 1:99:A:LEU:HD11 | 1:100:A:LYS:HG3  | 7        | 0.19          |
| (1,1447) | 1:99:A:LEU:HD12 | 1:100:A:LYS:HG2  | 7        | 0.19          |
| (1,1447) | 1:99:A:LEU:HD12 | 1:100:A:LYS:HG3  | 7        | 0.19          |
| (1,1447) | 1:99:A:LEU:HD13 | 1:100:A:LYS:HG2  | 7        | 0.19          |
| (1,1447) | 1:99:A:LEU:HD13 | 1:100:A:LYS:HG3  | 7        | 0.19          |
| (1,1324) | 1:44:A:ILE:HD11 | 1:76:A:GLU:HB2   | 10       | 0.19          |
| (1,1324) | 1:44:A:ILE:HD11 | 1:76:A:GLU:HB3   | 10       | 0.19          |
| (1,1324) | 1:44:A:ILE:HD12 | 1:76:A:GLU:HB2   | 10       | 0.19          |
| (1,1324) | 1:44:A:ILE:HD12 | 1:76:A:GLU:HB3   | 10       | 0.19          |
| (1,1324) | 1:44:A:ILE:HD13 | 1:76:A:GLU:HB2   | 10       | 0.19          |
| (1,1324) | 1:44:A:ILE:HD13 | 1:76:A:GLU:HB3   | 10       | 0.19          |
| (1,1265) | 1:36:A:ASP:H    | 1:39:A:LYS:HD2   | 3        | 0.19          |
| (1,1265) | 1:36:A:ASP:H    | 1:39:A:LYS:HD3   | 3        | 0.19          |
| (1,1188) | 1:13:A:ARG:HG2  | 1:16:A:GLU:HB2   | 6        | 0.19          |
| (1,1188) | 1:13:A:ARG:HG2  | 1:16:A:GLU:HB3   | 6        | 0.19          |
| (1,1188) | 1:13:A:ARG:HG3  | 1:16:A:GLU:HB2   | 6        | 0.19          |
| (1,1188) | 1:13:A:ARG:HG3  | 1:16:A:GLU:HB3   | 6        | 0.19          |
| (1,1187) | 1:13:A:ARG:HB2  | 1:17:A:GLU:H     | 12       | 0.19          |
| (1,1187) | 1:13:A:ARG:HB3  | 1:17:A:GLU:H     | 12       | 0.19          |
| (1,1150) | 1:72:A:TYR:HE1  | 1:78:A:LEU:HD11  | 20       | 0.19          |
| (1,1150) | 1:72:A:TYR:HE1  | 1:78:A:LEU:HD12  | 20       | 0.19          |
| (1,1150) | 1:72:A:TYR:HE1  | 1:78:A:LEU:HD13  | 20       | 0.19          |
| (1,1150) | 1:72:A:TYR:HE2  | 1:78:A:LEU:HD11  | 20       | 0.19          |
| (1,1150) | 1:72:A:TYR:HE2  | 1:78:A:LEU:HD12  | 20       | 0.19          |
| (1,1150) | 1:72:A:TYR:HE2  | 1:78:A:LEU:HD13  | 20       | 0.19          |
| (1,1112) | 1:96:A:TYR:HE1  | 1:97:A:GLU:HB2   | 20       | 0.19          |
| (1,1112) | 1:96:A:TYR:HE1  | 1:97:A:GLU:HB3   | 20       | 0.19          |
| (1,1112) | 1:96:A:TYR:HE2  | 1:97:A:GLU:HB2   | 20       | 0.19          |
| (1,1112) | 1:96:A:TYR:HE2  | 1:97:A:GLU:HB3   | 20       | 0.19          |
| (1,997)  | 1:22:A:VAL:H    | 1:119:A:LEU:HD21 | 7        | 0.19          |
| (1,997)  | 1:22:A:VAL:H    | 1:119:A:LEU:HD22 | 7        | 0.19          |
| (1,997)  | 1:22:A:VAL:H    | 1:119:A:LEU:HD23 | 7        | 0.19          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,724)  | 1:58:A:ILE:HB   | 1:63:A:GLU:HB2  | 3        | 0.19          |
| (1,724)  | 1:58:A:ILE:HB   | 1:63:A:GLU:HB3  | 3        | 0.19          |
| (2,875)  | 1:84:A:LYS:HE2  | 1:85:A:VAL:HA   | 3        | 0.18          |
| (2,875)  | 1:84:A:LYS:HE3  | 1:85:A:VAL:HA   | 3        | 0.18          |
| (2,875)  | 1:84:A:LYS:HE2  | 1:85:A:VAL:HA   | 12       | 0.18          |
| (2,875)  | 1:84:A:LYS:HE3  | 1:85:A:VAL:HA   | 12       | 0.18          |
| (2,866)  | 1:81:A:LEU:HB2  | 1:83:A:ILE:HA   | 8        | 0.18          |
| (2,866)  | 1:81:A:LEU:HB3  | 1:83:A:ILE:HA   | 8        | 0.18          |
| (2,866)  | 1:81:A:LEU:HB2  | 1:83:A:ILE:HA   | 18       | 0.18          |
| (2,866)  | 1:81:A:LEU:HB3  | 1:83:A:ILE:HA   | 18       | 0.18          |
| (2,792)  | 1:28:A:ASN:HD21 | 1:52:A:ARG:HG2  | 18       | 0.18          |
| (2,792)  | 1:28:A:ASN:HD21 | 1:52:A:ARG:HG3  | 18       | 0.18          |
| (2,792)  | 1:28:A:ASN:HD22 | 1:52:A:ARG:HG2  | 18       | 0.18          |
| (2,792)  | 1:28:A:ASN:HD22 | 1:52:A:ARG:HG3  | 18       | 0.18          |
| (2,711)  | 1:8:A:VAL:HB    | 1:66:A:VAL:HG21 | 17       | 0.18          |
| (2,711)  | 1:8:A:VAL:HB    | 1:66:A:VAL:HG22 | 17       | 0.18          |
| (2,711)  | 1:8:A:VAL:HB    | 1:66:A:VAL:HG23 | 17       | 0.18          |
| (2,523)  | 1:27:A:PRO:HB3  | 1:28:A:ASN:HB2  | 2        | 0.18          |
| (2,523)  | 1:27:A:PRO:HB3  | 1:28:A:ASN:HB3  | 2        | 0.18          |
| (2,473)  | 1:124:A:GLU:HG2 | 1:125:A:LYS:HE2 | 10       | 0.18          |
| (2,473)  | 1:124:A:GLU:HG2 | 1:125:A:LYS:HE3 | 10       | 0.18          |
| (2,473)  | 1:124:A:GLU:HG3 | 1:125:A:LYS:HE2 | 10       | 0.18          |
| (2,473)  | 1:124:A:GLU:HG3 | 1:125:A:LYS:HE3 | 10       | 0.18          |
| (2,440)  | 1:72:A:TYR:HE1  | 1:78:A:LEU:HG   | 12       | 0.18          |
| (2,440)  | 1:72:A:TYR:HE2  | 1:78:A:LEU:HG   | 12       | 0.18          |
| (2,398)  | 1:4:A:VAL:H     | 1:81:A:LEU:HD11 | 19       | 0.18          |
| (2,398)  | 1:4:A:VAL:H     | 1:81:A:LEU:HD12 | 19       | 0.18          |
| (2,398)  | 1:4:A:VAL:H     | 1:81:A:LEU:HD13 | 19       | 0.18          |
| (2,398)  | 1:4:A:VAL:H     | 1:81:A:LEU:HD11 | 20       | 0.18          |
| (2,398)  | 1:4:A:VAL:H     | 1:81:A:LEU:HD12 | 20       | 0.18          |
| (2,398)  | 1:4:A:VAL:H     | 1:81:A:LEU:HD13 | 20       | 0.18          |
| (2,316)  | 1:107:A:ARG:HD2 | 1:108:A:VAL:H   | 12       | 0.18          |
| (2,315)  | 1:81:A:LEU:HB3  | 1:105:A:ASP:HB2 | 1        | 0.18          |
| (2,315)  | 1:81:A:LEU:HB3  | 1:105:A:ASP:HB2 | 4        | 0.18          |
| (2,78)   | 1:33:A:ARG:HD2  | 1:34:A:THR:H    | 20       | 0.18          |
| (1,1504) | 1:129:A:LEU:HB2 | 1:130:A:GLU:HB2 | 8        | 0.18          |
| (1,1504) | 1:129:A:LEU:HB2 | 1:130:A:GLU:HB3 | 8        | 0.18          |
| (1,1504) | 1:129:A:LEU:HB3 | 1:130:A:GLU:HB2 | 8        | 0.18          |
| (1,1504) | 1:129:A:LEU:HB3 | 1:130:A:GLU:HB3 | 8        | 0.18          |
| (1,1324) | 1:44:A:ILE:HD11 | 1:76:A:GLU:HB2  | 2        | 0.18          |
| (1,1324) | 1:44:A:ILE:HD11 | 1:76:A:GLU:HB3  | 2        | 0.18          |
| (1,1324) | 1:44:A:ILE:HD12 | 1:76:A:GLU:HB2  | 2        | 0.18          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1324) | 1:44:A:ILE:HD12 | 1:76:A:GLU:HB3   | 2        | 0.18          |
| (1,1324) | 1:44:A:ILE:HD13 | 1:76:A:GLU:HB2   | 2        | 0.18          |
| (1,1324) | 1:44:A:ILE:HD13 | 1:76:A:GLU:HB3   | 2        | 0.18          |
| (1,1324) | 1:44:A:ILE:HD11 | 1:76:A:GLU:HB2   | 5        | 0.18          |
| (1,1324) | 1:44:A:ILE:HD11 | 1:76:A:GLU:HB3   | 5        | 0.18          |
| (1,1324) | 1:44:A:ILE:HD12 | 1:76:A:GLU:HB2   | 5        | 0.18          |
| (1,1324) | 1:44:A:ILE:HD12 | 1:76:A:GLU:HB3   | 5        | 0.18          |
| (1,1324) | 1:44:A:ILE:HD13 | 1:76:A:GLU:HB2   | 5        | 0.18          |
| (1,1324) | 1:44:A:ILE:HD13 | 1:76:A:GLU:HB3   | 5        | 0.18          |
| (1,1324) | 1:44:A:ILE:HD11 | 1:76:A:GLU:HB2   | 12       | 0.18          |
| (1,1324) | 1:44:A:ILE:HD11 | 1:76:A:GLU:HB3   | 12       | 0.18          |
| (1,1324) | 1:44:A:ILE:HD12 | 1:76:A:GLU:HB2   | 12       | 0.18          |
| (1,1324) | 1:44:A:ILE:HD12 | 1:76:A:GLU:HB3   | 12       | 0.18          |
| (1,1324) | 1:44:A:ILE:HD13 | 1:76:A:GLU:HB2   | 12       | 0.18          |
| (1,1324) | 1:44:A:ILE:HD13 | 1:76:A:GLU:HB3   | 12       | 0.18          |
| (1,1226) | 1:24:A:LYS:HG2  | 1:26:A:ASP:H     | 16       | 0.18          |
| (1,1226) | 1:24:A:LYS:HG3  | 1:26:A:ASP:H     | 16       | 0.18          |
| (1,1221) | 1:21:A:VAL:HG21 | 1:120:A:LYS:HB2  | 8        | 0.18          |
| (1,1221) | 1:21:A:VAL:HG21 | 1:120:A:LYS:HB3  | 8        | 0.18          |
| (1,1221) | 1:21:A:VAL:HG22 | 1:120:A:LYS:HB2  | 8        | 0.18          |
| (1,1221) | 1:21:A:VAL:HG22 | 1:120:A:LYS:HB3  | 8        | 0.18          |
| (1,1221) | 1:21:A:VAL:HG23 | 1:120:A:LYS:HB2  | 8        | 0.18          |
| (1,1221) | 1:21:A:VAL:HG23 | 1:120:A:LYS:HB3  | 8        | 0.18          |
| (1,1187) | 1:13:A:ARG:HB2  | 1:17:A:GLU:H     | 8        | 0.18          |
| (1,1187) | 1:13:A:ARG:HB3  | 1:17:A:GLU:H     | 8        | 0.18          |
| (1,1119) | 1:96:A:TYR:HD1  | 1:106:A:VAL:HG11 | 4        | 0.18          |
| (1,1119) | 1:96:A:TYR:HD1  | 1:106:A:VAL:HG12 | 4        | 0.18          |
| (1,1119) | 1:96:A:TYR:HD1  | 1:106:A:VAL:HG13 | 4        | 0.18          |
| (1,1119) | 1:96:A:TYR:HD2  | 1:106:A:VAL:HG11 | 4        | 0.18          |
| (1,1119) | 1:96:A:TYR:HD2  | 1:106:A:VAL:HG12 | 4        | 0.18          |
| (1,1119) | 1:96:A:TYR:HD2  | 1:106:A:VAL:HG13 | 4        | 0.18          |
| (1,1117) | 1:96:A:TYR:HD1  | 1:106:A:VAL:HB   | 19       | 0.18          |
| (1,1117) | 1:96:A:TYR:HD2  | 1:106:A:VAL:HB   | 19       | 0.18          |
| (1,977)  | 1:64:A:GLU:HG2  | 1:65:A:VAL:HG11  | 15       | 0.18          |
| (1,977)  | 1:64:A:GLU:HG2  | 1:65:A:VAL:HG12  | 15       | 0.18          |
| (1,977)  | 1:64:A:GLU:HG2  | 1:65:A:VAL:HG13  | 15       | 0.18          |
| (1,977)  | 1:64:A:GLU:HG3  | 1:65:A:VAL:HG11  | 15       | 0.18          |
| (1,977)  | 1:64:A:GLU:HG3  | 1:65:A:VAL:HG12  | 15       | 0.18          |
| (1,977)  | 1:64:A:GLU:HG3  | 1:65:A:VAL:HG13  | 15       | 0.18          |
| (1,873)  | 1:87:A:GLN:H    | 1:88:A:ASP:HB2   | 7        | 0.18          |
| (1,873)  | 1:87:A:GLN:H    | 1:88:A:ASP:HB3   | 7        | 0.18          |
| (1,845)  | 1:37:A:LYS:HD2  | 1:65:A:VAL:HB    | 1        | 0.18          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,845)  | 1:37:A:LYS:HD3  | 1:65:A:VAL:HB    | 1        | 0.18          |
| (1,832)  | 1:113:A:ASP:HA  | 1:116:A:LYS:HB2  | 1        | 0.18          |
| (1,832)  | 1:113:A:ASP:HA  | 1:116:A:LYS:HB3  | 1        | 0.18          |
| (1,724)  | 1:58:A:ILE:HB   | 1:63:A:GLU:HB2   | 16       | 0.18          |
| (1,724)  | 1:58:A:ILE:HB   | 1:63:A:GLU:HB3   | 16       | 0.18          |
| (1,345)  | 1:19:A:LEU:HD21 | 1:23:A:LEU:H     | 11       | 0.18          |
| (1,345)  | 1:19:A:LEU:HD22 | 1:23:A:LEU:H     | 11       | 0.18          |
| (1,345)  | 1:19:A:LEU:HD23 | 1:23:A:LEU:H     | 11       | 0.18          |
| (1,299)  | 1:116:A:LYS:H   | 1:116:A:LYS:HD2  | 6        | 0.18          |
| (1,299)  | 1:116:A:LYS:H   | 1:116:A:LYS:HD3  | 6        | 0.18          |
| (1,282)  | 1:97:A:GLU:H    | 1:98:A:GLN:HB2   | 1        | 0.18          |
| (1,282)  | 1:97:A:GLU:H    | 1:98:A:GLN:HB3   | 1        | 0.18          |
| (1,282)  | 1:97:A:GLU:H    | 1:98:A:GLN:HB2   | 17       | 0.18          |
| (1,282)  | 1:97:A:GLU:H    | 1:98:A:GLN:HB3   | 17       | 0.18          |
| (2,887)  | 1:89:A:GLN:HB2  | 1:92:A:LEU:HD11  | 8        | 0.17          |
| (2,887)  | 1:89:A:GLN:HB2  | 1:92:A:LEU:HD12  | 8        | 0.17          |
| (2,887)  | 1:89:A:GLN:HB2  | 1:92:A:LEU:HD13  | 8        | 0.17          |
| (2,887)  | 1:89:A:GLN:HB3  | 1:92:A:LEU:HD11  | 8        | 0.17          |
| (2,887)  | 1:89:A:GLN:HB3  | 1:92:A:LEU:HD12  | 8        | 0.17          |
| (2,887)  | 1:89:A:GLN:HB3  | 1:92:A:LEU:HD13  | 8        | 0.17          |
| (2,866)  | 1:81:A:LEU:HB2  | 1:83:A:ILE:HA    | 12       | 0.17          |
| (2,866)  | 1:81:A:LEU:HB3  | 1:83:A:ILE:HA    | 12       | 0.17          |
| (2,866)  | 1:81:A:LEU:HB2  | 1:83:A:ILE:HA    | 14       | 0.17          |
| (2,866)  | 1:81:A:LEU:HB3  | 1:83:A:ILE:HA    | 14       | 0.17          |
| (2,687)  | 1:9:A:SER:HB2   | 1:84:A:LYS:HA    | 4        | 0.17          |
| (2,528)  | 1:31:A:THR:HB   | 1:32:A:VAL:HB    | 10       | 0.17          |
| (2,431)  | 1:81:A:LEU:HB3  | 1:105:A:ASP:HB3  | 19       | 0.17          |
| (2,398)  | 1:4:A:VAL:H     | 1:81:A:LEU:HD11  | 4        | 0.17          |
| (2,398)  | 1:4:A:VAL:H     | 1:81:A:LEU:HD12  | 4        | 0.17          |
| (2,398)  | 1:4:A:VAL:H     | 1:81:A:LEU:HD13  | 4        | 0.17          |
| (2,398)  | 1:4:A:VAL:H     | 1:81:A:LEU:HD11  | 11       | 0.17          |
| (2,398)  | 1:4:A:VAL:H     | 1:81:A:LEU:HD12  | 11       | 0.17          |
| (2,398)  | 1:4:A:VAL:H     | 1:81:A:LEU:HD13  | 11       | 0.17          |
| (2,363)  | 1:81:A:LEU:HG   | 1:105:A:ASP:HB2  | 6        | 0.17          |
| (2,168)  | 1:3:A:THR:HB    | 1:5:A:VAL:HB     | 15       | 0.17          |
| (1,1487) | 1:120:A:LYS:HG2 | 1:123:A:LEU:HD21 | 14       | 0.17          |
| (1,1487) | 1:120:A:LYS:HG2 | 1:123:A:LEU:HD22 | 14       | 0.17          |
| (1,1487) | 1:120:A:LYS:HG2 | 1:123:A:LEU:HD23 | 14       | 0.17          |
| (1,1487) | 1:120:A:LYS:HG3 | 1:123:A:LEU:HD21 | 14       | 0.17          |
| (1,1487) | 1:120:A:LYS:HG3 | 1:123:A:LEU:HD22 | 14       | 0.17          |
| (1,1487) | 1:120:A:LYS:HG3 | 1:123:A:LEU:HD23 | 14       | 0.17          |
| (1,1284) | 1:38:A:GLU:HG2  | 1:39:A:LYS:HB2   | 18       | 0.17          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1284) | 1:38:A:GLU:HG2  | 1:39:A:LYS:HB3   | 18       | 0.17          |
| (1,1284) | 1:38:A:GLU:HG3  | 1:39:A:LYS:HB2   | 18       | 0.17          |
| (1,1284) | 1:38:A:GLU:HG3  | 1:39:A:LYS:HB3   | 18       | 0.17          |
| (1,1198) | 1:16:A:GLU:HG2  | 1:19:A:LEU:HD11  | 13       | 0.17          |
| (1,1198) | 1:16:A:GLU:HG2  | 1:19:A:LEU:HD12  | 13       | 0.17          |
| (1,1198) | 1:16:A:GLU:HG2  | 1:19:A:LEU:HD13  | 13       | 0.17          |
| (1,1198) | 1:16:A:GLU:HG3  | 1:19:A:LEU:HD11  | 13       | 0.17          |
| (1,1198) | 1:16:A:GLU:HG3  | 1:19:A:LEU:HD12  | 13       | 0.17          |
| (1,1198) | 1:16:A:GLU:HG3  | 1:19:A:LEU:HD13  | 13       | 0.17          |
| (1,1187) | 1:13:A:ARG:HB2  | 1:17:A:GLU:H     | 1        | 0.17          |
| (1,1187) | 1:13:A:ARG:HB3  | 1:17:A:GLU:H     | 1        | 0.17          |
| (1,1179) | 1:9:A:SER:HB2   | 1:85:A:VAL:HB    | 10       | 0.17          |
| (1,1179) | 1:9:A:SER:HB3   | 1:85:A:VAL:HB    | 10       | 0.17          |
| (1,1150) | 1:72:A:TYR:HE1  | 1:78:A:LEU:HD11  | 4        | 0.17          |
| (1,1150) | 1:72:A:TYR:HE1  | 1:78:A:LEU:HD12  | 4        | 0.17          |
| (1,1150) | 1:72:A:TYR:HE1  | 1:78:A:LEU:HD13  | 4        | 0.17          |
| (1,1150) | 1:72:A:TYR:HE2  | 1:78:A:LEU:HD11  | 4        | 0.17          |
| (1,1150) | 1:72:A:TYR:HE2  | 1:78:A:LEU:HD12  | 4        | 0.17          |
| (1,1150) | 1:72:A:TYR:HE2  | 1:78:A:LEU:HD13  | 4        | 0.17          |
| (1,1114) | 1:96:A:TYR:HE1  | 1:106:A:VAL:HG21 | 17       | 0.17          |
| (1,1114) | 1:96:A:TYR:HE1  | 1:106:A:VAL:HG22 | 17       | 0.17          |
| (1,1114) | 1:96:A:TYR:HE1  | 1:106:A:VAL:HG23 | 17       | 0.17          |
| (1,1114) | 1:96:A:TYR:HE2  | 1:106:A:VAL:HG21 | 17       | 0.17          |
| (1,1114) | 1:96:A:TYR:HE2  | 1:106:A:VAL:HG22 | 17       | 0.17          |
| (1,1114) | 1:96:A:TYR:HE2  | 1:106:A:VAL:HG23 | 17       | 0.17          |
| (1,1078) | 1:15:A:LEU:HD21 | 1:57:A:PHE:HZ    | 1        | 0.17          |
| (1,1078) | 1:15:A:LEU:HD22 | 1:57:A:PHE:HZ    | 1        | 0.17          |
| (1,1078) | 1:15:A:LEU:HD23 | 1:57:A:PHE:HZ    | 1        | 0.17          |
| (1,1078) | 1:15:A:LEU:HD21 | 1:57:A:PHE:HZ    | 14       | 0.17          |
| (1,1078) | 1:15:A:LEU:HD22 | 1:57:A:PHE:HZ    | 14       | 0.17          |
| (1,1078) | 1:15:A:LEU:HD23 | 1:57:A:PHE:HZ    | 14       | 0.17          |
| (1,997)  | 1:22:A:VAL:H    | 1:119:A:LEU:HD21 | 15       | 0.17          |
| (1,997)  | 1:22:A:VAL:H    | 1:119:A:LEU:HD22 | 15       | 0.17          |
| (1,997)  | 1:22:A:VAL:H    | 1:119:A:LEU:HD23 | 15       | 0.17          |
| (1,997)  | 1:22:A:VAL:H    | 1:119:A:LEU:HD21 | 20       | 0.17          |
| (1,997)  | 1:22:A:VAL:H    | 1:119:A:LEU:HD22 | 20       | 0.17          |
| (1,997)  | 1:22:A:VAL:H    | 1:119:A:LEU:HD23 | 20       | 0.17          |
| (1,845)  | 1:37:A:LYS:HD2  | 1:65:A:VAL:HB    | 19       | 0.17          |
| (1,845)  | 1:37:A:LYS:HD3  | 1:65:A:VAL:HB    | 19       | 0.17          |
| (1,389)  | 1:70:A:VAL:HB   | 1:72:A:TYR:H     | 14       | 0.17          |
| (1,154)  | 1:36:A:ASP:H    | 1:40:A:VAL:H     | 3        | 0.17          |
| (2,780)  | 1:20:A:GLU:HG2  | 1:57:A:PHE:HE1   | 6        | 0.16          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (2,780)  | 1:20:A:GLU:HG2  | 1:57:A:PHE:HE2   | 6        | 0.16          |
| (2,780)  | 1:20:A:GLU:HG3  | 1:57:A:PHE:HE1   | 6        | 0.16          |
| (2,780)  | 1:20:A:GLU:HG3  | 1:57:A:PHE:HE2   | 6        | 0.16          |
| (2,711)  | 1:8:A:VAL:HB    | 1:66:A:VAL:HG21  | 9        | 0.16          |
| (2,711)  | 1:8:A:VAL:HB    | 1:66:A:VAL:HG22  | 9        | 0.16          |
| (2,711)  | 1:8:A:VAL:HB    | 1:66:A:VAL:HG23  | 9        | 0.16          |
| (2,704)  | 1:107:A:ARG:HD3 | 1:108:A:VAL:H    | 11       | 0.16          |
| (2,630)  | 1:74:A:GLN:HG2  | 1:104:A:VAL:HG11 | 18       | 0.16          |
| (2,630)  | 1:74:A:GLN:HG2  | 1:104:A:VAL:HG12 | 18       | 0.16          |
| (2,630)  | 1:74:A:GLN:HG2  | 1:104:A:VAL:HG13 | 18       | 0.16          |
| (2,581)  | 1:56:A:ILE:HD11 | 1:57:A:PHE:HB2   | 9        | 0.16          |
| (2,581)  | 1:56:A:ILE:HD12 | 1:57:A:PHE:HB2   | 9        | 0.16          |
| (2,581)  | 1:56:A:ILE:HD13 | 1:57:A:PHE:HB2   | 9        | 0.16          |
| (2,478)  | 1:100:A:LYS:HA  | 1:106:A:VAL:HG21 | 9        | 0.16          |
| (2,478)  | 1:100:A:LYS:HA  | 1:106:A:VAL:HG22 | 9        | 0.16          |
| (2,478)  | 1:100:A:LYS:HA  | 1:106:A:VAL:HG23 | 9        | 0.16          |
| (2,402)  | 1:80:A:VAL:H    | 1:81:A:LEU:HD21  | 10       | 0.16          |
| (2,402)  | 1:80:A:VAL:H    | 1:81:A:LEU:HD22  | 10       | 0.16          |
| (2,402)  | 1:80:A:VAL:H    | 1:81:A:LEU:HD23  | 10       | 0.16          |
| (2,398)  | 1:4:A:VAL:H     | 1:81:A:LEU:HD11  | 17       | 0.16          |
| (2,398)  | 1:4:A:VAL:H     | 1:81:A:LEU:HD12  | 17       | 0.16          |
| (2,398)  | 1:4:A:VAL:H     | 1:81:A:LEU:HD13  | 17       | 0.16          |
| (1,1487) | 1:120:A:LYS:HG2 | 1:123:A:LEU:HD21 | 8        | 0.16          |
| (1,1487) | 1:120:A:LYS:HG2 | 1:123:A:LEU:HD22 | 8        | 0.16          |
| (1,1487) | 1:120:A:LYS:HG2 | 1:123:A:LEU:HD23 | 8        | 0.16          |
| (1,1487) | 1:120:A:LYS:HG3 | 1:123:A:LEU:HD21 | 8        | 0.16          |
| (1,1487) | 1:120:A:LYS:HG3 | 1:123:A:LEU:HD22 | 8        | 0.16          |
| (1,1487) | 1:120:A:LYS:HG3 | 1:123:A:LEU:HD23 | 8        | 0.16          |
| (1,1447) | 1:99:A:LEU:HD11 | 1:100:A:LYS:HG2  | 6        | 0.16          |
| (1,1447) | 1:99:A:LEU:HD11 | 1:100:A:LYS:HG3  | 6        | 0.16          |
| (1,1447) | 1:99:A:LEU:HD12 | 1:100:A:LYS:HG2  | 6        | 0.16          |
| (1,1447) | 1:99:A:LEU:HD12 | 1:100:A:LYS:HG3  | 6        | 0.16          |
| (1,1447) | 1:99:A:LEU:HD13 | 1:100:A:LYS:HG2  | 6        | 0.16          |
| (1,1447) | 1:99:A:LEU:HD13 | 1:100:A:LYS:HG3  | 6        | 0.16          |
| (1,1447) | 1:99:A:LEU:HD11 | 1:100:A:LYS:HG2  | 14       | 0.16          |
| (1,1447) | 1:99:A:LEU:HD11 | 1:100:A:LYS:HG3  | 14       | 0.16          |
| (1,1447) | 1:99:A:LEU:HD12 | 1:100:A:LYS:HG2  | 14       | 0.16          |
| (1,1447) | 1:99:A:LEU:HD12 | 1:100:A:LYS:HG3  | 14       | 0.16          |
| (1,1447) | 1:99:A:LEU:HD13 | 1:100:A:LYS:HG2  | 14       | 0.16          |
| (1,1447) | 1:99:A:LEU:HD13 | 1:100:A:LYS:HG3  | 14       | 0.16          |
| (1,1427) | 1:84:A:LYS:HE2  | 1:96:A:TYR:HE1   | 9        | 0.16          |
| (1,1427) | 1:84:A:LYS:HE2  | 1:96:A:TYR:HE2   | 9        | 0.16          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1427) | 1:84:A:LYS:HE3  | 1:96:A:TYR:HE1  | 9        | 0.16          |
| (1,1427) | 1:84:A:LYS:HE3  | 1:96:A:TYR:HE2  | 9        | 0.16          |
| (1,1269) | 1:36:A:ASP:HB2  | 1:39:A:LYS:HA   | 11       | 0.16          |
| (1,1269) | 1:36:A:ASP:HB3  | 1:39:A:LYS:HA   | 11       | 0.16          |
| (1,1265) | 1:36:A:ASP:H    | 1:39:A:LYS:HD2  | 17       | 0.16          |
| (1,1265) | 1:36:A:ASP:H    | 1:39:A:LYS:HD3  | 17       | 0.16          |
| (1,1198) | 1:16:A:GLU:HG2  | 1:19:A:LEU:HD11 | 10       | 0.16          |
| (1,1198) | 1:16:A:GLU:HG2  | 1:19:A:LEU:HD12 | 10       | 0.16          |
| (1,1198) | 1:16:A:GLU:HG2  | 1:19:A:LEU:HD13 | 10       | 0.16          |
| (1,1198) | 1:16:A:GLU:HG3  | 1:19:A:LEU:HD11 | 10       | 0.16          |
| (1,1198) | 1:16:A:GLU:HG3  | 1:19:A:LEU:HD12 | 10       | 0.16          |
| (1,1198) | 1:16:A:GLU:HG3  | 1:19:A:LEU:HD13 | 10       | 0.16          |
| (1,1188) | 1:13:A:ARG:HG2  | 1:16:A:GLU:HB2  | 18       | 0.16          |
| (1,1188) | 1:13:A:ARG:HG2  | 1:16:A:GLU:HB3  | 18       | 0.16          |
| (1,1188) | 1:13:A:ARG:HG3  | 1:16:A:GLU:HB2  | 18       | 0.16          |
| (1,1188) | 1:13:A:ARG:HG3  | 1:16:A:GLU:HB3  | 18       | 0.16          |
| (1,1187) | 1:13:A:ARG:HB2  | 1:17:A:GLU:H    | 20       | 0.16          |
| (1,1187) | 1:13:A:ARG:HB3  | 1:17:A:GLU:H    | 20       | 0.16          |
| (1,1150) | 1:72:A:TYR:HE1  | 1:78:A:LEU:HD11 | 9        | 0.16          |
| (1,1150) | 1:72:A:TYR:HE1  | 1:78:A:LEU:HD12 | 9        | 0.16          |
| (1,1150) | 1:72:A:TYR:HE1  | 1:78:A:LEU:HD13 | 9        | 0.16          |
| (1,1150) | 1:72:A:TYR:HE2  | 1:78:A:LEU:HD11 | 9        | 0.16          |
| (1,1150) | 1:72:A:TYR:HE2  | 1:78:A:LEU:HD12 | 9        | 0.16          |
| (1,1150) | 1:72:A:TYR:HE2  | 1:78:A:LEU:HD13 | 9        | 0.16          |
| (1,1150) | 1:72:A:TYR:HE1  | 1:78:A:LEU:HD11 | 12       | 0.16          |
| (1,1150) | 1:72:A:TYR:HE1  | 1:78:A:LEU:HD12 | 12       | 0.16          |
| (1,1150) | 1:72:A:TYR:HE1  | 1:78:A:LEU:HD13 | 12       | 0.16          |
| (1,1150) | 1:72:A:TYR:HE2  | 1:78:A:LEU:HD11 | 12       | 0.16          |
| (1,1150) | 1:72:A:TYR:HE2  | 1:78:A:LEU:HD12 | 12       | 0.16          |
| (1,1150) | 1:72:A:TYR:HE2  | 1:78:A:LEU:HD13 | 12       | 0.16          |
| (1,1112) | 1:96:A:TYR:HE1  | 1:97:A:GLU:HB2  | 4        | 0.16          |
| (1,1112) | 1:96:A:TYR:HE1  | 1:97:A:GLU:HB3  | 4        | 0.16          |
| (1,1112) | 1:96:A:TYR:HE2  | 1:97:A:GLU:HB2  | 4        | 0.16          |
| (1,1112) | 1:96:A:TYR:HE2  | 1:97:A:GLU:HB3  | 4        | 0.16          |
| (1,1078) | 1:15:A:LEU:HD21 | 1:57:A:PHE:HZ   | 13       | 0.16          |
| (1,1078) | 1:15:A:LEU:HD22 | 1:57:A:PHE:HZ   | 13       | 0.16          |
| (1,1078) | 1:15:A:LEU:HD23 | 1:57:A:PHE:HZ   | 13       | 0.16          |
| (1,902)  | 1:95:A:PHE:HA   | 1:97:A:GLU:HB2  | 4        | 0.16          |
| (1,902)  | 1:95:A:PHE:HA   | 1:97:A:GLU:HB3  | 4        | 0.16          |
| (1,601)  | 1:114:A:GLU:HB2 | 1:117:A:LYS:HD2 | 13       | 0.16          |
| (1,601)  | 1:114:A:GLU:HB2 | 1:117:A:LYS:HD3 | 13       | 0.16          |
| (1,601)  | 1:114:A:GLU:HB3 | 1:117:A:LYS:HD2 | 13       | 0.16          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,601)  | 1:114:A:GLU:HB3 | 1:117:A:LYS:HD3  | 13       | 0.16          |
| (1,389)  | 1:70:A:VAL:HB   | 1:72:A:TYR:H     | 2        | 0.16          |
| (1,77)   | 1:22:A:VAL:H    | 1:23:A:LEU:HB3   | 13       | 0.16          |
| (1,77)   | 1:22:A:VAL:H    | 1:23:A:LEU:HB3   | 20       | 0.16          |
| (2,875)  | 1:84:A:LYS:HE2  | 1:85:A:VAL:HA    | 17       | 0.15          |
| (2,875)  | 1:84:A:LYS:HE3  | 1:85:A:VAL:HA    | 17       | 0.15          |
| (2,780)  | 1:20:A:GLU:HG2  | 1:57:A:PHE:HE1   | 10       | 0.15          |
| (2,780)  | 1:20:A:GLU:HG2  | 1:57:A:PHE:HE2   | 10       | 0.15          |
| (2,780)  | 1:20:A:GLU:HG3  | 1:57:A:PHE:HE1   | 10       | 0.15          |
| (2,780)  | 1:20:A:GLU:HG3  | 1:57:A:PHE:HE2   | 10       | 0.15          |
| (2,765)  | 1:9:A:SER:H     | 1:63:A:GLU:HG2   | 9        | 0.15          |
| (2,765)  | 1:9:A:SER:H     | 1:63:A:GLU:HG3   | 9        | 0.15          |
| (2,720)  | 1:6:A:ILE:HB    | 1:55:A:VAL:HG11  | 1        | 0.15          |
| (2,720)  | 1:6:A:ILE:HB    | 1:55:A:VAL:HG12  | 1        | 0.15          |
| (2,720)  | 1:6:A:ILE:HB    | 1:55:A:VAL:HG13  | 1        | 0.15          |
| (2,528)  | 1:31:A:THR:HB   | 1:32:A:VAL:HB    | 8        | 0.15          |
| (2,523)  | 1:27:A:PRO:HB3  | 1:28:A:ASN:HB2   | 20       | 0.15          |
| (2,523)  | 1:27:A:PRO:HB3  | 1:28:A:ASN:HB3   | 20       | 0.15          |
| (2,402)  | 1:80:A:VAL:H    | 1:81:A:LEU:HD21  | 8        | 0.15          |
| (2,402)  | 1:80:A:VAL:H    | 1:81:A:LEU:HD22  | 8        | 0.15          |
| (2,402)  | 1:80:A:VAL:H    | 1:81:A:LEU:HD23  | 8        | 0.15          |
| (2,402)  | 1:80:A:VAL:H    | 1:81:A:LEU:HD21  | 14       | 0.15          |
| (2,402)  | 1:80:A:VAL:H    | 1:81:A:LEU:HD22  | 14       | 0.15          |
| (2,402)  | 1:80:A:VAL:H    | 1:81:A:LEU:HD23  | 14       | 0.15          |
| (2,363)  | 1:81:A:LEU:HG   | 1:105:A:ASP:HB2  | 14       | 0.15          |
| (2,315)  | 1:81:A:LEU:HB3  | 1:105:A:ASP:HB2  | 8        | 0.15          |
| (2,237)  | 1:97:A:GLU:HB2  | 1:101:A:LYS:HE2  | 9        | 0.15          |
| (2,237)  | 1:97:A:GLU:HB2  | 1:101:A:LYS:HE3  | 9        | 0.15          |
| (2,237)  | 1:97:A:GLU:HB3  | 1:101:A:LYS:HE2  | 9        | 0.15          |
| (2,237)  | 1:97:A:GLU:HB3  | 1:101:A:LYS:HE3  | 9        | 0.15          |
| (2,236)  | 1:37:A:LYS:HE2  | 1:38:A:GLU:HB2   | 12       | 0.15          |
| (2,236)  | 1:37:A:LYS:HE2  | 1:38:A:GLU:HB3   | 12       | 0.15          |
| (2,236)  | 1:37:A:LYS:HE3  | 1:38:A:GLU:HB2   | 12       | 0.15          |
| (2,236)  | 1:37:A:LYS:HE3  | 1:38:A:GLU:HB3   | 12       | 0.15          |
| (1,1490) | 1:121:A:GLU:HB2 | 1:122:A:LEU:HG   | 9        | 0.15          |
| (1,1490) | 1:121:A:GLU:HB3 | 1:122:A:LEU:HG   | 9        | 0.15          |
| (1,1487) | 1:120:A:LYS:HG2 | 1:123:A:LEU:HD21 | 3        | 0.15          |
| (1,1487) | 1:120:A:LYS:HG2 | 1:123:A:LEU:HD22 | 3        | 0.15          |
| (1,1487) | 1:120:A:LYS:HG2 | 1:123:A:LEU:HD23 | 3        | 0.15          |
| (1,1487) | 1:120:A:LYS:HG3 | 1:123:A:LEU:HD21 | 3        | 0.15          |
| (1,1487) | 1:120:A:LYS:HG3 | 1:123:A:LEU:HD22 | 3        | 0.15          |
| (1,1487) | 1:120:A:LYS:HG3 | 1:123:A:LEU:HD23 | 3        | 0.15          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1455) | 1:106:A:VAL:H   | 1:107:A:ARG:HG2  | 15       | 0.15          |
| (1,1455) | 1:106:A:VAL:H   | 1:107:A:ARG:HG3  | 15       | 0.15          |
| (1,1428) | 1:85:A:VAL:HG21 | 1:111:A:ASN:HB2  | 5        | 0.15          |
| (1,1428) | 1:85:A:VAL:HG21 | 1:111:A:ASN:HB3  | 5        | 0.15          |
| (1,1428) | 1:85:A:VAL:HG22 | 1:111:A:ASN:HB2  | 5        | 0.15          |
| (1,1428) | 1:85:A:VAL:HG22 | 1:111:A:ASN:HB3  | 5        | 0.15          |
| (1,1428) | 1:85:A:VAL:HG23 | 1:111:A:ASN:HB2  | 5        | 0.15          |
| (1,1428) | 1:85:A:VAL:HG23 | 1:111:A:ASN:HB3  | 5        | 0.15          |
| (1,1427) | 1:84:A:LYS:HE2  | 1:96:A:TYR:HE1   | 8        | 0.15          |
| (1,1427) | 1:84:A:LYS:HE2  | 1:96:A:TYR:HE2   | 8        | 0.15          |
| (1,1427) | 1:84:A:LYS:HE3  | 1:96:A:TYR:HE1   | 8        | 0.15          |
| (1,1427) | 1:84:A:LYS:HE3  | 1:96:A:TYR:HE2   | 8        | 0.15          |
| (1,1427) | 1:84:A:LYS:HE2  | 1:96:A:TYR:HE1   | 18       | 0.15          |
| (1,1427) | 1:84:A:LYS:HE2  | 1:96:A:TYR:HE2   | 18       | 0.15          |
| (1,1427) | 1:84:A:LYS:HE3  | 1:96:A:TYR:HE1   | 18       | 0.15          |
| (1,1427) | 1:84:A:LYS:HE3  | 1:96:A:TYR:HE2   | 18       | 0.15          |
| (1,1346) | 1:53:A:PRO:HB2  | 1:126:A:VAL:HG11 | 15       | 0.15          |
| (1,1346) | 1:53:A:PRO:HB2  | 1:126:A:VAL:HG12 | 15       | 0.15          |
| (1,1346) | 1:53:A:PRO:HB2  | 1:126:A:VAL:HG13 | 15       | 0.15          |
| (1,1346) | 1:53:A:PRO:HB2  | 1:126:A:VAL:HG21 | 15       | 0.15          |
| (1,1346) | 1:53:A:PRO:HB2  | 1:126:A:VAL:HG22 | 15       | 0.15          |
| (1,1346) | 1:53:A:PRO:HB2  | 1:126:A:VAL:HG23 | 15       | 0.15          |
| (1,1187) | 1:13:A:ARG:HB2  | 1:17:A:GLU:H     | 3        | 0.15          |
| (1,1187) | 1:13:A:ARG:HB3  | 1:17:A:GLU:H     | 3        | 0.15          |
| (1,1187) | 1:13:A:ARG:HB2  | 1:17:A:GLU:H     | 19       | 0.15          |
| (1,1187) | 1:13:A:ARG:HB3  | 1:17:A:GLU:H     | 19       | 0.15          |
| (1,1129) | 1:61:A:ALA:H    | 1:62:A:TYR:HD1   | 17       | 0.15          |
| (1,1129) | 1:61:A:ALA:H    | 1:62:A:TYR:HD2   | 17       | 0.15          |
| (1,1112) | 1:96:A:TYR:HE1  | 1:97:A:GLU:HB2   | 1        | 0.15          |
| (1,1112) | 1:96:A:TYR:HE1  | 1:97:A:GLU:HB3   | 1        | 0.15          |
| (1,1112) | 1:96:A:TYR:HE2  | 1:97:A:GLU:HB2   | 1        | 0.15          |
| (1,1112) | 1:96:A:TYR:HE2  | 1:97:A:GLU:HB3   | 1        | 0.15          |
| (1,1112) | 1:96:A:TYR:HE1  | 1:97:A:GLU:HB2   | 14       | 0.15          |
| (1,1112) | 1:96:A:TYR:HE1  | 1:97:A:GLU:HB3   | 14       | 0.15          |
| (1,1112) | 1:96:A:TYR:HE2  | 1:97:A:GLU:HB2   | 14       | 0.15          |
| (1,1112) | 1:96:A:TYR:HE2  | 1:97:A:GLU:HB3   | 14       | 0.15          |
| (1,1078) | 1:15:A:LEU:HD21 | 1:57:A:PHE:HZ    | 10       | 0.15          |
| (1,1078) | 1:15:A:LEU:HD22 | 1:57:A:PHE:HZ    | 10       | 0.15          |
| (1,1078) | 1:15:A:LEU:HD23 | 1:57:A:PHE:HZ    | 10       | 0.15          |
| (1,997)  | 1:22:A:VAL:H    | 1:119:A:LEU:HD21 | 18       | 0.15          |
| (1,997)  | 1:22:A:VAL:H    | 1:119:A:LEU:HD22 | 18       | 0.15          |
| (1,997)  | 1:22:A:VAL:H    | 1:119:A:LEU:HD23 | 18       | 0.15          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,902) | 1:95:A:PHE:HA   | 1:97:A:GLU:HB2  | 11       | 0.15          |
| (1,902) | 1:95:A:PHE:HA   | 1:97:A:GLU:HB3  | 11       | 0.15          |
| (1,836) | 1:62:A:TYR:HA   | 1:64:A:GLU:HG2  | 5        | 0.15          |
| (1,836) | 1:62:A:TYR:HA   | 1:64:A:GLU:HG3  | 5        | 0.15          |
| (1,767) | 1:37:A:LYS:HE2  | 1:65:A:VAL:HB   | 16       | 0.15          |
| (1,767) | 1:37:A:LYS:HE3  | 1:65:A:VAL:HB   | 16       | 0.15          |
| (1,724) | 1:58:A:ILE:HB   | 1:63:A:GLU:HB2  | 2        | 0.15          |
| (1,724) | 1:58:A:ILE:HB   | 1:63:A:GLU:HB3  | 2        | 0.15          |
| (1,581) | 1:23:A:LEU:HA   | 1:23:A:LEU:HD21 | 6        | 0.15          |
| (1,581) | 1:23:A:LEU:HA   | 1:23:A:LEU:HD22 | 6        | 0.15          |
| (1,581) | 1:23:A:LEU:HA   | 1:23:A:LEU:HD23 | 6        | 0.15          |
| (1,322) | 1:6:A:ILE:H     | 1:83:A:ILE:HD11 | 10       | 0.15          |
| (1,322) | 1:6:A:ILE:H     | 1:83:A:ILE:HD12 | 10       | 0.15          |
| (1,322) | 1:6:A:ILE:H     | 1:83:A:ILE:HD13 | 10       | 0.15          |
| (1,77)  | 1:22:A:VAL:H    | 1:23:A:LEU:HB3  | 18       | 0.15          |
| (2,892) | 1:97:A:GLU:HB2  | 1:98:A:GLN:HE21 | 13       | 0.14          |
| (2,892) | 1:97:A:GLU:HB2  | 1:98:A:GLN:HE22 | 13       | 0.14          |
| (2,892) | 1:97:A:GLU:HB3  | 1:98:A:GLN:HE21 | 13       | 0.14          |
| (2,892) | 1:97:A:GLU:HB3  | 1:98:A:GLN:HE22 | 13       | 0.14          |
| (2,889) | 1:92:A:LEU:HD21 | 1:110:A:ASP:HB2 | 3        | 0.14          |
| (2,889) | 1:92:A:LEU:HD21 | 1:110:A:ASP:HB3 | 3        | 0.14          |
| (2,889) | 1:92:A:LEU:HD22 | 1:110:A:ASP:HB2 | 3        | 0.14          |
| (2,889) | 1:92:A:LEU:HD22 | 1:110:A:ASP:HB3 | 3        | 0.14          |
| (2,889) | 1:92:A:LEU:HD23 | 1:110:A:ASP:HB2 | 3        | 0.14          |
| (2,889) | 1:92:A:LEU:HD23 | 1:110:A:ASP:HB3 | 3        | 0.14          |
| (2,875) | 1:84:A:LYS:HE2  | 1:85:A:VAL:HA   | 9        | 0.14          |
| (2,875) | 1:84:A:LYS:HE3  | 1:85:A:VAL:HA   | 9        | 0.14          |
| (2,875) | 1:84:A:LYS:HE2  | 1:85:A:VAL:HA   | 14       | 0.14          |
| (2,875) | 1:84:A:LYS:HE3  | 1:85:A:VAL:HA   | 14       | 0.14          |
| (2,875) | 1:84:A:LYS:HE2  | 1:85:A:VAL:HA   | 19       | 0.14          |
| (2,875) | 1:84:A:LYS:HE3  | 1:85:A:VAL:HA   | 19       | 0.14          |
| (2,866) | 1:81:A:LEU:HB2  | 1:83:A:ILE:HA   | 4        | 0.14          |
| (2,866) | 1:81:A:LEU:HB3  | 1:83:A:ILE:HA   | 4        | 0.14          |
| (2,792) | 1:28:A:ASN:HD21 | 1:52:A:ARG:HG2  | 2        | 0.14          |
| (2,792) | 1:28:A:ASN:HD21 | 1:52:A:ARG:HG3  | 2        | 0.14          |
| (2,792) | 1:28:A:ASN:HD22 | 1:52:A:ARG:HG2  | 2        | 0.14          |
| (2,792) | 1:28:A:ASN:HD22 | 1:52:A:ARG:HG3  | 2        | 0.14          |
| (2,765) | 1:9:A:SER:H     | 1:63:A:GLU:HG2  | 17       | 0.14          |
| (2,765) | 1:9:A:SER:H     | 1:63:A:GLU:HG3  | 17       | 0.14          |
| (2,720) | 1:6:A:ILE:HB    | 1:55:A:VAL:HG11 | 4        | 0.14          |
| (2,720) | 1:6:A:ILE:HB    | 1:55:A:VAL:HG12 | 4        | 0.14          |
| (2,720) | 1:6:A:ILE:HB    | 1:55:A:VAL:HG13 | 4        | 0.14          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (2,709)  | 1:99:A:LEU:HD11 | 1:100:A:LYS:HD2  | 11       | 0.14          |
| (2,709)  | 1:99:A:LEU:HD11 | 1:100:A:LYS:HD3  | 11       | 0.14          |
| (2,709)  | 1:99:A:LEU:HD12 | 1:100:A:LYS:HD2  | 11       | 0.14          |
| (2,709)  | 1:99:A:LEU:HD12 | 1:100:A:LYS:HD3  | 11       | 0.14          |
| (2,709)  | 1:99:A:LEU:HD13 | 1:100:A:LYS:HD2  | 11       | 0.14          |
| (2,709)  | 1:99:A:LEU:HD13 | 1:100:A:LYS:HD3  | 11       | 0.14          |
| (2,630)  | 1:74:A:GLN:HG2  | 1:104:A:VAL:HG11 | 6        | 0.14          |
| (2,630)  | 1:74:A:GLN:HG2  | 1:104:A:VAL:HG12 | 6        | 0.14          |
| (2,630)  | 1:74:A:GLN:HG2  | 1:104:A:VAL:HG13 | 6        | 0.14          |
| (2,520)  | 1:22:A:VAL:HB   | 1:23:A:LEU:HG    | 6        | 0.14          |
| (2,473)  | 1:124:A:GLU:HG2 | 1:125:A:LYS:HE2  | 3        | 0.14          |
| (2,473)  | 1:124:A:GLU:HG2 | 1:125:A:LYS:HE3  | 3        | 0.14          |
| (2,473)  | 1:124:A:GLU:HG3 | 1:125:A:LYS:HE2  | 3        | 0.14          |
| (2,473)  | 1:124:A:GLU:HG3 | 1:125:A:LYS:HE3  | 3        | 0.14          |
| (2,402)  | 1:80:A:VAL:H    | 1:81:A:LEU:HD21  | 4        | 0.14          |
| (2,402)  | 1:80:A:VAL:H    | 1:81:A:LEU:HD22  | 4        | 0.14          |
| (2,402)  | 1:80:A:VAL:H    | 1:81:A:LEU:HD23  | 4        | 0.14          |
| (2,348)  | 1:129:A:LEU:HG  | 1:130:A:GLU:HA   | 3        | 0.14          |
| (2,315)  | 1:81:A:LEU:HB3  | 1:105:A:ASP:HB2  | 2        | 0.14          |
| (2,315)  | 1:81:A:LEU:HB3  | 1:105:A:ASP:HB2  | 6        | 0.14          |
| (1,1487) | 1:120:A:LYS:HG2 | 1:123:A:LEU:HD21 | 4        | 0.14          |
| (1,1487) | 1:120:A:LYS:HG2 | 1:123:A:LEU:HD22 | 4        | 0.14          |
| (1,1487) | 1:120:A:LYS:HG2 | 1:123:A:LEU:HD23 | 4        | 0.14          |
| (1,1487) | 1:120:A:LYS:HG3 | 1:123:A:LEU:HD21 | 4        | 0.14          |
| (1,1487) | 1:120:A:LYS:HG3 | 1:123:A:LEU:HD22 | 4        | 0.14          |
| (1,1487) | 1:120:A:LYS:HG3 | 1:123:A:LEU:HD23 | 4        | 0.14          |
| (1,1447) | 1:99:A:LEU:HD11 | 1:100:A:LYS:HG2  | 10       | 0.14          |
| (1,1447) | 1:99:A:LEU:HD11 | 1:100:A:LYS:HG3  | 10       | 0.14          |
| (1,1447) | 1:99:A:LEU:HD12 | 1:100:A:LYS:HG2  | 10       | 0.14          |
| (1,1447) | 1:99:A:LEU:HD12 | 1:100:A:LYS:HG3  | 10       | 0.14          |
| (1,1447) | 1:99:A:LEU:HD13 | 1:100:A:LYS:HG2  | 10       | 0.14          |
| (1,1447) | 1:99:A:LEU:HD13 | 1:100:A:LYS:HG3  | 10       | 0.14          |
| (1,1429) | 1:86:A:ALA:HB1  | 1:87:A:GLN:HB2   | 19       | 0.14          |
| (1,1429) | 1:86:A:ALA:HB1  | 1:87:A:GLN:HB3   | 19       | 0.14          |
| (1,1429) | 1:86:A:ALA:HB2  | 1:87:A:GLN:HB2   | 19       | 0.14          |
| (1,1429) | 1:86:A:ALA:HB2  | 1:87:A:GLN:HB3   | 19       | 0.14          |
| (1,1429) | 1:86:A:ALA:HB3  | 1:87:A:GLN:HB2   | 19       | 0.14          |
| (1,1429) | 1:86:A:ALA:HB3  | 1:87:A:GLN:HB3   | 19       | 0.14          |
| (1,1428) | 1:85:A:VAL:HG21 | 1:111:A:ASN:HB2  | 12       | 0.14          |
| (1,1428) | 1:85:A:VAL:HG21 | 1:111:A:ASN:HB3  | 12       | 0.14          |
| (1,1428) | 1:85:A:VAL:HG22 | 1:111:A:ASN:HB2  | 12       | 0.14          |
| (1,1428) | 1:85:A:VAL:HG22 | 1:111:A:ASN:HB3  | 12       | 0.14          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1428) | 1:85:A:VAL:HG23 | 1:111:A:ASN:HB2  | 12       | 0.14          |
| (1,1428) | 1:85:A:VAL:HG23 | 1:111:A:ASN:HB3  | 12       | 0.14          |
| (1,1324) | 1:44:A:ILE:HD11 | 1:76:A:GLU:HB2   | 1        | 0.14          |
| (1,1324) | 1:44:A:ILE:HD11 | 1:76:A:GLU:HB3   | 1        | 0.14          |
| (1,1324) | 1:44:A:ILE:HD12 | 1:76:A:GLU:HB2   | 1        | 0.14          |
| (1,1324) | 1:44:A:ILE:HD12 | 1:76:A:GLU:HB3   | 1        | 0.14          |
| (1,1324) | 1:44:A:ILE:HD13 | 1:76:A:GLU:HB2   | 1        | 0.14          |
| (1,1324) | 1:44:A:ILE:HD13 | 1:76:A:GLU:HB3   | 1        | 0.14          |
| (1,1324) | 1:44:A:ILE:HD11 | 1:76:A:GLU:HB2   | 18       | 0.14          |
| (1,1324) | 1:44:A:ILE:HD11 | 1:76:A:GLU:HB3   | 18       | 0.14          |
| (1,1324) | 1:44:A:ILE:HD12 | 1:76:A:GLU:HB2   | 18       | 0.14          |
| (1,1324) | 1:44:A:ILE:HD12 | 1:76:A:GLU:HB3   | 18       | 0.14          |
| (1,1324) | 1:44:A:ILE:HD13 | 1:76:A:GLU:HB2   | 18       | 0.14          |
| (1,1324) | 1:44:A:ILE:HD13 | 1:76:A:GLU:HB3   | 18       | 0.14          |
| (1,1324) | 1:44:A:ILE:HD11 | 1:76:A:GLU:HB2   | 20       | 0.14          |
| (1,1324) | 1:44:A:ILE:HD11 | 1:76:A:GLU:HB3   | 20       | 0.14          |
| (1,1324) | 1:44:A:ILE:HD12 | 1:76:A:GLU:HB2   | 20       | 0.14          |
| (1,1324) | 1:44:A:ILE:HD12 | 1:76:A:GLU:HB3   | 20       | 0.14          |
| (1,1324) | 1:44:A:ILE:HD13 | 1:76:A:GLU:HB2   | 20       | 0.14          |
| (1,1324) | 1:44:A:ILE:HD13 | 1:76:A:GLU:HB3   | 20       | 0.14          |
| (1,1226) | 1:24:A:LYS:HG2  | 1:26:A:ASP:H     | 14       | 0.14          |
| (1,1226) | 1:24:A:LYS:HG3  | 1:26:A:ASP:H     | 14       | 0.14          |
| (1,1215) | 1:21:A:VAL:HG11 | 1:24:A:LYS:HG2   | 16       | 0.14          |
| (1,1215) | 1:21:A:VAL:HG11 | 1:24:A:LYS:HG3   | 16       | 0.14          |
| (1,1215) | 1:21:A:VAL:HG12 | 1:24:A:LYS:HG2   | 16       | 0.14          |
| (1,1215) | 1:21:A:VAL:HG12 | 1:24:A:LYS:HG3   | 16       | 0.14          |
| (1,1215) | 1:21:A:VAL:HG13 | 1:24:A:LYS:HG2   | 16       | 0.14          |
| (1,1215) | 1:21:A:VAL:HG13 | 1:24:A:LYS:HG3   | 16       | 0.14          |
| (1,1188) | 1:13:A:ARG:HG2  | 1:16:A:GLU:HB2   | 8        | 0.14          |
| (1,1188) | 1:13:A:ARG:HG2  | 1:16:A:GLU:HB3   | 8        | 0.14          |
| (1,1188) | 1:13:A:ARG:HG3  | 1:16:A:GLU:HB2   | 8        | 0.14          |
| (1,1188) | 1:13:A:ARG:HG3  | 1:16:A:GLU:HB3   | 8        | 0.14          |
| (1,1187) | 1:13:A:ARG:HB2  | 1:17:A:GLU:H     | 6        | 0.14          |
| (1,1187) | 1:13:A:ARG:HB3  | 1:17:A:GLU:H     | 6        | 0.14          |
| (1,1187) | 1:13:A:ARG:HB2  | 1:17:A:GLU:H     | 17       | 0.14          |
| (1,1187) | 1:13:A:ARG:HB3  | 1:17:A:GLU:H     | 17       | 0.14          |
| (1,1187) | 1:13:A:ARG:HB2  | 1:17:A:GLU:H     | 18       | 0.14          |
| (1,1187) | 1:13:A:ARG:HB3  | 1:17:A:GLU:H     | 18       | 0.14          |
| (1,1117) | 1:96:A:TYR:HD1  | 1:106:A:VAL:HB   | 11       | 0.14          |
| (1,1117) | 1:96:A:TYR:HD2  | 1:106:A:VAL:HB   | 11       | 0.14          |
| (1,1114) | 1:96:A:TYR:HE1  | 1:106:A:VAL:HG21 | 18       | 0.14          |
| (1,1114) | 1:96:A:TYR:HE1  | 1:106:A:VAL:HG22 | 18       | 0.14          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1114) | 1:96:A:TYR:HE1  | 1:106:A:VAL:HG23 | 18       | 0.14          |
| (1,1114) | 1:96:A:TYR:HE2  | 1:106:A:VAL:HG21 | 18       | 0.14          |
| (1,1114) | 1:96:A:TYR:HE2  | 1:106:A:VAL:HG22 | 18       | 0.14          |
| (1,1114) | 1:96:A:TYR:HE2  | 1:106:A:VAL:HG23 | 18       | 0.14          |
| (1,1113) | 1:96:A:TYR:HE1  | 1:106:A:VAL:HB   | 7        | 0.14          |
| (1,1113) | 1:96:A:TYR:HE2  | 1:106:A:VAL:HB   | 7        | 0.14          |
| (1,997)  | 1:22:A:VAL:H    | 1:119:A:LEU:HD21 | 13       | 0.14          |
| (1,997)  | 1:22:A:VAL:H    | 1:119:A:LEU:HD22 | 13       | 0.14          |
| (1,997)  | 1:22:A:VAL:H    | 1:119:A:LEU:HD23 | 13       | 0.14          |
| (1,955)  | 1:34:A:THR:HG21 | 1:37:A:LYS:H     | 19       | 0.14          |
| (1,955)  | 1:34:A:THR:HG22 | 1:37:A:LYS:H     | 19       | 0.14          |
| (1,955)  | 1:34:A:THR:HG23 | 1:37:A:LYS:H     | 19       | 0.14          |
| (1,902)  | 1:95:A:PHE:HA   | 1:97:A:GLU:HB2   | 6        | 0.14          |
| (1,902)  | 1:95:A:PHE:HA   | 1:97:A:GLU:HB3   | 6        | 0.14          |
| (1,836)  | 1:62:A:TYR:HA   | 1:64:A:GLU:HG2   | 10       | 0.14          |
| (1,836)  | 1:62:A:TYR:HA   | 1:64:A:GLU:HG3   | 10       | 0.14          |
| (1,836)  | 1:62:A:TYR:HA   | 1:64:A:GLU:HG2   | 20       | 0.14          |
| (1,836)  | 1:62:A:TYR:HA   | 1:64:A:GLU:HG3   | 20       | 0.14          |
| (1,821)  | 1:29:A:VAL:HG21 | 1:53:A:PRO:HB2   | 4        | 0.14          |
| (1,821)  | 1:29:A:VAL:HG22 | 1:53:A:PRO:HB2   | 4        | 0.14          |
| (1,821)  | 1:29:A:VAL:HG23 | 1:53:A:PRO:HB2   | 4        | 0.14          |
| (1,767)  | 1:37:A:LYS:HE2  | 1:65:A:VAL:HB    | 2        | 0.14          |
| (1,767)  | 1:37:A:LYS:HE3  | 1:65:A:VAL:HB    | 2        | 0.14          |
| (1,767)  | 1:37:A:LYS:HE2  | 1:65:A:VAL:HB    | 9        | 0.14          |
| (1,767)  | 1:37:A:LYS:HE3  | 1:65:A:VAL:HB    | 9        | 0.14          |
| (1,724)  | 1:58:A:ILE:HB   | 1:63:A:GLU:HB2   | 4        | 0.14          |
| (1,724)  | 1:58:A:ILE:HB   | 1:63:A:GLU:HB3   | 4        | 0.14          |
| (1,724)  | 1:58:A:ILE:HB   | 1:63:A:GLU:HB2   | 5        | 0.14          |
| (1,724)  | 1:58:A:ILE:HB   | 1:63:A:GLU:HB3   | 5        | 0.14          |
| (1,678)  | 1:24:A:LYS:HA   | 1:24:A:LYS:HE2   | 1        | 0.14          |
| (1,678)  | 1:24:A:LYS:HA   | 1:24:A:LYS:HE3   | 1        | 0.14          |
| (1,658)  | 1:129:A:LEU:HG  | 1:130:A:GLU:HG2  | 15       | 0.14          |
| (1,658)  | 1:129:A:LEU:HG  | 1:130:A:GLU:HG3  | 15       | 0.14          |
| (1,453)  | 1:80:A:VAL:H    | 1:104:A:VAL:HG21 | 5        | 0.14          |
| (1,453)  | 1:80:A:VAL:H    | 1:104:A:VAL:HG22 | 5        | 0.14          |
| (1,453)  | 1:80:A:VAL:H    | 1:104:A:VAL:HG23 | 5        | 0.14          |
| (1,391)  | 1:73:A:ALA:H    | 1:78:A:LEU:HD11  | 1        | 0.14          |
| (1,391)  | 1:73:A:ALA:H    | 1:78:A:LEU:HD12  | 1        | 0.14          |
| (1,391)  | 1:73:A:ALA:H    | 1:78:A:LEU:HD13  | 1        | 0.14          |
| (1,345)  | 1:19:A:LEU:HD21 | 1:23:A:LEU:H     | 4        | 0.14          |
| (1,345)  | 1:19:A:LEU:HD22 | 1:23:A:LEU:H     | 4        | 0.14          |
| (1,345)  | 1:19:A:LEU:HD23 | 1:23:A:LEU:H     | 4        | 0.14          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,299) | 1:116:A:LYS:H   | 1:116:A:LYS:HD2 | 20       | 0.14          |
| (1,299) | 1:116:A:LYS:H   | 1:116:A:LYS:HD3 | 20       | 0.14          |
| (1,282) | 1:97:A:GLU:H    | 1:98:A:GLN:HB2  | 20       | 0.14          |
| (1,282) | 1:97:A:GLU:H    | 1:98:A:GLN:HB3  | 20       | 0.14          |
| (1,77)  | 1:22:A:VAL:H    | 1:23:A:LEU:HB3  | 2        | 0.14          |
| (1,77)  | 1:22:A:VAL:H    | 1:23:A:LEU:HB3  | 16       | 0.14          |
| (1,77)  | 1:22:A:VAL:H    | 1:23:A:LEU:HB3  | 19       | 0.14          |
| (2,892) | 1:97:A:GLU:HB2  | 1:98:A:GLN:HE21 | 11       | 0.13          |
| (2,892) | 1:97:A:GLU:HB2  | 1:98:A:GLN:HE22 | 11       | 0.13          |
| (2,892) | 1:97:A:GLU:HB3  | 1:98:A:GLN:HE21 | 11       | 0.13          |
| (2,892) | 1:97:A:GLU:HB3  | 1:98:A:GLN:HE22 | 11       | 0.13          |
| (2,885) | 1:87:A:GLN:HA   | 1:89:A:GLN:HG2  | 11       | 0.13          |
| (2,885) | 1:87:A:GLN:HA   | 1:89:A:GLN:HG3  | 11       | 0.13          |
| (2,872) | 1:84:A:LYS:HB2  | 1:109:A:THR:H   | 20       | 0.13          |
| (2,872) | 1:84:A:LYS:HB3  | 1:109:A:THR:H   | 20       | 0.13          |
| (2,765) | 1:9:A:SER:H     | 1:63:A:GLU:HG2  | 7        | 0.13          |
| (2,765) | 1:9:A:SER:H     | 1:63:A:GLU:HG3  | 7        | 0.13          |
| (2,736) | 1:67:A:ARG:HD3  | 1:99:A:LEU:HD11 | 17       | 0.13          |
| (2,736) | 1:67:A:ARG:HD3  | 1:99:A:LEU:HD12 | 17       | 0.13          |
| (2,736) | 1:67:A:ARG:HD3  | 1:99:A:LEU:HD13 | 17       | 0.13          |
| (2,709) | 1:99:A:LEU:HD11 | 1:100:A:LYS:HD2 | 14       | 0.13          |
| (2,709) | 1:99:A:LEU:HD11 | 1:100:A:LYS:HD3 | 14       | 0.13          |
| (2,709) | 1:99:A:LEU:HD12 | 1:100:A:LYS:HD2 | 14       | 0.13          |
| (2,709) | 1:99:A:LEU:HD12 | 1:100:A:LYS:HD3 | 14       | 0.13          |
| (2,709) | 1:99:A:LEU:HD13 | 1:100:A:LYS:HD2 | 14       | 0.13          |
| (2,709) | 1:99:A:LEU:HD13 | 1:100:A:LYS:HD3 | 14       | 0.13          |
| (2,604) | 1:36:A:ASP:H    | 1:65:A:VAL:HG21 | 6        | 0.13          |
| (2,604) | 1:36:A:ASP:H    | 1:65:A:VAL:HG22 | 6        | 0.13          |
| (2,604) | 1:36:A:ASP:H    | 1:65:A:VAL:HG23 | 6        | 0.13          |
| (2,544) | 1:40:A:VAL:HB   | 1:66:A:VAL:HA   | 10       | 0.13          |
| (2,426) | 1:100:A:LYS:HE2 | 1:106:A:VAL:H   | 6        | 0.13          |
| (2,426) | 1:100:A:LYS:HE3 | 1:106:A:VAL:H   | 6        | 0.13          |
| (2,402) | 1:80:A:VAL:H    | 1:81:A:LEU:HD21 | 1        | 0.13          |
| (2,402) | 1:80:A:VAL:H    | 1:81:A:LEU:HD22 | 1        | 0.13          |
| (2,402) | 1:80:A:VAL:H    | 1:81:A:LEU:HD23 | 1        | 0.13          |
| (2,402) | 1:80:A:VAL:H    | 1:81:A:LEU:HD21 | 2        | 0.13          |
| (2,402) | 1:80:A:VAL:H    | 1:81:A:LEU:HD22 | 2        | 0.13          |
| (2,402) | 1:80:A:VAL:H    | 1:81:A:LEU:HD23 | 2        | 0.13          |
| (2,335) | 1:59:A:ARG:HB2  | 1:61:A:ALA:HB1  | 7        | 0.13          |
| (2,335) | 1:59:A:ARG:HB2  | 1:61:A:ALA:HB2  | 7        | 0.13          |
| (2,335) | 1:59:A:ARG:HB2  | 1:61:A:ALA:HB3  | 7        | 0.13          |
| (2,326) | 1:126:A:VAL:HB  | 1:127:A:GLY:HA2 | 8        | 0.13          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (2,315)  | 1:81:A:LEU:HB3  | 1:105:A:ASP:HB2  | 14       | 0.13          |
| (2,163)  | 1:74:A:GLN:HE21 | 1:103:A:GLY:H    | 11       | 0.13          |
| (1,1487) | 1:120:A:LYS:HG2 | 1:123:A:LEU:HD21 | 6        | 0.13          |
| (1,1487) | 1:120:A:LYS:HG2 | 1:123:A:LEU:HD22 | 6        | 0.13          |
| (1,1487) | 1:120:A:LYS:HG2 | 1:123:A:LEU:HD23 | 6        | 0.13          |
| (1,1487) | 1:120:A:LYS:HG3 | 1:123:A:LEU:HD21 | 6        | 0.13          |
| (1,1487) | 1:120:A:LYS:HG3 | 1:123:A:LEU:HD22 | 6        | 0.13          |
| (1,1487) | 1:120:A:LYS:HG3 | 1:123:A:LEU:HD23 | 6        | 0.13          |
| (1,1324) | 1:44:A:ILE:HD11 | 1:76:A:GLU:HB2   | 9        | 0.13          |
| (1,1324) | 1:44:A:ILE:HD11 | 1:76:A:GLU:HB3   | 9        | 0.13          |
| (1,1324) | 1:44:A:ILE:HD12 | 1:76:A:GLU:HB2   | 9        | 0.13          |
| (1,1324) | 1:44:A:ILE:HD12 | 1:76:A:GLU:HB3   | 9        | 0.13          |
| (1,1324) | 1:44:A:ILE:HD13 | 1:76:A:GLU:HB2   | 9        | 0.13          |
| (1,1324) | 1:44:A:ILE:HD13 | 1:76:A:GLU:HB3   | 9        | 0.13          |
| (1,1324) | 1:44:A:ILE:HD11 | 1:76:A:GLU:HB2   | 11       | 0.13          |
| (1,1324) | 1:44:A:ILE:HD11 | 1:76:A:GLU:HB3   | 11       | 0.13          |
| (1,1324) | 1:44:A:ILE:HD12 | 1:76:A:GLU:HB2   | 11       | 0.13          |
| (1,1324) | 1:44:A:ILE:HD12 | 1:76:A:GLU:HB3   | 11       | 0.13          |
| (1,1324) | 1:44:A:ILE:HD13 | 1:76:A:GLU:HB2   | 11       | 0.13          |
| (1,1324) | 1:44:A:ILE:HD13 | 1:76:A:GLU:HB3   | 11       | 0.13          |
| (1,1269) | 1:36:A:ASP:HB2  | 1:39:A:LYS:HA    | 15       | 0.13          |
| (1,1269) | 1:36:A:ASP:HB3  | 1:39:A:LYS:HA    | 15       | 0.13          |
| (1,1269) | 1:36:A:ASP:HB2  | 1:39:A:LYS:HA    | 19       | 0.13          |
| (1,1269) | 1:36:A:ASP:HB3  | 1:39:A:LYS:HA    | 19       | 0.13          |
| (1,1252) | 1:30:A:LYS:HD2  | 1:31:A:THR:H     | 5        | 0.13          |
| (1,1252) | 1:30:A:LYS:HD3  | 1:31:A:THR:H     | 5        | 0.13          |
| (1,1196) | 1:16:A:GLU:H    | 1:16:A:GLU:HG2   | 18       | 0.13          |
| (1,1196) | 1:16:A:GLU:H    | 1:16:A:GLU:HG3   | 18       | 0.13          |
| (1,1187) | 1:13:A:ARG:HB2  | 1:17:A:GLU:H     | 2        | 0.13          |
| (1,1187) | 1:13:A:ARG:HB3  | 1:17:A:GLU:H     | 2        | 0.13          |
| (1,1187) | 1:13:A:ARG:HB2  | 1:17:A:GLU:H     | 13       | 0.13          |
| (1,1187) | 1:13:A:ARG:HB3  | 1:17:A:GLU:H     | 13       | 0.13          |
| (1,1187) | 1:13:A:ARG:HB2  | 1:17:A:GLU:H     | 15       | 0.13          |
| (1,1187) | 1:13:A:ARG:HB3  | 1:17:A:GLU:H     | 15       | 0.13          |
| (1,1150) | 1:72:A:TYR:HE1  | 1:78:A:LEU:HD11  | 17       | 0.13          |
| (1,1150) | 1:72:A:TYR:HE1  | 1:78:A:LEU:HD12  | 17       | 0.13          |
| (1,1150) | 1:72:A:TYR:HE1  | 1:78:A:LEU:HD13  | 17       | 0.13          |
| (1,1150) | 1:72:A:TYR:HE2  | 1:78:A:LEU:HD11  | 17       | 0.13          |
| (1,1150) | 1:72:A:TYR:HE2  | 1:78:A:LEU:HD12  | 17       | 0.13          |
| (1,1150) | 1:72:A:TYR:HE2  | 1:78:A:LEU:HD13  | 17       | 0.13          |
| (1,1117) | 1:96:A:TYR:HD1  | 1:106:A:VAL:HB   | 9        | 0.13          |
| (1,1117) | 1:96:A:TYR:HD2  | 1:106:A:VAL:HB   | 9        | 0.13          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1113) | 1:96:A:TYR:HE1  | 1:106:A:VAL:HB   | 16       | 0.13          |
| (1,1113) | 1:96:A:TYR:HE2  | 1:106:A:VAL:HB   | 16       | 0.13          |
| (1,1078) | 1:15:A:LEU:HD21 | 1:57:A:PHE:HZ    | 8        | 0.13          |
| (1,1078) | 1:15:A:LEU:HD22 | 1:57:A:PHE:HZ    | 8        | 0.13          |
| (1,1078) | 1:15:A:LEU:HD23 | 1:57:A:PHE:HZ    | 8        | 0.13          |
| (1,1078) | 1:15:A:LEU:HD21 | 1:57:A:PHE:HZ    | 11       | 0.13          |
| (1,1078) | 1:15:A:LEU:HD22 | 1:57:A:PHE:HZ    | 11       | 0.13          |
| (1,1078) | 1:15:A:LEU:HD23 | 1:57:A:PHE:HZ    | 11       | 0.13          |
| (1,997)  | 1:22:A:VAL:H    | 1:119:A:LEU:HD21 | 1        | 0.13          |
| (1,997)  | 1:22:A:VAL:H    | 1:119:A:LEU:HD22 | 1        | 0.13          |
| (1,997)  | 1:22:A:VAL:H    | 1:119:A:LEU:HD23 | 1        | 0.13          |
| (1,997)  | 1:22:A:VAL:H    | 1:119:A:LEU:HD21 | 11       | 0.13          |
| (1,997)  | 1:22:A:VAL:H    | 1:119:A:LEU:HD22 | 11       | 0.13          |
| (1,997)  | 1:22:A:VAL:H    | 1:119:A:LEU:HD23 | 11       | 0.13          |
| (1,880)  | 1:83:A:ILE:HD11 | 1:115:A:ALA:HA   | 6        | 0.13          |
| (1,880)  | 1:83:A:ILE:HD12 | 1:115:A:ALA:HA   | 6        | 0.13          |
| (1,880)  | 1:83:A:ILE:HD13 | 1:115:A:ALA:HA   | 6        | 0.13          |
| (1,873)  | 1:87:A:GLN:H    | 1:88:A:ASP:HB2   | 13       | 0.13          |
| (1,873)  | 1:87:A:GLN:H    | 1:88:A:ASP:HB3   | 13       | 0.13          |
| (1,724)  | 1:58:A:ILE:HB   | 1:63:A:GLU:HB2   | 14       | 0.13          |
| (1,724)  | 1:58:A:ILE:HB   | 1:63:A:GLU:HB3   | 14       | 0.13          |
| (1,640)  | 1:34:A:THR:HB   | 1:39:A:LYS:HG2   | 12       | 0.13          |
| (1,640)  | 1:34:A:THR:HB   | 1:39:A:LYS:HG3   | 12       | 0.13          |
| (1,282)  | 1:97:A:GLU:H    | 1:98:A:GLN:HB2   | 18       | 0.13          |
| (1,282)  | 1:97:A:GLU:H    | 1:98:A:GLN:HB3   | 18       | 0.13          |
| (1,154)  | 1:36:A:ASP:H    | 1:40:A:VAL:H     | 6        | 0.13          |
| (1,103)  | 1:28:A:ASN:H    | 1:28:A:ASN:HD22  | 7        | 0.13          |
| (2,892)  | 1:97:A:GLU:HB2  | 1:98:A:GLN:HE21  | 2        | 0.12          |
| (2,892)  | 1:97:A:GLU:HB2  | 1:98:A:GLN:HE22  | 2        | 0.12          |
| (2,892)  | 1:97:A:GLU:HB3  | 1:98:A:GLN:HE21  | 2        | 0.12          |
| (2,892)  | 1:97:A:GLU:HB3  | 1:98:A:GLN:HE22  | 2        | 0.12          |
| (2,892)  | 1:97:A:GLU:HB2  | 1:98:A:GLN:HE21  | 16       | 0.12          |
| (2,892)  | 1:97:A:GLU:HB2  | 1:98:A:GLN:HE22  | 16       | 0.12          |
| (2,892)  | 1:97:A:GLU:HB3  | 1:98:A:GLN:HE21  | 16       | 0.12          |
| (2,892)  | 1:97:A:GLU:HB3  | 1:98:A:GLN:HE22  | 16       | 0.12          |
| (2,875)  | 1:84:A:LYS:HE2  | 1:85:A:VAL:HA    | 5        | 0.12          |
| (2,875)  | 1:84:A:LYS:HE3  | 1:85:A:VAL:HA    | 5        | 0.12          |
| (2,875)  | 1:84:A:LYS:HE2  | 1:85:A:VAL:HA    | 18       | 0.12          |
| (2,875)  | 1:84:A:LYS:HE3  | 1:85:A:VAL:HA    | 18       | 0.12          |
| (2,866)  | 1:81:A:LEU:HB2  | 1:83:A:ILE:HA    | 11       | 0.12          |
| (2,866)  | 1:81:A:LEU:HB3  | 1:83:A:ILE:HA    | 11       | 0.12          |
| (2,866)  | 1:81:A:LEU:HB2  | 1:83:A:ILE:HA    | 15       | 0.12          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,866)  | 1:81:A:LEU:HB3   | 1:83:A:ILE:HA    | 15       | 0.12          |
| (2,765)  | 1:9:A:SER:H      | 1:63:A:GLU:HG2   | 2        | 0.12          |
| (2,765)  | 1:9:A:SER:H      | 1:63:A:GLU:HG3   | 2        | 0.12          |
| (2,765)  | 1:9:A:SER:H      | 1:63:A:GLU:HG2   | 18       | 0.12          |
| (2,765)  | 1:9:A:SER:H      | 1:63:A:GLU:HG3   | 18       | 0.12          |
| (2,731)  | 1:9:A:SER:H      | 1:58:A:ILE:HG12  | 12       | 0.12          |
| (2,731)  | 1:9:A:SER:H      | 1:58:A:ILE:HG13  | 12       | 0.12          |
| (2,719)  | 1:55:A:VAL:HG11  | 1:123:A:LEU:HG   | 11       | 0.12          |
| (2,719)  | 1:55:A:VAL:HG12  | 1:123:A:LEU:HG   | 11       | 0.12          |
| (2,719)  | 1:55:A:VAL:HG13  | 1:123:A:LEU:HG   | 11       | 0.12          |
| (2,676)  | 1:89:A:GLN:HA    | 1:92:A:LEU:HD11  | 20       | 0.12          |
| (2,676)  | 1:89:A:GLN:HA    | 1:92:A:LEU:HD12  | 20       | 0.12          |
| (2,676)  | 1:89:A:GLN:HA    | 1:92:A:LEU:HD13  | 20       | 0.12          |
| (2,629)  | 1:74:A:GLN:HG3   | 1:104:A:VAL:HG11 | 17       | 0.12          |
| (2,629)  | 1:74:A:GLN:HG3   | 1:104:A:VAL:HG12 | 17       | 0.12          |
| (2,629)  | 1:74:A:GLN:HG3   | 1:104:A:VAL:HG13 | 17       | 0.12          |
| (2,584)  | 1:8:A:VAL:H      | 1:55:A:VAL:HG11  | 8        | 0.12          |
| (2,584)  | 1:8:A:VAL:H      | 1:55:A:VAL:HG12  | 8        | 0.12          |
| (2,584)  | 1:8:A:VAL:H      | 1:55:A:VAL:HG13  | 8        | 0.12          |
| (2,398)  | 1:4:A:VAL:H      | 1:81:A:LEU:HD11  | 5        | 0.12          |
| (2,398)  | 1:4:A:VAL:H      | 1:81:A:LEU:HD12  | 5        | 0.12          |
| (2,398)  | 1:4:A:VAL:H      | 1:81:A:LEU:HD13  | 5        | 0.12          |
| (2,348)  | 1:129:A:LEU:HG   | 1:130:A:GLU:HA   | 15       | 0.12          |
| (2,318)  | 1:87:A:GLN:HA    | 1:110:A:ASP:HB3  | 4        | 0.12          |
| (2,163)  | 1:74:A:GLN:HE21  | 1:103:A:GLY:H    | 13       | 0.12          |
| (2,160)  | 1:85:A:VAL:HG21  | 1:110:A:ASP:H    | 9        | 0.12          |
| (2,160)  | 1:85:A:VAL:HG22  | 1:110:A:ASP:H    | 9        | 0.12          |
| (2,160)  | 1:85:A:VAL:HG23  | 1:110:A:ASP:H    | 9        | 0.12          |
| (1,1487) | 1:120:A:LYS:HG2  | 1:123:A:LEU:HD21 | 7        | 0.12          |
| (1,1487) | 1:120:A:LYS:HG2  | 1:123:A:LEU:HD22 | 7        | 0.12          |
| (1,1487) | 1:120:A:LYS:HG2  | 1:123:A:LEU:HD23 | 7        | 0.12          |
| (1,1487) | 1:120:A:LYS:HG3  | 1:123:A:LEU:HD21 | 7        | 0.12          |
| (1,1487) | 1:120:A:LYS:HG3  | 1:123:A:LEU:HD22 | 7        | 0.12          |
| (1,1487) | 1:120:A:LYS:HG3  | 1:123:A:LEU:HD23 | 7        | 0.12          |
| (1,1487) | 1:120:A:LYS:HG2  | 1:123:A:LEU:HD21 | 17       | 0.12          |
| (1,1487) | 1:120:A:LYS:HG2  | 1:123:A:LEU:HD22 | 17       | 0.12          |
| (1,1487) | 1:120:A:LYS:HG2  | 1:123:A:LEU:HD23 | 17       | 0.12          |
| (1,1487) | 1:120:A:LYS:HG3  | 1:123:A:LEU:HD21 | 17       | 0.12          |
| (1,1487) | 1:120:A:LYS:HG3  | 1:123:A:LEU:HD22 | 17       | 0.12          |
| (1,1487) | 1:120:A:LYS:HG3  | 1:123:A:LEU:HD23 | 17       | 0.12          |
| (1,1462) | 1:111:A:ASN:HD21 | 1:112:A:GLU:HG2  | 5        | 0.12          |
| (1,1462) | 1:111:A:ASN:HD21 | 1:112:A:GLU:HG3  | 5        | 0.12          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1462) | 1:111:A:ASN:HD22 | 1:112:A:GLU:HG2 | 5        | 0.12          |
| (1,1462) | 1:111:A:ASN:HD22 | 1:112:A:GLU:HG3 | 5        | 0.12          |
| (1,1458) | 1:111:A:ASN:HB2  | 1:112:A:GLU:HG2 | 18       | 0.12          |
| (1,1458) | 1:111:A:ASN:HB2  | 1:112:A:GLU:HG3 | 18       | 0.12          |
| (1,1458) | 1:111:A:ASN:HB3  | 1:112:A:GLU:HG2 | 18       | 0.12          |
| (1,1458) | 1:111:A:ASN:HB3  | 1:112:A:GLU:HG3 | 18       | 0.12          |
| (1,1438) | 1:96:A:TYR:HD1   | 1:100:A:LYS:HG2 | 6        | 0.12          |
| (1,1438) | 1:96:A:TYR:HD1   | 1:100:A:LYS:HG3 | 6        | 0.12          |
| (1,1438) | 1:96:A:TYR:HD2   | 1:100:A:LYS:HG2 | 6        | 0.12          |
| (1,1438) | 1:96:A:TYR:HD2   | 1:100:A:LYS:HG3 | 6        | 0.12          |
| (1,1428) | 1:85:A:VAL:HG21  | 1:111:A:ASN:HB2 | 16       | 0.12          |
| (1,1428) | 1:85:A:VAL:HG21  | 1:111:A:ASN:HB3 | 16       | 0.12          |
| (1,1428) | 1:85:A:VAL:HG22  | 1:111:A:ASN:HB2 | 16       | 0.12          |
| (1,1428) | 1:85:A:VAL:HG22  | 1:111:A:ASN:HB3 | 16       | 0.12          |
| (1,1428) | 1:85:A:VAL:HG23  | 1:111:A:ASN:HB2 | 16       | 0.12          |
| (1,1428) | 1:85:A:VAL:HG23  | 1:111:A:ASN:HB3 | 16       | 0.12          |
| (1,1422) | 1:84:A:LYS:HG2   | 1:95:A:PHE:HD1  | 14       | 0.12          |
| (1,1422) | 1:84:A:LYS:HG2   | 1:95:A:PHE:HD2  | 14       | 0.12          |
| (1,1422) | 1:84:A:LYS:HG3   | 1:95:A:PHE:HD1  | 14       | 0.12          |
| (1,1422) | 1:84:A:LYS:HG3   | 1:95:A:PHE:HD2  | 14       | 0.12          |
| (1,1422) | 1:84:A:LYS:HG2   | 1:95:A:PHE:HD1  | 17       | 0.12          |
| (1,1422) | 1:84:A:LYS:HG2   | 1:95:A:PHE:HD2  | 17       | 0.12          |
| (1,1422) | 1:84:A:LYS:HG3   | 1:95:A:PHE:HD1  | 17       | 0.12          |
| (1,1422) | 1:84:A:LYS:HG3   | 1:95:A:PHE:HD2  | 17       | 0.12          |
| (1,1411) | 1:83:A:ILE:HG12  | 1:107:A:ARG:HA  | 10       | 0.12          |
| (1,1411) | 1:83:A:ILE:HG13  | 1:107:A:ARG:HA  | 10       | 0.12          |
| (1,1262) | 1:35:A:ASP:HB2   | 1:58:A:ILE:HB   | 1        | 0.12          |
| (1,1262) | 1:35:A:ASP:HB3   | 1:58:A:ILE:HB   | 1        | 0.12          |
| (1,1221) | 1:21:A:VAL:HG21  | 1:120:A:LYS:HB2 | 4        | 0.12          |
| (1,1221) | 1:21:A:VAL:HG21  | 1:120:A:LYS:HB3 | 4        | 0.12          |
| (1,1221) | 1:21:A:VAL:HG22  | 1:120:A:LYS:HB2 | 4        | 0.12          |
| (1,1221) | 1:21:A:VAL:HG22  | 1:120:A:LYS:HB3 | 4        | 0.12          |
| (1,1221) | 1:21:A:VAL:HG23  | 1:120:A:LYS:HB2 | 4        | 0.12          |
| (1,1221) | 1:21:A:VAL:HG23  | 1:120:A:LYS:HB3 | 4        | 0.12          |
| (1,1188) | 1:13:A:ARG:HG2   | 1:16:A:GLU:HB2  | 3        | 0.12          |
| (1,1188) | 1:13:A:ARG:HG2   | 1:16:A:GLU:HB3  | 3        | 0.12          |
| (1,1188) | 1:13:A:ARG:HG3   | 1:16:A:GLU:HB2  | 3        | 0.12          |
| (1,1188) | 1:13:A:ARG:HG3   | 1:16:A:GLU:HB3  | 3        | 0.12          |
| (1,1187) | 1:13:A:ARG:HB2   | 1:17:A:GLU:H    | 9        | 0.12          |
| (1,1187) | 1:13:A:ARG:HB3   | 1:17:A:GLU:H    | 9        | 0.12          |
| (1,1178) | 1:9:A:SER:HB2    | 1:59:A:ARG:HG2  | 1        | 0.12          |
| (1,1178) | 1:9:A:SER:HB2    | 1:59:A:ARG:HG3  | 1        | 0.12          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1178) | 1:9:A:SER:HB3   | 1:59:A:ARG:HG2   | 1        | 0.12          |
| (1,1178) | 1:9:A:SER:HB3   | 1:59:A:ARG:HG3   | 1        | 0.12          |
| (1,1113) | 1:96:A:TYR:HE1  | 1:106:A:VAL:HB   | 11       | 0.12          |
| (1,1113) | 1:96:A:TYR:HE2  | 1:106:A:VAL:HB   | 11       | 0.12          |
| (1,1112) | 1:96:A:TYR:HE1  | 1:97:A:GLU:HB2   | 8        | 0.12          |
| (1,1112) | 1:96:A:TYR:HE1  | 1:97:A:GLU:HB3   | 8        | 0.12          |
| (1,1112) | 1:96:A:TYR:HE2  | 1:97:A:GLU:HB2   | 8        | 0.12          |
| (1,1112) | 1:96:A:TYR:HE2  | 1:97:A:GLU:HB3   | 8        | 0.12          |
| (1,997)  | 1:22:A:VAL:H    | 1:119:A:LEU:HD21 | 16       | 0.12          |
| (1,997)  | 1:22:A:VAL:H    | 1:119:A:LEU:HD22 | 16       | 0.12          |
| (1,997)  | 1:22:A:VAL:H    | 1:119:A:LEU:HD23 | 16       | 0.12          |
| (1,977)  | 1:64:A:GLU:HG2  | 1:65:A:VAL:HG11  | 1        | 0.12          |
| (1,977)  | 1:64:A:GLU:HG2  | 1:65:A:VAL:HG12  | 1        | 0.12          |
| (1,977)  | 1:64:A:GLU:HG2  | 1:65:A:VAL:HG13  | 1        | 0.12          |
| (1,977)  | 1:64:A:GLU:HG3  | 1:65:A:VAL:HG11  | 1        | 0.12          |
| (1,977)  | 1:64:A:GLU:HG3  | 1:65:A:VAL:HG12  | 1        | 0.12          |
| (1,977)  | 1:64:A:GLU:HG3  | 1:65:A:VAL:HG13  | 1        | 0.12          |
| (1,880)  | 1:83:A:ILE:HD11 | 1:115:A:ALA:HA   | 1        | 0.12          |
| (1,880)  | 1:83:A:ILE:HD12 | 1:115:A:ALA:HA   | 1        | 0.12          |
| (1,880)  | 1:83:A:ILE:HD13 | 1:115:A:ALA:HA   | 1        | 0.12          |
| (1,724)  | 1:58:A:ILE:HB   | 1:63:A:GLU:HB2   | 10       | 0.12          |
| (1,724)  | 1:58:A:ILE:HB   | 1:63:A:GLU:HB3   | 10       | 0.12          |
| (1,724)  | 1:58:A:ILE:HB   | 1:63:A:GLU:HB2   | 19       | 0.12          |
| (1,724)  | 1:58:A:ILE:HB   | 1:63:A:GLU:HB3   | 19       | 0.12          |
| (1,658)  | 1:129:A:LEU:HG  | 1:130:A:GLU:HG2  | 17       | 0.12          |
| (1,658)  | 1:129:A:LEU:HG  | 1:130:A:GLU:HG3  | 17       | 0.12          |
| (1,557)  | 1:19:A:LEU:HD21 | 1:23:A:LEU:HD11  | 6        | 0.12          |
| (1,557)  | 1:19:A:LEU:HD21 | 1:23:A:LEU:HD12  | 6        | 0.12          |
| (1,557)  | 1:19:A:LEU:HD21 | 1:23:A:LEU:HD13  | 6        | 0.12          |
| (1,557)  | 1:19:A:LEU:HD22 | 1:23:A:LEU:HD11  | 6        | 0.12          |
| (1,557)  | 1:19:A:LEU:HD22 | 1:23:A:LEU:HD12  | 6        | 0.12          |
| (1,557)  | 1:19:A:LEU:HD22 | 1:23:A:LEU:HD13  | 6        | 0.12          |
| (1,557)  | 1:19:A:LEU:HD23 | 1:23:A:LEU:HD11  | 6        | 0.12          |
| (1,557)  | 1:19:A:LEU:HD23 | 1:23:A:LEU:HD12  | 6        | 0.12          |
| (1,557)  | 1:19:A:LEU:HD23 | 1:23:A:LEU:HD13  | 6        | 0.12          |
| (1,345)  | 1:19:A:LEU:HD21 | 1:23:A:LEU:H     | 6        | 0.12          |
| (1,345)  | 1:19:A:LEU:HD22 | 1:23:A:LEU:H     | 6        | 0.12          |
| (1,345)  | 1:19:A:LEU:HD23 | 1:23:A:LEU:H     | 6        | 0.12          |
| (1,282)  | 1:97:A:GLU:H    | 1:98:A:GLN:HB2   | 5        | 0.12          |
| (1,282)  | 1:97:A:GLU:H    | 1:98:A:GLN:HB3   | 5        | 0.12          |
| (1,282)  | 1:97:A:GLU:H    | 1:98:A:GLN:HB2   | 7        | 0.12          |
| (1,282)  | 1:97:A:GLU:H    | 1:98:A:GLN:HB3   | 7        | 0.12          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,282) | 1:97:A:GLU:H     | 1:98:A:GLN:HB2   | 8        | 0.12          |
| (1,282) | 1:97:A:GLU:H     | 1:98:A:GLN:HB3   | 8        | 0.12          |
| (1,77)  | 1:22:A:VAL:H     | 1:23:A:LEU:HB3   | 5        | 0.12          |
| (2,886) | 1:87:A:GLN:HB2   | 1:92:A:LEU:HD11  | 15       | 0.11          |
| (2,886) | 1:87:A:GLN:HB2   | 1:92:A:LEU:HD12  | 15       | 0.11          |
| (2,886) | 1:87:A:GLN:HB2   | 1:92:A:LEU:HD13  | 15       | 0.11          |
| (2,886) | 1:87:A:GLN:HB3   | 1:92:A:LEU:HD11  | 15       | 0.11          |
| (2,886) | 1:87:A:GLN:HB3   | 1:92:A:LEU:HD12  | 15       | 0.11          |
| (2,886) | 1:87:A:GLN:HB3   | 1:92:A:LEU:HD13  | 15       | 0.11          |
| (2,873) | 1:84:A:LYS:HG2   | 1:86:A:ALA:HA    | 14       | 0.11          |
| (2,873) | 1:84:A:LYS:HG3   | 1:86:A:ALA:HA    | 14       | 0.11          |
| (2,765) | 1:9:A:SER:H      | 1:63:A:GLU:HG2   | 5        | 0.11          |
| (2,765) | 1:9:A:SER:H      | 1:63:A:GLU:HG3   | 5        | 0.11          |
| (2,720) | 1:6:A:ILE:HB     | 1:55:A:VAL:HG11  | 6        | 0.11          |
| (2,720) | 1:6:A:ILE:HB     | 1:55:A:VAL:HG12  | 6        | 0.11          |
| (2,720) | 1:6:A:ILE:HB     | 1:55:A:VAL:HG13  | 6        | 0.11          |
| (2,674) | 1:92:A:LEU:HD11  | 1:96:A:TYR:HB3   | 17       | 0.11          |
| (2,674) | 1:92:A:LEU:HD12  | 1:96:A:TYR:HB3   | 17       | 0.11          |
| (2,674) | 1:92:A:LEU:HD13  | 1:96:A:TYR:HB3   | 17       | 0.11          |
| (2,630) | 1:74:A:GLN:HG2   | 1:104:A:VAL:HG11 | 12       | 0.11          |
| (2,630) | 1:74:A:GLN:HG2   | 1:104:A:VAL:HG12 | 12       | 0.11          |
| (2,630) | 1:74:A:GLN:HG2   | 1:104:A:VAL:HG13 | 12       | 0.11          |
| (2,627) | 1:74:A:GLN:HA    | 1:78:A:LEU:HD11  | 19       | 0.11          |
| (2,627) | 1:74:A:GLN:HA    | 1:78:A:LEU:HD12  | 19       | 0.11          |
| (2,627) | 1:74:A:GLN:HA    | 1:78:A:LEU:HD13  | 19       | 0.11          |
| (2,584) | 1:8:A:VAL:H      | 1:55:A:VAL:HG11  | 10       | 0.11          |
| (2,584) | 1:8:A:VAL:H      | 1:55:A:VAL:HG12  | 10       | 0.11          |
| (2,584) | 1:8:A:VAL:H      | 1:55:A:VAL:HG13  | 10       | 0.11          |
| (2,575) | 1:47:A:ALA:HB1   | 1:50:A:GLN:HG3   | 4        | 0.11          |
| (2,575) | 1:47:A:ALA:HB2   | 1:50:A:GLN:HG3   | 4        | 0.11          |
| (2,575) | 1:47:A:ALA:HB3   | 1:50:A:GLN:HG3   | 4        | 0.11          |
| (2,544) | 1:40:A:VAL:HB    | 1:66:A:VAL:HA    | 12       | 0.11          |
| (2,509) | 1:32:A:VAL:HG11  | 1:56:A:ILE:HB    | 14       | 0.11          |
| (2,509) | 1:32:A:VAL:HG12  | 1:56:A:ILE:HB    | 14       | 0.11          |
| (2,509) | 1:32:A:VAL:HG13  | 1:56:A:ILE:HB    | 14       | 0.11          |
| (2,468) | 1:11:A:ASP:HA    | 1:14:A:ILE:HG21  | 15       | 0.11          |
| (2,468) | 1:11:A:ASP:HA    | 1:14:A:ILE:HG22  | 15       | 0.11          |
| (2,468) | 1:11:A:ASP:HA    | 1:14:A:ILE:HG23  | 15       | 0.11          |
| (2,457) | 1:122:A:LEU:HD21 | 1:125:A:LYS:HE2  | 16       | 0.11          |
| (2,457) | 1:122:A:LEU:HD21 | 1:125:A:LYS:HE3  | 16       | 0.11          |
| (2,457) | 1:122:A:LEU:HD22 | 1:125:A:LYS:HE2  | 16       | 0.11          |
| (2,457) | 1:122:A:LEU:HD22 | 1:125:A:LYS:HE3  | 16       | 0.11          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,457)  | 1:122:A:LEU:HD23 | 1:125:A:LYS:HE2  | 16       | 0.11          |
| (2,457)  | 1:122:A:LEU:HD23 | 1:125:A:LYS:HE3  | 16       | 0.11          |
| (2,440)  | 1:72:A:TYR:HE1   | 1:78:A:LEU:HG    | 19       | 0.11          |
| (2,440)  | 1:72:A:TYR:HE2   | 1:78:A:LEU:HG    | 19       | 0.11          |
| (2,402)  | 1:80:A:VAL:H     | 1:81:A:LEU:HD21  | 17       | 0.11          |
| (2,402)  | 1:80:A:VAL:H     | 1:81:A:LEU:HD22  | 17       | 0.11          |
| (2,402)  | 1:80:A:VAL:H     | 1:81:A:LEU:HD23  | 17       | 0.11          |
| (2,384)  | 1:97:A:GLU:H     | 1:106:A:VAL:HG11 | 14       | 0.11          |
| (2,384)  | 1:97:A:GLU:H     | 1:106:A:VAL:HG12 | 14       | 0.11          |
| (2,384)  | 1:97:A:GLU:H     | 1:106:A:VAL:HG13 | 14       | 0.11          |
| (2,384)  | 1:97:A:GLU:H     | 1:106:A:VAL:HG11 | 18       | 0.11          |
| (2,384)  | 1:97:A:GLU:H     | 1:106:A:VAL:HG12 | 18       | 0.11          |
| (2,384)  | 1:97:A:GLU:H     | 1:106:A:VAL:HG13 | 18       | 0.11          |
| (2,363)  | 1:81:A:LEU:HG    | 1:105:A:ASP:HB2  | 2        | 0.11          |
| (2,335)  | 1:59:A:ARG:HB2   | 1:61:A:ALA:HB1   | 6        | 0.11          |
| (2,335)  | 1:59:A:ARG:HB2   | 1:61:A:ALA:HB2   | 6        | 0.11          |
| (2,335)  | 1:59:A:ARG:HB2   | 1:61:A:ALA:HB3   | 6        | 0.11          |
| (2,318)  | 1:87:A:GLN:HA    | 1:110:A:ASP:HB3  | 17       | 0.11          |
| (2,242)  | 1:49:A:LYS:HD2   | 1:50:A:GLN:HA    | 15       | 0.11          |
| (2,242)  | 1:49:A:LYS:HD3   | 1:50:A:GLN:HA    | 15       | 0.11          |
| (2,74)   | 1:31:A:THR:H     | 1:54:A:ILE:HD11  | 4        | 0.11          |
| (2,74)   | 1:31:A:THR:H     | 1:54:A:ILE:HD12  | 4        | 0.11          |
| (2,74)   | 1:31:A:THR:H     | 1:54:A:ILE:HD13  | 4        | 0.11          |
| (1,1458) | 1:111:A:ASN:HB2  | 1:112:A:GLU:HG2  | 5        | 0.11          |
| (1,1458) | 1:111:A:ASN:HB2  | 1:112:A:GLU:HG3  | 5        | 0.11          |
| (1,1458) | 1:111:A:ASN:HB3  | 1:112:A:GLU:HG2  | 5        | 0.11          |
| (1,1458) | 1:111:A:ASN:HB3  | 1:112:A:GLU:HG3  | 5        | 0.11          |
| (1,1448) | 1:99:A:LEU:HD21  | 1:100:A:LYS:HG2  | 3        | 0.11          |
| (1,1448) | 1:99:A:LEU:HD21  | 1:100:A:LYS:HG3  | 3        | 0.11          |
| (1,1448) | 1:99:A:LEU:HD22  | 1:100:A:LYS:HG2  | 3        | 0.11          |
| (1,1448) | 1:99:A:LEU:HD22  | 1:100:A:LYS:HG3  | 3        | 0.11          |
| (1,1448) | 1:99:A:LEU:HD23  | 1:100:A:LYS:HG2  | 3        | 0.11          |
| (1,1448) | 1:99:A:LEU:HD23  | 1:100:A:LYS:HG3  | 3        | 0.11          |
| (1,1447) | 1:99:A:LEU:HD11  | 1:100:A:LYS:HG2  | 4        | 0.11          |
| (1,1447) | 1:99:A:LEU:HD11  | 1:100:A:LYS:HG3  | 4        | 0.11          |
| (1,1447) | 1:99:A:LEU:HD12  | 1:100:A:LYS:HG2  | 4        | 0.11          |
| (1,1447) | 1:99:A:LEU:HD12  | 1:100:A:LYS:HG3  | 4        | 0.11          |
| (1,1447) | 1:99:A:LEU:HD13  | 1:100:A:LYS:HG2  | 4        | 0.11          |
| (1,1447) | 1:99:A:LEU:HD13  | 1:100:A:LYS:HG3  | 4        | 0.11          |
| (1,1447) | 1:99:A:LEU:HD11  | 1:100:A:LYS:HG2  | 9        | 0.11          |
| (1,1447) | 1:99:A:LEU:HD11  | 1:100:A:LYS:HG3  | 9        | 0.11          |
| (1,1447) | 1:99:A:LEU:HD12  | 1:100:A:LYS:HG2  | 9        | 0.11          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1447) | 1:99:A:LEU:HD12 | 1:100:A:LYS:HG3 | 9        | 0.11          |
| (1,1447) | 1:99:A:LEU:HD13 | 1:100:A:LYS:HG2 | 9        | 0.11          |
| (1,1447) | 1:99:A:LEU:HD13 | 1:100:A:LYS:HG3 | 9        | 0.11          |
| (1,1427) | 1:84:A:LYS:HE2  | 1:96:A:TYR:HE1  | 19       | 0.11          |
| (1,1427) | 1:84:A:LYS:HE2  | 1:96:A:TYR:HE2  | 19       | 0.11          |
| (1,1427) | 1:84:A:LYS:HE3  | 1:96:A:TYR:HE1  | 19       | 0.11          |
| (1,1427) | 1:84:A:LYS:HE3  | 1:96:A:TYR:HE2  | 19       | 0.11          |
| (1,1419) | 1:84:A:LYS:HB2  | 1:96:A:TYR:HB2  | 13       | 0.11          |
| (1,1419) | 1:84:A:LYS:HB2  | 1:96:A:TYR:HB3  | 13       | 0.11          |
| (1,1419) | 1:84:A:LYS:HB3  | 1:96:A:TYR:HB2  | 13       | 0.11          |
| (1,1419) | 1:84:A:LYS:HB3  | 1:96:A:TYR:HB3  | 13       | 0.11          |
| (1,1411) | 1:83:A:ILE:HG12 | 1:107:A:ARG:HA  | 9        | 0.11          |
| (1,1411) | 1:83:A:ILE:HG13 | 1:107:A:ARG:HA  | 9        | 0.11          |
| (1,1403) | 1:81:A:LEU:HB2  | 1:107:A:ARG:HD2 | 18       | 0.11          |
| (1,1403) | 1:81:A:LEU:HB2  | 1:107:A:ARG:HD3 | 18       | 0.11          |
| (1,1403) | 1:81:A:LEU:HB3  | 1:107:A:ARG:HD2 | 18       | 0.11          |
| (1,1403) | 1:81:A:LEU:HB3  | 1:107:A:ARG:HD3 | 18       | 0.11          |
| (1,1324) | 1:44:A:ILE:HD11 | 1:76:A:GLU:HB2  | 17       | 0.11          |
| (1,1324) | 1:44:A:ILE:HD11 | 1:76:A:GLU:HB3  | 17       | 0.11          |
| (1,1324) | 1:44:A:ILE:HD12 | 1:76:A:GLU:HB2  | 17       | 0.11          |
| (1,1324) | 1:44:A:ILE:HD12 | 1:76:A:GLU:HB3  | 17       | 0.11          |
| (1,1324) | 1:44:A:ILE:HD13 | 1:76:A:GLU:HB2  | 17       | 0.11          |
| (1,1324) | 1:44:A:ILE:HD13 | 1:76:A:GLU:HB3  | 17       | 0.11          |
| (1,1255) | 1:32:A:VAL:HG21 | 1:39:A:LYS:HE2  | 16       | 0.11          |
| (1,1255) | 1:32:A:VAL:HG21 | 1:39:A:LYS:HE3  | 16       | 0.11          |
| (1,1255) | 1:32:A:VAL:HG22 | 1:39:A:LYS:HE2  | 16       | 0.11          |
| (1,1255) | 1:32:A:VAL:HG22 | 1:39:A:LYS:HE3  | 16       | 0.11          |
| (1,1255) | 1:32:A:VAL:HG23 | 1:39:A:LYS:HE2  | 16       | 0.11          |
| (1,1255) | 1:32:A:VAL:HG23 | 1:39:A:LYS:HE3  | 16       | 0.11          |
| (1,1245) | 1:29:A:VAL:HG21 | 1:53:A:PRO:HG2  | 10       | 0.11          |
| (1,1245) | 1:29:A:VAL:HG21 | 1:53:A:PRO:HG3  | 10       | 0.11          |
| (1,1245) | 1:29:A:VAL:HG22 | 1:53:A:PRO:HG2  | 10       | 0.11          |
| (1,1245) | 1:29:A:VAL:HG22 | 1:53:A:PRO:HG3  | 10       | 0.11          |
| (1,1245) | 1:29:A:VAL:HG23 | 1:53:A:PRO:HG2  | 10       | 0.11          |
| (1,1245) | 1:29:A:VAL:HG23 | 1:53:A:PRO:HG3  | 10       | 0.11          |
| (1,1129) | 1:61:A:ALA:H    | 1:62:A:TYR:HD1  | 13       | 0.11          |
| (1,1129) | 1:61:A:ALA:H    | 1:62:A:TYR:HD2  | 13       | 0.11          |
| (1,1113) | 1:96:A:TYR:HE1  | 1:106:A:VAL:HB  | 2        | 0.11          |
| (1,1113) | 1:96:A:TYR:HE2  | 1:106:A:VAL:HB  | 2        | 0.11          |
| (1,1078) | 1:15:A:LEU:HD21 | 1:57:A:PHE:HZ   | 7        | 0.11          |
| (1,1078) | 1:15:A:LEU:HD22 | 1:57:A:PHE:HZ   | 7        | 0.11          |
| (1,1078) | 1:15:A:LEU:HD23 | 1:57:A:PHE:HZ   | 7        | 0.11          |

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| Key     | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (1,997) | 1:22:A:VAL:H    | 1:119:A:LEU:HD21 | 3        | 0.11          |
| (1,997) | 1:22:A:VAL:H    | 1:119:A:LEU:HD22 | 3        | 0.11          |
| (1,997) | 1:22:A:VAL:H    | 1:119:A:LEU:HD23 | 3        | 0.11          |
| (1,968) | 1:29:A:VAL:HG21 | 1:54:A:ILE:HA    | 9        | 0.11          |
| (1,968) | 1:29:A:VAL:HG22 | 1:54:A:ILE:HA    | 9        | 0.11          |
| (1,968) | 1:29:A:VAL:HG23 | 1:54:A:ILE:HA    | 9        | 0.11          |
| (1,968) | 1:29:A:VAL:HG21 | 1:54:A:ILE:HA    | 19       | 0.11          |
| (1,968) | 1:29:A:VAL:HG22 | 1:54:A:ILE:HA    | 19       | 0.11          |
| (1,968) | 1:29:A:VAL:HG23 | 1:54:A:ILE:HA    | 19       | 0.11          |
| (1,902) | 1:95:A:PHE:HA   | 1:97:A:GLU:HB2   | 16       | 0.11          |
| (1,902) | 1:95:A:PHE:HA   | 1:97:A:GLU:HB3   | 16       | 0.11          |
| (1,556) | 1:19:A:LEU:HD11 | 1:23:A:LEU:HD21  | 15       | 0.11          |
| (1,556) | 1:19:A:LEU:HD11 | 1:23:A:LEU:HD22  | 15       | 0.11          |
| (1,556) | 1:19:A:LEU:HD11 | 1:23:A:LEU:HD23  | 15       | 0.11          |
| (1,556) | 1:19:A:LEU:HD12 | 1:23:A:LEU:HD21  | 15       | 0.11          |
| (1,556) | 1:19:A:LEU:HD12 | 1:23:A:LEU:HD22  | 15       | 0.11          |
| (1,556) | 1:19:A:LEU:HD12 | 1:23:A:LEU:HD23  | 15       | 0.11          |
| (1,556) | 1:19:A:LEU:HD13 | 1:23:A:LEU:HD21  | 15       | 0.11          |
| (1,556) | 1:19:A:LEU:HD13 | 1:23:A:LEU:HD22  | 15       | 0.11          |
| (1,556) | 1:19:A:LEU:HD13 | 1:23:A:LEU:HD23  | 15       | 0.11          |
| (1,453) | 1:80:A:VAL:H    | 1:104:A:VAL:HG21 | 12       | 0.11          |
| (1,453) | 1:80:A:VAL:H    | 1:104:A:VAL:HG22 | 12       | 0.11          |
| (1,453) | 1:80:A:VAL:H    | 1:104:A:VAL:HG23 | 12       | 0.11          |
| (1,77)  | 1:22:A:VAL:H    | 1:23:A:LEU:HB3   | 7        | 0.11          |
| (2,792) | 1:28:A:ASN:HD21 | 1:52:A:ARG:HG2   | 15       | 0.1           |
| (2,792) | 1:28:A:ASN:HD21 | 1:52:A:ARG:HG3   | 15       | 0.1           |
| (2,792) | 1:28:A:ASN:HD22 | 1:52:A:ARG:HG2   | 15       | 0.1           |
| (2,792) | 1:28:A:ASN:HD22 | 1:52:A:ARG:HG3   | 15       | 0.1           |
| (2,765) | 1:9:A:SER:H     | 1:63:A:GLU:HG2   | 6        | 0.1           |
| (2,765) | 1:9:A:SER:H     | 1:63:A:GLU:HG3   | 6        | 0.1           |
| (2,687) | 1:9:A:SER:HB2   | 1:84:A:LYS:HA    | 1        | 0.1           |
| (2,687) | 1:9:A:SER:HB2   | 1:84:A:LYS:HA    | 3        | 0.1           |
| (2,687) | 1:9:A:SER:HB2   | 1:84:A:LYS:HA    | 6        | 0.1           |
| (2,684) | 1:9:A:SER:HB3   | 1:84:A:LYS:HA    | 17       | 0.1           |
| (2,415) | 1:87:A:GLN:H    | 1:89:A:GLN:HG3   | 13       | 0.1           |
| (2,402) | 1:80:A:VAL:H    | 1:81:A:LEU:HD21  | 15       | 0.1           |
| (2,402) | 1:80:A:VAL:H    | 1:81:A:LEU:HD22  | 15       | 0.1           |
| (2,402) | 1:80:A:VAL:H    | 1:81:A:LEU:HD23  | 15       | 0.1           |
| (2,363) | 1:81:A:LEU:HG   | 1:105:A:ASP:HB2  | 15       | 0.1           |
| (2,335) | 1:59:A:ARG:HB2  | 1:61:A:ALA:HB1   | 10       | 0.1           |
| (2,335) | 1:59:A:ARG:HB2  | 1:61:A:ALA:HB2   | 10       | 0.1           |
| (2,335) | 1:59:A:ARG:HB2  | 1:61:A:ALA:HB3   | 10       | 0.1           |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (2,318)  | 1:87:A:GLN:HA   | 1:110:A:ASP:HB3  | 5        | 0.1           |
| (2,259)  | 1:9:A:SER:HA    | 1:59:A:ARG:HG2   | 13       | 0.1           |
| (2,237)  | 1:97:A:GLU:HB2  | 1:101:A:LYS:HE2  | 12       | 0.1           |
| (2,237)  | 1:97:A:GLU:HB2  | 1:101:A:LYS:HE3  | 12       | 0.1           |
| (2,237)  | 1:97:A:GLU:HB3  | 1:101:A:LYS:HE2  | 12       | 0.1           |
| (2,237)  | 1:97:A:GLU:HB3  | 1:101:A:LYS:HE3  | 12       | 0.1           |
| (1,1475) | 1:118:A:ARG:HG2 | 1:121:A:GLU:HB2  | 8        | 0.1           |
| (1,1475) | 1:118:A:ARG:HG2 | 1:121:A:GLU:HB3  | 8        | 0.1           |
| (1,1475) | 1:118:A:ARG:HG3 | 1:121:A:GLU:HB2  | 8        | 0.1           |
| (1,1475) | 1:118:A:ARG:HG3 | 1:121:A:GLU:HB3  | 8        | 0.1           |
| (1,1458) | 1:111:A:ASN:HB2 | 1:112:A:GLU:HG2  | 12       | 0.1           |
| (1,1458) | 1:111:A:ASN:HB2 | 1:112:A:GLU:HG3  | 12       | 0.1           |
| (1,1458) | 1:111:A:ASN:HB3 | 1:112:A:GLU:HG2  | 12       | 0.1           |
| (1,1458) | 1:111:A:ASN:HB3 | 1:112:A:GLU:HG3  | 12       | 0.1           |
| (1,1448) | 1:99:A:LEU:HD21 | 1:100:A:LYS:HG2  | 14       | 0.1           |
| (1,1448) | 1:99:A:LEU:HD21 | 1:100:A:LYS:HG3  | 14       | 0.1           |
| (1,1448) | 1:99:A:LEU:HD22 | 1:100:A:LYS:HG2  | 14       | 0.1           |
| (1,1448) | 1:99:A:LEU:HD22 | 1:100:A:LYS:HG3  | 14       | 0.1           |
| (1,1448) | 1:99:A:LEU:HD23 | 1:100:A:LYS:HG2  | 14       | 0.1           |
| (1,1448) | 1:99:A:LEU:HD23 | 1:100:A:LYS:HG3  | 14       | 0.1           |
| (1,1447) | 1:99:A:LEU:HD11 | 1:100:A:LYS:HG2  | 11       | 0.1           |
| (1,1447) | 1:99:A:LEU:HD11 | 1:100:A:LYS:HG3  | 11       | 0.1           |
| (1,1447) | 1:99:A:LEU:HD12 | 1:100:A:LYS:HG2  | 11       | 0.1           |
| (1,1447) | 1:99:A:LEU:HD12 | 1:100:A:LYS:HG3  | 11       | 0.1           |
| (1,1447) | 1:99:A:LEU:HD13 | 1:100:A:LYS:HG2  | 11       | 0.1           |
| (1,1447) | 1:99:A:LEU:HD13 | 1:100:A:LYS:HG3  | 11       | 0.1           |
| (1,1411) | 1:83:A:ILE:HG12 | 1:107:A:ARG:HA   | 2        | 0.1           |
| (1,1411) | 1:83:A:ILE:HG13 | 1:107:A:ARG:HA   | 2        | 0.1           |
| (1,1269) | 1:36:A:ASP:HB2  | 1:39:A:LYS:HA    | 2        | 0.1           |
| (1,1269) | 1:36:A:ASP:HB3  | 1:39:A:LYS:HA    | 2        | 0.1           |
| (1,1196) | 1:16:A:GLU:H    | 1:16:A:GLU:HG2   | 10       | 0.1           |
| (1,1196) | 1:16:A:GLU:H    | 1:16:A:GLU:HG3   | 10       | 0.1           |
| (1,1196) | 1:16:A:GLU:H    | 1:16:A:GLU:HG2   | 13       | 0.1           |
| (1,1196) | 1:16:A:GLU:H    | 1:16:A:GLU:HG3   | 13       | 0.1           |
| (1,1187) | 1:13:A:ARG:HB2  | 1:17:A:GLU:H     | 14       | 0.1           |
| (1,1187) | 1:13:A:ARG:HB3  | 1:17:A:GLU:H     | 14       | 0.1           |
| (1,1129) | 1:61:A:ALA:H    | 1:62:A:TYR:HD1   | 10       | 0.1           |
| (1,1129) | 1:61:A:ALA:H    | 1:62:A:TYR:HD2   | 10       | 0.1           |
| (1,1114) | 1:96:A:TYR:HE1  | 1:106:A:VAL:HG21 | 8        | 0.1           |
| (1,1114) | 1:96:A:TYR:HE1  | 1:106:A:VAL:HG22 | 8        | 0.1           |
| (1,1114) | 1:96:A:TYR:HE1  | 1:106:A:VAL:HG23 | 8        | 0.1           |
| (1,1114) | 1:96:A:TYR:HE2  | 1:106:A:VAL:HG21 | 8        | 0.1           |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1114) | 1:96:A:TYR:HE2  | 1:106:A:VAL:HG22 | 8        | 0.1           |
| (1,1114) | 1:96:A:TYR:HE2  | 1:106:A:VAL:HG23 | 8        | 0.1           |
| (1,1114) | 1:96:A:TYR:HE1  | 1:106:A:VAL:HG21 | 14       | 0.1           |
| (1,1114) | 1:96:A:TYR:HE1  | 1:106:A:VAL:HG22 | 14       | 0.1           |
| (1,1114) | 1:96:A:TYR:HE1  | 1:106:A:VAL:HG23 | 14       | 0.1           |
| (1,1114) | 1:96:A:TYR:HE2  | 1:106:A:VAL:HG21 | 14       | 0.1           |
| (1,1114) | 1:96:A:TYR:HE2  | 1:106:A:VAL:HG22 | 14       | 0.1           |
| (1,1114) | 1:96:A:TYR:HE2  | 1:106:A:VAL:HG23 | 14       | 0.1           |
| (1,874)  | 1:89:A:GLN:HA   | 1:92:A:LEU:HD21  | 7        | 0.1           |
| (1,874)  | 1:89:A:GLN:HA   | 1:92:A:LEU:HD22  | 7        | 0.1           |
| (1,874)  | 1:89:A:GLN:HA   | 1:92:A:LEU:HD23  | 7        | 0.1           |
| (1,854)  | 1:53:A:PRO:HB2  | 1:126:A:VAL:HA   | 5        | 0.1           |
| (1,724)  | 1:58:A:ILE:HB   | 1:63:A:GLU:HB2   | 17       | 0.1           |
| (1,724)  | 1:58:A:ILE:HB   | 1:63:A:GLU:HB3   | 17       | 0.1           |
| (1,689)  | 1:29:A:VAL:HG21 | 1:53:A:PRO:HD3   | 10       | 0.1           |
| (1,689)  | 1:29:A:VAL:HG22 | 1:53:A:PRO:HD3   | 10       | 0.1           |
| (1,689)  | 1:29:A:VAL:HG23 | 1:53:A:PRO:HD3   | 10       | 0.1           |
| (1,658)  | 1:129:A:LEU:HG  | 1:130:A:GLU:HG2  | 7        | 0.1           |
| (1,658)  | 1:129:A:LEU:HG  | 1:130:A:GLU:HG3  | 7        | 0.1           |
| (1,500)  | 1:23:A:LEU:HG   | 1:31:A:THR:HG21  | 7        | 0.1           |
| (1,500)  | 1:23:A:LEU:HG   | 1:31:A:THR:HG22  | 7        | 0.1           |
| (1,500)  | 1:23:A:LEU:HG   | 1:31:A:THR:HG23  | 7        | 0.1           |
| (1,453)  | 1:80:A:VAL:H    | 1:104:A:VAL:HG21 | 11       | 0.1           |
| (1,453)  | 1:80:A:VAL:H    | 1:104:A:VAL:HG22 | 11       | 0.1           |
| (1,453)  | 1:80:A:VAL:H    | 1:104:A:VAL:HG23 | 11       | 0.1           |
| (1,282)  | 1:97:A:GLU:H    | 1:98:A:GLN:HB2   | 15       | 0.1           |
| (1,282)  | 1:97:A:GLU:H    | 1:98:A:GLN:HB3   | 15       | 0.1           |
| (1,154)  | 1:36:A:ASP:H    | 1:40:A:VAL:H     | 10       | 0.1           |
| (1,154)  | 1:36:A:ASP:H    | 1:40:A:VAL:H     | 16       | 0.1           |

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

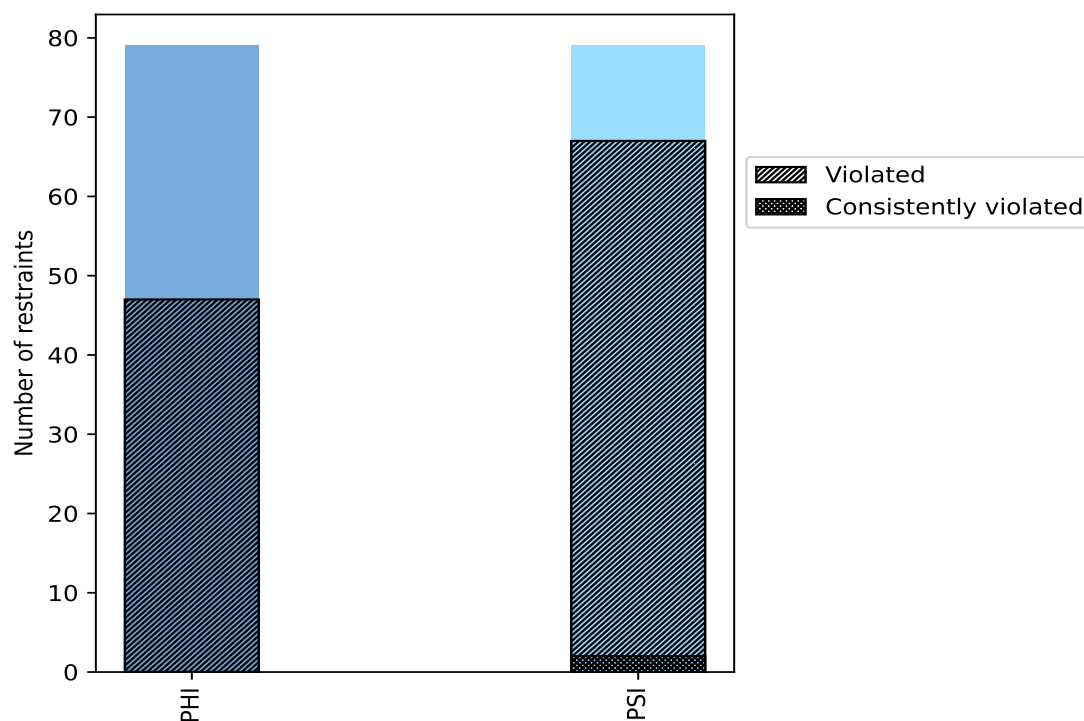
### 10.1 Summary of dihedral-angle violations [i](#)

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

| Angle type | Count | % <sup>1</sup> | Violated <sup>3</sup> |                |                | Consistently Violated <sup>4</sup> |                |                |
|------------|-------|----------------|-----------------------|----------------|----------------|------------------------------------|----------------|----------------|
|            |       |                | Count                 | % <sup>2</sup> | % <sup>1</sup> | Count                              | % <sup>2</sup> | % <sup>1</sup> |
| PHI        | 79    | 50.0           | 47                    | 59.5           | 29.7           | 0                                  | 0.0            | 0.0            |
| PSI        | 79    | 50.0           | 67                    | 84.8           | 42.4           | 2                                  | 2.5            | 1.3            |
| Total      | 158   | 100.0          | 114                   | 72.2           | 72.2           | 2                                  | 1.3            | 1.3            |

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

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



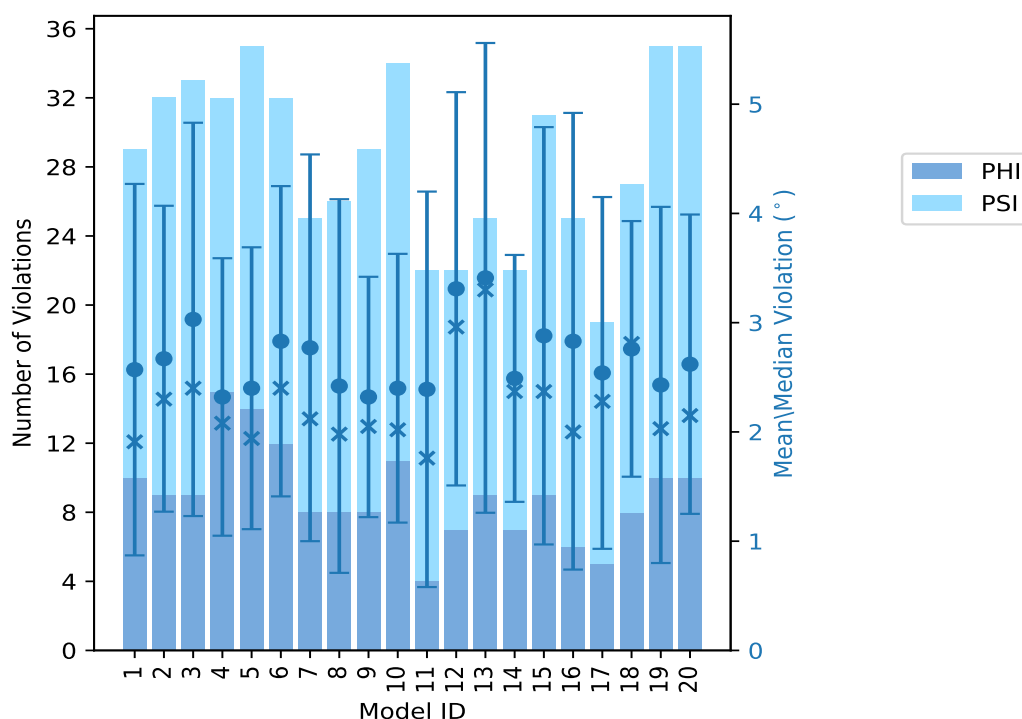
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

## 10.2 Dihedral-angle violation statistics for each model ⓘ

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

| Model ID | Number of violations |     |       | Mean (°) | Max (°) | SD (°) | Median (°) |
|----------|----------------------|-----|-------|----------|---------|--------|------------|
|          | PHI                  | PSI | Total |          |         |        |            |
| 1        | 10                   | 19  | 29    | 2.57     | 9.84    | 1.7    | 1.91       |
| 2        | 9                    | 23  | 32    | 2.67     | 5.86    | 1.4    | 2.3        |
| 3        | 9                    | 24  | 33    | 3.03     | 7.95    | 1.8    | 2.4        |
| 4        | 15                   | 17  | 32    | 2.32     | 7.59    | 1.27   | 2.08       |
| 5        | 14                   | 21  | 35    | 2.4      | 7.02    | 1.29   | 1.94       |
| 6        | 12                   | 20  | 32    | 2.83     | 6.11    | 1.42   | 2.4        |
| 7        | 8                    | 17  | 25    | 2.77     | 7.18    | 1.77   | 2.12       |
| 8        | 8                    | 18  | 26    | 2.42     | 9.85    | 1.71   | 1.98       |
| 9        | 8                    | 21  | 29    | 2.32     | 5.29    | 1.1    | 2.05       |
| 10       | 11                   | 23  | 34    | 2.4      | 6.48    | 1.23   | 2.02       |
| 11       | 4                    | 18  | 22    | 2.39     | 9.15    | 1.81   | 1.76       |
| 12       | 7                    | 15  | 22    | 3.31     | 9.06    | 1.8    | 2.96       |
| 13       | 9                    | 16  | 25    | 3.41     | 9.51    | 2.15   | 3.3        |
| 14       | 7                    | 15  | 22    | 2.49     | 5.62    | 1.13   | 2.37       |
| 15       | 9                    | 22  | 31    | 2.88     | 9.97    | 1.91   | 2.37       |
| 16       | 6                    | 19  | 25    | 2.83     | 10.86   | 2.09   | 2.0        |
| 17       | 5                    | 14  | 19    | 2.54     | 8.71    | 1.61   | 2.28       |
| 18       | 8                    | 19  | 27    | 2.76     | 5.43    | 1.17   | 2.81       |
| 19       | 10                   | 25  | 35    | 2.43     | 8.29    | 1.63   | 2.03       |
| 20       | 10                   | 25  | 35    | 2.62     | 6.29    | 1.37   | 2.15       |

### 10.2.1 Bar graph : Dihedral violation statistics for each model [i](#)



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

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

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

| Number of violated restraints |     |       | Fraction of the ensemble |      |
|-------------------------------|-----|-------|--------------------------|------|
| PHI                           | PSI | Total | Count <sup>1</sup>       | %    |
| 17                            | 12  | 29    | 1                        | 5.0  |
| 7                             | 7   | 14    | 2                        | 10.0 |
| 6                             | 8   | 14    | 3                        | 15.0 |
| 3                             | 9   | 12    | 4                        | 20.0 |
| 3                             | 6   | 9     | 5                        | 25.0 |
| 3                             | 3   | 6     | 6                        | 30.0 |
| 0                             | 1   | 1     | 7                        | 35.0 |
| 3                             | 3   | 6     | 8                        | 40.0 |
| 0                             | 4   | 4     | 9                        | 45.0 |
| 3                             | 2   | 5     | 10                       | 50.0 |
| 0                             | 3   | 3     | 11                       | 55.0 |

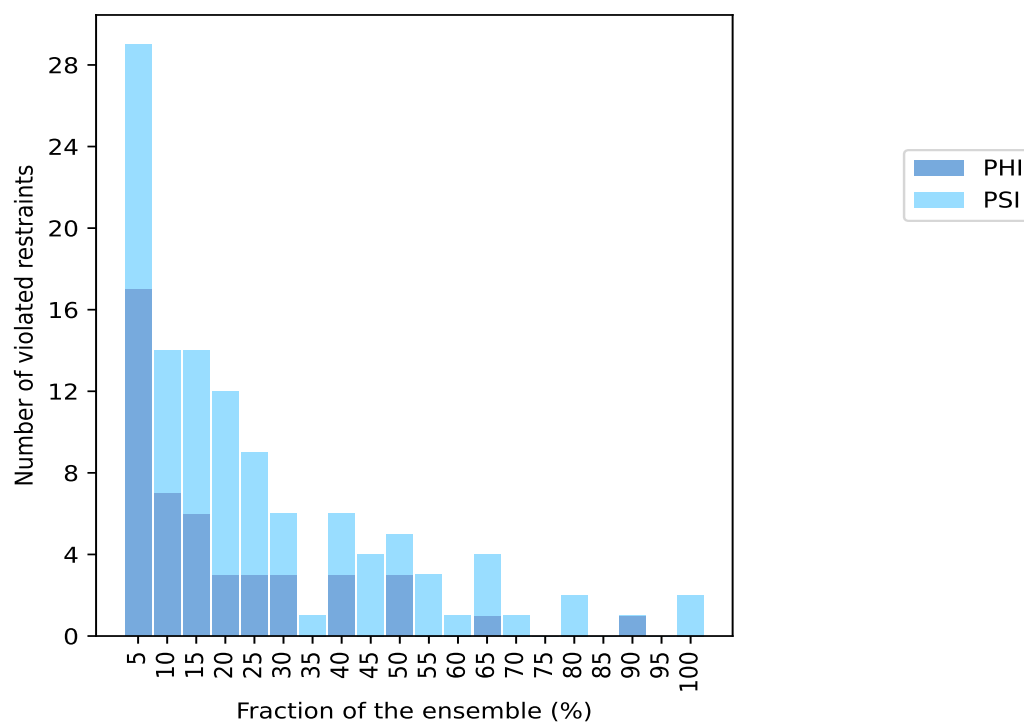
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| Number of violated restraints |     |       | Fraction of the ensemble |       |
|-------------------------------|-----|-------|--------------------------|-------|
| PHI                           | PSI | Total | Count <sup>1</sup>       | %     |
| 0                             | 1   | 1     | 12                       | 60.0  |
| 1                             | 3   | 4     | 13                       | 65.0  |
| 0                             | 1   | 1     | 14                       | 70.0  |
| 0                             | 0   | 0     | 15                       | 75.0  |
| 0                             | 2   | 2     | 16                       | 80.0  |
| 0                             | 0   | 0     | 17                       | 85.0  |
| 1                             | 0   | 1     | 18                       | 90.0  |
| 0                             | 0   | 0     | 19                       | 95.0  |
| 0                             | 2   | 2     | 20                       | 100.0 |

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

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

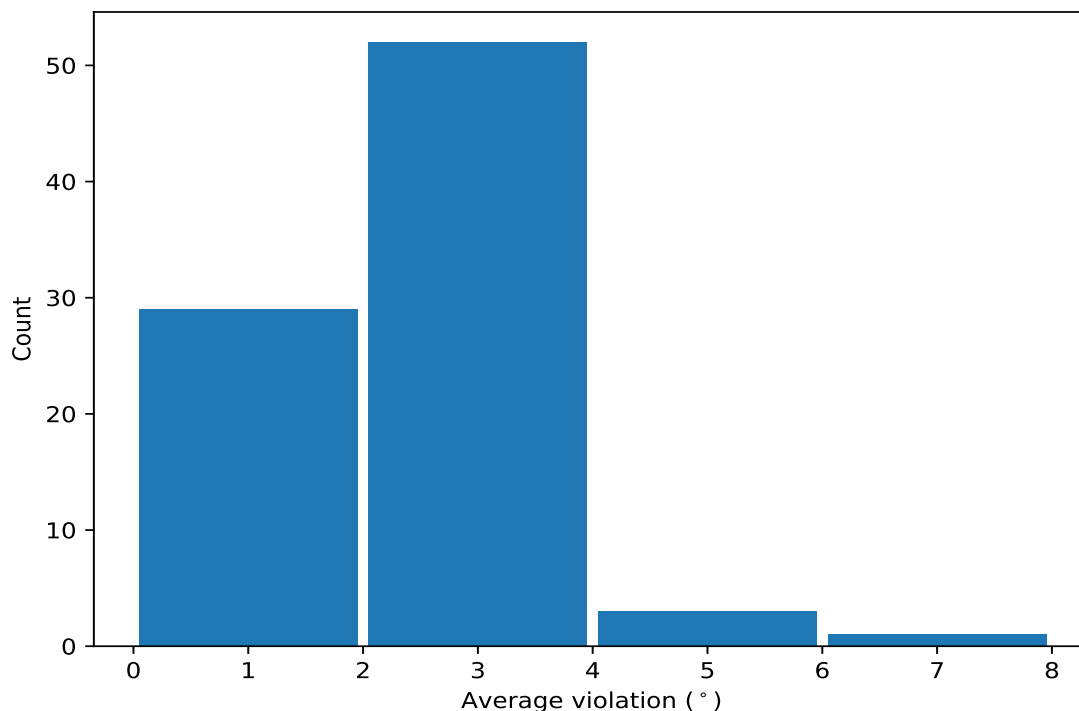


## 10.4 Most violated dihedral-angle restraints in the ensemble ⓘ

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

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

in the ensemble



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

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

| Key     | Atom-1        | Atom-2         | Atom-3        | Atom-4        | Models <sup>1</sup> | Mean | SD <sup>2</sup> | Median |
|---------|---------------|----------------|---------------|---------------|---------------------|------|-----------------|--------|
| (1,70)  | 1:62:A:TYR:N  | 1:62:A:TYR:CA  | 1:62:A:TYR:C  | 1:63:A:GLU:N  | 20                  | 7.46 | 2.0             | 7.44   |
| (1,2)   | 1:4:A:VAL:N   | 1:4:A:VAL:CA   | 1:4:A:VAL:C   | 1:5:A:VAL:N   | 20                  | 4.24 | 1.17            | 4.05   |
| (1,7)   | 1:6:A:ILE:C   | 1:7:A:VAL:N    | 1:7:A:VAL:CA  | 1:7:A:VAL:C   | 18                  | 3.31 | 1.05            | 3.2    |
| (1,98)  | 1:81:A:LEU:N  | 1:81:A:LEU:CA  | 1:81:A:LEU:C  | 1:82:A:VAL:N  | 16                  | 3.01 | 1.16            | 3.1    |
| (1,12)  | 1:13:A:ARG:N  | 1:13:A:ARG:CA  | 1:13:A:ARG:C  | 1:14:A:ILE:N  | 16                  | 1.97 | 0.82            | 1.9    |
| (1,102) | 1:83:A:ILE:N  | 1:83:A:ILE:CA  | 1:83:A:ILE:C  | 1:84:A:LYS:N  | 14                  | 3.08 | 1.81            | 2.64   |
| (1,100) | 1:82:A:VAL:N  | 1:82:A:VAL:CA  | 1:82:A:VAL:C  | 1:83:A:ILE:N  | 13                  | 3.88 | 1.18            | 4.38   |
| (1,132) | 1:107:A:ARG:N | 1:107:A:ARG:CA | 1:107:A:ARG:C | 1:108:A:VAL:N | 13                  | 3.41 | 1.4             | 2.92   |
| (1,105) | 1:84:A:LYS:C  | 1:85:A:VAL:N   | 1:85:A:VAL:CA | 1:85:A:VAL:C  | 13                  | 2.6  | 1.75            | 2.04   |
| (1,4)   | 1:5:A:VAL:N   | 1:5:A:VAL:CA   | 1:5:A:VAL:C   | 1:6:A:ILE:N   | 13                  | 2.47 | 0.97            | 2.28   |
| (1,78)  | 1:66:A:VAL:N  | 1:66:A:VAL:CA  | 1:66:A:VAL:C  | 1:67:A:ARG:N  | 12                  | 1.92 | 0.77            | 1.71   |
| (1,92)  | 1:73:A:ALA:N  | 1:73:A:ALA:CA  | 1:73:A:ALA:C  | 1:74:A:GLN:N  | 11                  | 2.48 | 1.23            | 2.16   |
| (1,22)  | 1:18:A:LEU:N  | 1:18:A:LEU:CA  | 1:18:A:LEU:C  | 1:19:A:LEU:N  | 11                  | 2.46 | 0.79            | 2.38   |
| (1,36)  | 1:32:A:VAL:N  | 1:32:A:VAL:CA  | 1:32:A:VAL:C  | 1:33:A:ARG:N  | 11                  | 2.46 | 0.88            | 2.56   |
| (1,101) | 1:82:A:VAL:C  | 1:83:A:ILE:N   | 1:83:A:ILE:CA | 1:83:A:ILE:C  | 10                  | 2.78 | 1.28            | 2.72   |
| (1,95)  | 1:79:A:ARG:C  | 1:80:A:VAL:N   | 1:80:A:VAL:CA | 1:80:A:VAL:C  | 10                  | 2.73 | 1.09            | 2.74   |
| (1,72)  | 1:63:A:GLU:N  | 1:63:A:GLU:CA  | 1:63:A:GLU:C  | 1:64:A:GLU:N  | 10                  | 2.72 | 1.32            | 2.72   |
| (1,97)  | 1:80:A:VAL:C  | 1:81:A:LEU:N   | 1:81:A:LEU:CA | 1:81:A:LEU:C  | 10                  | 2.27 | 0.95            | 2.1    |
| (1,116) | 1:94:A:ARG:N  | 1:94:A:ARG:CA  | 1:94:A:ARG:C  | 1:95:A:PHE:N  | 10                  | 2.22 | 0.73            | 2.23   |
| (1,134) | 1:108:A:VAL:N | 1:108:A:VAL:CA | 1:108:A:VAL:C | 1:109:A:THR:N | 9                   | 2.56 | 1.28            | 2.3    |

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| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Models <sup>1</sup> | Mean | SD <sup>2</sup> | Median |
|---------|---------------|----------------|----------------|---------------|---------------------|------|-----------------|--------|
| (1,136) | 1:113:A:ASP:N | 1:113:A:ASP:CA | 1:113:A:ASP:C  | 1:114:A:GLU:N | 9                   | 2.36 | 0.76            | 2.11   |
| (1,130) | 1:106:A:VAL:N | 1:106:A:VAL:CA | 1:106:A:VAL:C  | 1:107:A:ARG:N | 9                   | 2.31 | 0.82            | 2.34   |
| (1,62)  | 1:55:A:VAL:N  | 1:55:A:VAL:CA  | 1:55:A:VAL:C   | 1:56:A:ILE:N  | 9                   | 2.02 | 0.8             | 1.87   |
| (1,104) | 1:84:A:LYS:N  | 1:84:A:LYS:CA  | 1:84:A:LYS:C   | 1:85:A:VAL:N  | 8                   | 4.21 | 1.58            | 4.7    |
| (1,71)  | 1:62:A:TYR:C  | 1:63:A:GLU:N   | 1:63:A:GLU:CA  | 1:63:A:GLU:C  | 8                   | 2.61 | 0.81            | 2.57   |
| (1,76)  | 1:65:A:VAL:N  | 1:65:A:VAL:CA  | 1:65:A:VAL:C   | 1:66:A:VAL:N  | 8                   | 2.31 | 1.42            | 1.86   |
| (1,146) | 1:118:A:ARG:N | 1:118:A:ARG:CA | 1:118:A:ARG:C  | 1:119:A:LEU:N | 8                   | 2.25 | 1.41            | 1.86   |
| (1,73)  | 1:63:A:GLU:C  | 1:64:A:GLU:N   | 1:64:A:GLU:CA  | 1:64:A:GLU:C  | 8                   | 2.08 | 0.97            | 1.84   |
| (1,65)  | 1:56:A:ILE:C  | 1:57:A:PHE:N   | 1:57:A:PHE:CA  | 1:57:A:PHE:C  | 8                   | 2.07 | 0.77            | 1.88   |
| (1,60)  | 1:48:A:ARG:N  | 1:48:A:ARG:CA  | 1:48:A:ARG:C   | 1:49:A:LYS:N  | 7                   | 1.94 | 0.6             | 1.88   |
| (1,108) | 1:90:A:GLU:N  | 1:90:A:GLU:CA  | 1:90:A:GLU:C   | 1:91:A:LEU:N  | 6                   | 2.51 | 1.52            | 2.0    |
| (1,133) | 1:107:A:ARG:C | 1:108:A:VAL:N  | 1:108:A:VAL:CA | 1:108:A:VAL:C | 6                   | 2.22 | 0.8             | 2.11   |
| (1,58)  | 1:47:A:ALA:N  | 1:47:A:ALA:CA  | 1:47:A:ALA:C   | 1:48:A:ARG:N  | 6                   | 2.2  | 1.22            | 1.6    |
| (1,117) | 1:94:A:ARG:C  | 1:95:A:PHE:N   | 1:95:A:PHE:CA  | 1:95:A:PHE:C  | 6                   | 2.15 | 0.56            | 1.93   |
| (1,26)  | 1:20:A:GLU:N  | 1:20:A:GLU:CA  | 1:20:A:GLU:C   | 1:21:A:VAL:N  | 6                   | 1.86 | 0.71            | 1.68   |
| (1,119) | 1:95:A:PHE:C  | 1:96:A:TYR:N   | 1:96:A:TYR:CA  | 1:96:A:TYR:C  | 6                   | 1.21 | 0.13            | 1.17   |
| (1,50)  | 1:43:A:GLU:N  | 1:43:A:GLU:CA  | 1:43:A:GLU:C   | 1:44:A:ILE:N  | 5                   | 5.28 | 3.15            | 4.51   |
| (1,38)  | 1:33:A:ARG:N  | 1:33:A:ARG:CA  | 1:33:A:ARG:C   | 1:34:A:THR:N  | 5                   | 3.33 | 1.39            | 3.51   |
| (1,103) | 1:83:A:ILE:C  | 1:84:A:LYS:N   | 1:84:A:LYS:CA  | 1:84:A:LYS:C  | 5                   | 2.9  | 0.78            | 3.04   |
| (1,84)  | 1:69:A:ILE:N  | 1:69:A:ILE:CA  | 1:69:A:ILE:C   | 1:70:A:VAL:N  | 5                   | 2.44 | 0.9             | 2.81   |
| (1,126) | 1:99:A:LEU:N  | 1:99:A:LEU:CA  | 1:99:A:LEU:C   | 1:100:A:LYS:N | 5                   | 2.04 | 0.27            | 2.22   |
| (1,129) | 1:105:A:ASP:C | 1:106:A:VAL:N  | 1:106:A:VAL:CA | 1:106:A:VAL:C | 5                   | 1.94 | 0.37            | 1.87   |
| (1,77)  | 1:65:A:VAL:C  | 1:66:A:VAL:N   | 1:66:A:VAL:CA  | 1:66:A:VAL:C  | 5                   | 1.8  | 0.77            | 1.54   |
| (1,20)  | 1:17:A:GLU:N  | 1:17:A:GLU:CA  | 1:17:A:GLU:C   | 1:18:A:LEU:N  | 5                   | 1.78 | 0.4             | 1.65   |
| (1,158) | 1:124:A:GLU:N | 1:124:A:GLU:CA | 1:124:A:GLU:C  | 1:125:A:LYS:N | 5                   | 1.46 | 0.23            | 1.5    |
| (1,110) | 1:91:A:LEU:N  | 1:91:A:LEU:CA  | 1:91:A:LEU:C   | 1:92:A:LEU:N  | 4                   | 3.24 | 0.49            | 3.16   |
| (1,74)  | 1:64:A:GLU:N  | 1:64:A:GLU:CA  | 1:64:A:GLU:C   | 1:65:A:VAL:N  | 4                   | 2.99 | 0.62            | 3.18   |
| (1,154) | 1:122:A:LEU:N | 1:122:A:LEU:CA | 1:122:A:LEU:C  | 1:123:A:LEU:N | 4                   | 2.87 | 1.21            | 2.42   |
| (1,152) | 1:121:A:GLU:N | 1:121:A:GLU:CA | 1:121:A:GLU:C  | 1:122:A:LEU:N | 4                   | 2.77 | 0.95            | 2.94   |
| (1,79)  | 1:66:A:VAL:C  | 1:67:A:ARG:N   | 1:67:A:ARG:CA  | 1:67:A:ARG:C  | 4                   | 2.57 | 1.52            | 1.71   |
| (1,144) | 1:117:A:LYS:N | 1:117:A:LYS:CA | 1:117:A:LYS:C  | 1:118:A:ARG:N | 4                   | 2.47 | 0.29            | 2.49   |
| (1,114) | 1:93:A:GLU:N  | 1:93:A:GLU:CA  | 1:93:A:GLU:C   | 1:94:A:ARG:N  | 4                   | 2.26 | 0.77            | 2.31   |
| (1,35)  | 1:31:A:THR:C  | 1:32:A:VAL:N   | 1:32:A:VAL:CA  | 1:32:A:VAL:C  | 4                   | 2.25 | 1.04            | 2.24   |
| (1,96)  | 1:80:A:VAL:N  | 1:80:A:VAL:CA  | 1:80:A:VAL:C   | 1:81:A:LEU:N  | 4                   | 1.97 | 0.58            | 2.1    |
| (1,48)  | 1:42:A:GLU:N  | 1:42:A:GLU:CA  | 1:42:A:GLU:C   | 1:43:A:GLU:N  | 4                   | 1.78 | 0.8             | 1.5    |
| (1,131) | 1:106:A:VAL:C | 1:107:A:ARG:N  | 1:107:A:ARG:CA | 1:107:A:ARG:C | 4                   | 1.74 | 0.99            | 1.23   |
| (1,8)   | 1:7:A:VAL:N   | 1:7:A:VAL:CA   | 1:7:A:VAL:C    | 1:8:A:VAL:N   | 4                   | 1.56 | 0.48            | 1.44   |
| (1,111) | 1:91:A:LEU:C  | 1:92:A:LEU:N   | 1:92:A:LEU:CA  | 1:92:A:LEU:C  | 3                   | 3.02 | 1.62            | 2.17   |
| (1,86)  | 1:70:A:VAL:N  | 1:70:A:VAL:CA  | 1:70:A:VAL:C   | 1:71:A:GLU:N  | 3                   | 2.38 | 0.81            | 2.2    |
| (1,28)  | 1:21:A:VAL:N  | 1:21:A:VAL:CA  | 1:21:A:VAL:C   | 1:22:A:VAL:N  | 3                   | 2.29 | 0.96            | 2.29   |
| (1,156) | 1:123:A:LEU:N | 1:123:A:LEU:CA | 1:123:A:LEU:C  | 1:124:A:GLU:N | 3                   | 2.23 | 1.19            | 1.53   |
| (1,81)  | 1:67:A:ARG:C  | 1:68:A:ASP:N   | 1:68:A:ASP:CA  | 1:68:A:ASP:C  | 3                   | 2.2  | 0.94            | 1.81   |
| (1,142) | 1:116:A:LYS:N | 1:116:A:LYS:CA | 1:116:A:LYS:C  | 1:117:A:LYS:N | 3                   | 2.02 | 0.52            | 1.98   |
| (1,99)  | 1:81:A:LEU:C  | 1:82:A:VAL:N   | 1:82:A:VAL:CA  | 1:82:A:VAL:C  | 3                   | 1.74 | 0.14            | 1.73   |
| (1,1)   | 1:3:A:THR:C   | 1:4:A:VAL:N    | 1:4:A:VAL:CA   | 1:4:A:VAL:C   | 3                   | 1.73 | 0.47            | 2.05   |
| (1,64)  | 1:56:A:ILE:N  | 1:56:A:ILE:CA  | 1:56:A:ILE:C   | 1:57:A:PHE:N  | 3                   | 1.65 | 0.42            | 1.68   |
| (1,124) | 1:98:A:GLN:N  | 1:98:A:GLN:CA  | 1:98:A:GLN:C   | 1:99:A:LEU:N  | 3                   | 1.63 | 0.44            | 1.92   |
| (1,138) | 1:114:A:GLU:N | 1:114:A:GLU:CA | 1:114:A:GLU:C  | 1:115:A:ALA:N | 3                   | 1.58 | 0.31            | 1.72   |
| (1,151) | 1:120:A:LYS:C | 1:121:A:GLU:N  | 1:121:A:GLU:CA | 1:121:A:GLU:C | 3                   | 1.58 | 0.37            | 1.56   |
| (1,128) | 1:100:A:LYS:N | 1:100:A:LYS:CA | 1:100:A:LYS:C  | 1:101:A:LYS:N | 3                   | 1.49 | 0.3             | 1.36   |
| (1,141) | 1:115:A:ALA:C | 1:116:A:LYS:N  | 1:116:A:LYS:CA | 1:116:A:LYS:C | 3                   | 1.49 | 0.36            | 1.5    |

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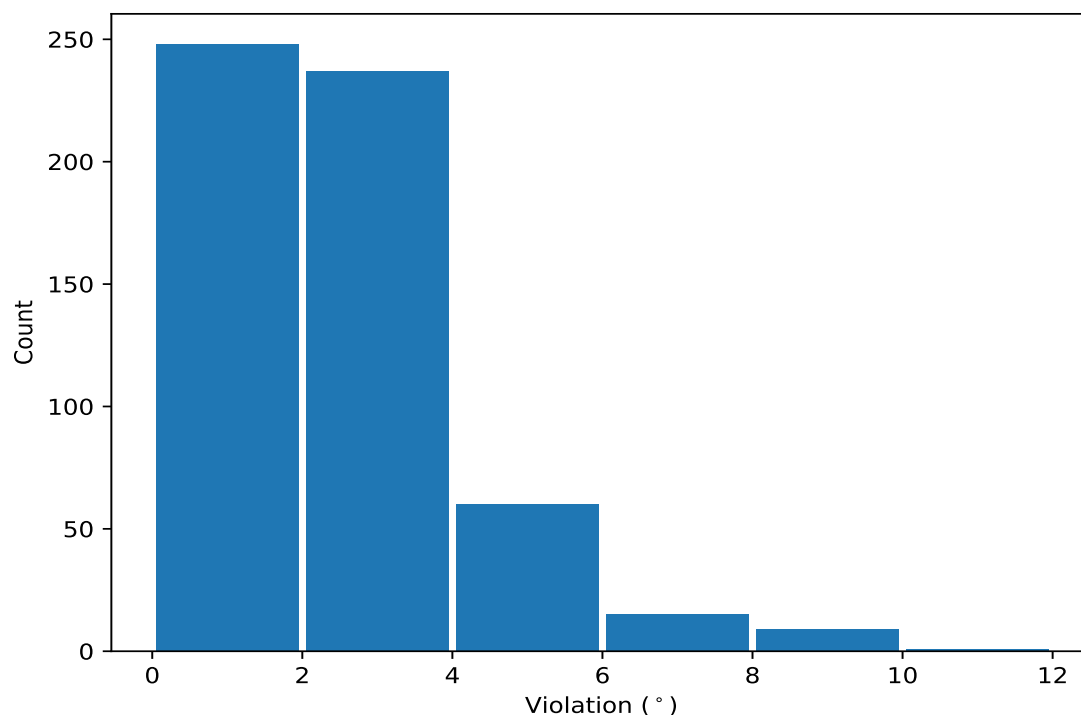
| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Models <sup>1</sup> | Mean | SD <sup>2</sup> | Median |
|---------|---------------|----------------|----------------|---------------|---------------------|------|-----------------|--------|
| (1,44)  | 1:40:A:VAL:N  | 1:40:A:VAL:CA  | 1:40:A:VAL:C   | 1:41:A:LYS:N  | 2                   | 3.89 | 0.62            | 3.89   |
| (1,153) | 1:121:A:GLU:C | 1:122:A:LEU:N  | 1:122:A:LEU:CA | 1:122:A:LEU:C | 2                   | 2.69 | 0.7             | 2.69   |
| (1,56)  | 1:46:A:LYS:N  | 1:46:A:LYS:CA  | 1:46:A:LYS:C   | 1:47:A:ALA:N  | 2                   | 2.64 | 0.7             | 2.64   |
| (1,120) | 1:96:A:TYR:N  | 1:96:A:TYR:CA  | 1:96:A:TYR:C   | 1:97:A:GLU:N  | 2                   | 2.28 | 0.56            | 2.28   |
| (1,59)  | 1:47:A:ALA:C  | 1:48:A:ARG:N   | 1:48:A:ARG:CA  | 1:48:A:ARG:C  | 2                   | 2.17 | 0.72            | 2.17   |
| (1,148) | 1:119:A:LEU:N | 1:119:A:LEU:CA | 1:119:A:LEU:C  | 1:120:A:LYS:N | 2                   | 2.02 | 0.39            | 2.02   |
| (1,94)  | 1:74:A:GLN:N  | 1:74:A:GLN:CA  | 1:74:A:GLN:C   | 1:75:A:LYS:N  | 2                   | 1.81 | 0.72            | 1.81   |
| (1,140) | 1:115:A:ALA:N | 1:115:A:ALA:CA | 1:115:A:ALA:C  | 1:116:A:LYS:N | 2                   | 1.64 | 0.54            | 1.64   |
| (1,107) | 1:89:A:GLN:C  | 1:90:A:GLU:N   | 1:90:A:GLU:CA  | 1:90:A:GLU:C  | 2                   | 1.53 | 0.44            | 1.53   |
| (1,49)  | 1:42:A:GLU:C  | 1:43:A:GLU:N   | 1:43:A:GLU:CA  | 1:43:A:GLU:C  | 2                   | 1.48 | 0.44            | 1.48   |
| (1,85)  | 1:69:A:ILE:C  | 1:70:A:VAL:N   | 1:70:A:VAL:CA  | 1:70:A:VAL:C  | 2                   | 1.27 | 0.0             | 1.27   |
| (1,135) | 1:112:A:GLU:C | 1:113:A:ASP:N  | 1:113:A:ASP:CA | 1:113:A:ASP:C | 2                   | 1.26 | 0.07            | 1.26   |
| (1,39)  | 1:37:A:LYS:C  | 1:38:A:GLU:N   | 1:38:A:GLU:CA  | 1:38:A:GLU:C  | 2                   | 1.2  | 0.17            | 1.2    |
| (1,6)   | 1:6:A:ILE:N   | 1:6:A:ILE:CA   | 1:6:A:ILE:C    | 1:7:A:VAL:N   | 2                   | 1.13 | 0.08            | 1.13   |

<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 (°) |
|---------|---------------|----------------|---------------|---------------|----------|---------------|
| (1,70)  | 1:62:A:TYR:N  | 1:62:A:TYR:CA  | 1:62:A:TYR:C  | 1:63:A:GLU:N  | 16       | 10.86         |
| (1,70)  | 1:62:A:TYR:N  | 1:62:A:TYR:CA  | 1:62:A:TYR:C  | 1:63:A:GLU:N  | 15       | 9.97          |
| (1,70)  | 1:62:A:TYR:N  | 1:62:A:TYR:CA  | 1:62:A:TYR:C  | 1:63:A:GLU:N  | 8        | 9.85          |
| (1,70)  | 1:62:A:TYR:N  | 1:62:A:TYR:CA  | 1:62:A:TYR:C  | 1:63:A:GLU:N  | 1        | 9.84          |
| (1,50)  | 1:43:A:GLU:N  | 1:43:A:GLU:CA  | 1:43:A:GLU:C  | 1:44:A:ILE:N  | 13       | 9.51          |
| (1,70)  | 1:62:A:TYR:N  | 1:62:A:TYR:CA  | 1:62:A:TYR:C  | 1:63:A:GLU:N  | 11       | 9.15          |
| (1,70)  | 1:62:A:TYR:N  | 1:62:A:TYR:CA  | 1:62:A:TYR:C  | 1:63:A:GLU:N  | 12       | 9.06          |
| (1,70)  | 1:62:A:TYR:N  | 1:62:A:TYR:CA  | 1:62:A:TYR:C  | 1:63:A:GLU:N  | 17       | 8.71          |
| (1,70)  | 1:62:A:TYR:N  | 1:62:A:TYR:CA  | 1:62:A:TYR:C  | 1:63:A:GLU:N  | 13       | 8.41          |
| (1,50)  | 1:43:A:GLU:N  | 1:43:A:GLU:CA  | 1:43:A:GLU:C  | 1:44:A:ILE:N  | 19       | 8.29          |
| (1,70)  | 1:62:A:TYR:N  | 1:62:A:TYR:CA  | 1:62:A:TYR:C  | 1:63:A:GLU:N  | 3        | 7.95          |
| (1,70)  | 1:62:A:TYR:N  | 1:62:A:TYR:CA  | 1:62:A:TYR:C  | 1:63:A:GLU:N  | 4        | 7.59          |
| (1,70)  | 1:62:A:TYR:N  | 1:62:A:TYR:CA  | 1:62:A:TYR:C  | 1:63:A:GLU:N  | 19       | 7.28          |
| (1,70)  | 1:62:A:TYR:N  | 1:62:A:TYR:CA  | 1:62:A:TYR:C  | 1:63:A:GLU:N  | 7        | 7.18          |
| (1,70)  | 1:62:A:TYR:N  | 1:62:A:TYR:CA  | 1:62:A:TYR:C  | 1:63:A:GLU:N  | 5        | 7.02          |
| (1,105) | 1:84:A:LYS:C  | 1:85:A:VAL:N   | 1:85:A:VAL:CA | 1:85:A:VAL:C  | 7        | 6.85          |
| (1,70)  | 1:62:A:TYR:N  | 1:62:A:TYR:CA  | 1:62:A:TYR:C  | 1:63:A:GLU:N  | 10       | 6.48          |
| (1,102) | 1:83:A:ILE:N  | 1:83:A:ILE:CA  | 1:83:A:ILE:C  | 1:84:A:LYS:N  | 3        | 6.45          |
| (1,2)   | 1:4:A:VAL:N   | 1:4:A:VAL:CA   | 1:4:A:VAL:C   | 1:5:A:VAL:N   | 19       | 6.42          |
| (1,2)   | 1:4:A:VAL:N   | 1:4:A:VAL:CA   | 1:4:A:VAL:C   | 1:5:A:VAL:N   | 20       | 6.29          |
| (1,102) | 1:83:A:ILE:N  | 1:83:A:ILE:CA  | 1:83:A:ILE:C  | 1:84:A:LYS:N  | 12       | 6.22          |
| (1,102) | 1:83:A:ILE:N  | 1:83:A:ILE:CA  | 1:83:A:ILE:C  | 1:84:A:LYS:N  | 6        | 6.11          |
| (1,105) | 1:84:A:LYS:C  | 1:85:A:VAL:N   | 1:85:A:VAL:CA | 1:85:A:VAL:C  | 3        | 6.1           |
| (1,72)  | 1:63:A:GLU:N  | 1:63:A:GLU:CA  | 1:63:A:GLU:C  | 1:64:A:GLU:N  | 15       | 6.06          |
| (1,104) | 1:84:A:LYS:N  | 1:84:A:LYS:CA  | 1:84:A:LYS:C  | 1:85:A:VAL:N  | 3        | 6.05          |
| (1,70)  | 1:62:A:TYR:N  | 1:62:A:TYR:CA  | 1:62:A:TYR:C  | 1:63:A:GLU:N  | 6        | 5.99          |
| (1,104) | 1:84:A:LYS:N  | 1:84:A:LYS:CA  | 1:84:A:LYS:C  | 1:85:A:VAL:N  | 7        | 5.97          |
| (1,100) | 1:82:A:VAL:N  | 1:82:A:VAL:CA  | 1:82:A:VAL:C  | 1:83:A:ILE:N  | 13       | 5.87          |
| (1,76)  | 1:65:A:VAL:N  | 1:65:A:VAL:CA  | 1:65:A:VAL:C  | 1:66:A:VAL:N  | 2        | 5.86          |
| (1,2)   | 1:4:A:VAL:N   | 1:4:A:VAL:CA   | 1:4:A:VAL:C   | 1:5:A:VAL:N   | 16       | 5.82          |
| (1,132) | 1:107:A:ARG:N | 1:107:A:ARG:CA | 1:107:A:ARG:C | 1:108:A:VAL:N | 15       | 5.78          |
| (1,2)   | 1:4:A:VAL:N   | 1:4:A:VAL:CA   | 1:4:A:VAL:C   | 1:5:A:VAL:N   | 13       | 5.63          |
| (1,70)  | 1:62:A:TYR:N  | 1:62:A:TYR:CA  | 1:62:A:TYR:C  | 1:63:A:GLU:N  | 14       | 5.62          |
| (1,146) | 1:118:A:ARG:N | 1:118:A:ARG:CA | 1:118:A:ARG:C | 1:119:A:LEU:N | 10       | 5.54          |
| (1,134) | 1:108:A:VAL:N | 1:108:A:VAL:CA | 1:108:A:VAL:C | 1:109:A:THR:N | 16       | 5.53          |
| (1,108) | 1:90:A:GLU:N  | 1:90:A:GLU:CA  | 1:90:A:GLU:C  | 1:91:A:LEU:N  | 12       | 5.45          |
| (1,132) | 1:107:A:ARG:N | 1:107:A:ARG:CA | 1:107:A:ARG:C | 1:108:A:VAL:N | 20       | 5.43          |
| (1,70)  | 1:62:A:TYR:N  | 1:62:A:TYR:CA  | 1:62:A:TYR:C  | 1:63:A:GLU:N  | 18       | 5.43          |
| (1,2)   | 1:4:A:VAL:N   | 1:4:A:VAL:CA   | 1:4:A:VAL:C   | 1:5:A:VAL:N   | 3        | 5.43          |
| (1,38)  | 1:33:A:ARG:N  | 1:33:A:ARG:CA  | 1:33:A:ARG:C  | 1:34:A:THR:N  | 20       | 5.42          |
| (1,111) | 1:91:A:LEU:C  | 1:92:A:LEU:N   | 1:92:A:LEU:CA | 1:92:A:LEU:C  | 9        | 5.29          |
| (1,79)  | 1:66:A:VAL:C  | 1:67:A:ARG:N   | 1:67:A:ARG:CA | 1:67:A:ARG:C  | 3        | 5.2           |
| (1,101) | 1:82:A:VAL:C  | 1:83:A:ILE:N   | 1:83:A:ILE:CA | 1:83:A:ILE:C  | 1        | 5.12          |
| (1,132) | 1:107:A:ARG:N | 1:107:A:ARG:CA | 1:107:A:ARG:C | 1:108:A:VAL:N | 6        | 5.1           |
| (1,2)   | 1:4:A:VAL:N   | 1:4:A:VAL:CA   | 1:4:A:VAL:C   | 1:5:A:VAL:N   | 11       | 5.07          |
| (1,104) | 1:84:A:LYS:N  | 1:84:A:LYS:CA  | 1:84:A:LYS:C  | 1:85:A:VAL:N  | 2        | 4.96          |
| (1,92)  | 1:73:A:ALA:N  | 1:73:A:ALA:CA  | 1:73:A:ALA:C  | 1:74:A:GLN:N  | 2        | 4.95          |

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| Key     | Atom-1        | Atom-2         | Atom-3        | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|---------------|---------------|----------|---------------|
| (1,7)   | 1:6:A:ILE:C   | 1:7:A:VAL:N    | 1:7:A:VAL:CA  | 1:7:A:VAL:C   | 2        | 4.95          |
| (1,104) | 1:84:A:LYS:N  | 1:84:A:LYS:CA  | 1:84:A:LYS:C  | 1:85:A:VAL:N  | 6        | 4.89          |
| (1,70)  | 1:62:A:TYR:N  | 1:62:A:TYR:CA  | 1:62:A:TYR:C  | 1:63:A:GLU:N  | 20       | 4.88          |
| (1,2)   | 1:4:A:VAL:N   | 1:4:A:VAL:CA   | 1:4:A:VAL:C   | 1:5:A:VAL:N   | 12       | 4.87          |
| (1,7)   | 1:6:A:ILE:C   | 1:7:A:VAL:N    | 1:7:A:VAL:CA  | 1:7:A:VAL:C   | 5        | 4.82          |
| (1,154) | 1:122:A:LEU:N | 1:122:A:LEU:CA | 1:122:A:LEU:C | 1:123:A:LEU:N | 6        | 4.81          |
| (1,95)  | 1:79:A:ARG:C  | 1:80:A:VAL:N   | 1:80:A:VAL:CA | 1:80:A:VAL:C  | 8        | 4.75          |
| (1,100) | 1:82:A:VAL:N  | 1:82:A:VAL:CA  | 1:82:A:VAL:C  | 1:83:A:ILE:N  | 9        | 4.74          |
| (1,98)  | 1:81:A:LEU:N  | 1:81:A:LEU:CA  | 1:81:A:LEU:C  | 1:82:A:VAL:N  | 7        | 4.74          |
| (1,98)  | 1:81:A:LEU:N  | 1:81:A:LEU:CA  | 1:81:A:LEU:C  | 1:82:A:VAL:N  | 2        | 4.72          |
| (1,100) | 1:82:A:VAL:N  | 1:82:A:VAL:CA  | 1:82:A:VAL:C  | 1:83:A:ILE:N  | 3        | 4.71          |
| (1,100) | 1:82:A:VAL:N  | 1:82:A:VAL:CA  | 1:82:A:VAL:C  | 1:83:A:ILE:N  | 7        | 4.71          |
| (1,98)  | 1:81:A:LEU:N  | 1:81:A:LEU:CA  | 1:81:A:LEU:C  | 1:82:A:VAL:N  | 13       | 4.7           |
| (1,7)   | 1:6:A:ILE:C   | 1:7:A:VAL:N    | 1:7:A:VAL:CA  | 1:7:A:VAL:C   | 15       | 4.68          |
| (1,7)   | 1:6:A:ILE:C   | 1:7:A:VAL:N    | 1:7:A:VAL:CA  | 1:7:A:VAL:C   | 18       | 4.68          |
| (1,70)  | 1:62:A:TYR:N  | 1:62:A:TYR:CA  | 1:62:A:TYR:C  | 1:63:A:GLU:N  | 2        | 4.65          |
| (1,4)   | 1:5:A:VAL:N   | 1:5:A:VAL:CA   | 1:5:A:VAL:C   | 1:6:A:ILE:N   | 15       | 4.63          |
| (1,100) | 1:82:A:VAL:N  | 1:82:A:VAL:CA  | 1:82:A:VAL:C  | 1:83:A:ILE:N  | 16       | 4.57          |
| (1,44)  | 1:40:A:VAL:N  | 1:40:A:VAL:CA  | 1:40:A:VAL:C  | 1:41:A:LYS:N  | 20       | 4.52          |
| (1,50)  | 1:43:A:GLU:N  | 1:43:A:GLU:CA  | 1:43:A:GLU:C  | 1:44:A:ILE:N  | 3        | 4.51          |
| (1,104) | 1:84:A:LYS:N  | 1:84:A:LYS:CA  | 1:84:A:LYS:C  | 1:85:A:VAL:N  | 13       | 4.5           |
| (1,100) | 1:82:A:VAL:N  | 1:82:A:VAL:CA  | 1:82:A:VAL:C  | 1:83:A:ILE:N  | 20       | 4.46          |
| (1,100) | 1:82:A:VAL:N  | 1:82:A:VAL:CA  | 1:82:A:VAL:C  | 1:83:A:ILE:N  | 2        | 4.38          |
| (1,22)  | 1:18:A:LEU:N  | 1:18:A:LEU:CA  | 1:18:A:LEU:C  | 1:19:A:LEU:N  | 5        | 4.37          |
| (1,92)  | 1:73:A:ALA:N  | 1:73:A:ALA:CA  | 1:73:A:ALA:C  | 1:74:A:GLN:N  | 13       | 4.36          |
| (1,101) | 1:82:A:VAL:C  | 1:83:A:ILE:N   | 1:83:A:ILE:CA | 1:83:A:ILE:C  | 12       | 4.35          |
| (1,7)   | 1:6:A:ILE:C   | 1:7:A:VAL:N    | 1:7:A:VAL:CA  | 1:7:A:VAL:C   | 6        | 4.29          |
| (1,132) | 1:107:A:ARG:N | 1:107:A:ARG:CA | 1:107:A:ARG:C | 1:108:A:VAL:N | 18       | 4.28          |
| (1,58)  | 1:47:A:ALA:N  | 1:47:A:ALA:CA  | 1:47:A:ALA:C  | 1:48:A:ARG:N  | 15       | 4.23          |
| (1,2)   | 1:4:A:VAL:N   | 1:4:A:VAL:CA   | 1:4:A:VAL:C   | 1:5:A:VAL:N   | 18       | 4.2           |
| (1,132) | 1:107:A:ARG:N | 1:107:A:ARG:CA | 1:107:A:ARG:C | 1:108:A:VAL:N | 13       | 4.19          |
| (1,12)  | 1:13:A:ARG:N  | 1:13:A:ARG:CA  | 1:13:A:ARG:C  | 1:14:A:ILE:N  | 16       | 4.18          |
| (1,73)  | 1:63:A:GLU:C  | 1:64:A:GLU:N   | 1:64:A:GLU:CA | 1:64:A:GLU:C  | 15       | 4.12          |
| (1,2)   | 1:4:A:VAL:N   | 1:4:A:VAL:CA   | 1:4:A:VAL:C   | 1:5:A:VAL:N   | 8        | 4.08          |
| (1,2)   | 1:4:A:VAL:N   | 1:4:A:VAL:CA   | 1:4:A:VAL:C   | 1:5:A:VAL:N   | 4        | 4.07          |
| (1,98)  | 1:81:A:LEU:N  | 1:81:A:LEU:CA  | 1:81:A:LEU:C  | 1:82:A:VAL:N  | 9        | 4.03          |
| (1,2)   | 1:4:A:VAL:N   | 1:4:A:VAL:CA   | 1:4:A:VAL:C   | 1:5:A:VAL:N   | 6        | 4.03          |
| (1,38)  | 1:33:A:ARG:N  | 1:33:A:ARG:CA  | 1:33:A:ARG:C  | 1:34:A:THR:N  | 5        | 4.02          |
| (1,110) | 1:91:A:LEU:N  | 1:91:A:LEU:CA  | 1:91:A:LEU:C  | 1:92:A:LEU:N  | 13       | 3.99          |
| (1,136) | 1:113:A:ASP:N | 1:113:A:ASP:CA | 1:113:A:ASP:C | 1:114:A:GLU:N | 20       | 3.95          |
| (1,71)  | 1:62:A:TYR:C  | 1:63:A:GLU:N   | 1:63:A:GLU:CA | 1:63:A:GLU:C  | 12       | 3.95          |
| (1,2)   | 1:4:A:VAL:N   | 1:4:A:VAL:CA   | 1:4:A:VAL:C   | 1:5:A:VAL:N   | 15       | 3.94          |
| (1,132) | 1:107:A:ARG:N | 1:107:A:ARG:CA | 1:107:A:ARG:C | 1:108:A:VAL:N | 1        | 3.93          |
| (1,97)  | 1:80:A:VAL:C  | 1:81:A:LEU:N   | 1:81:A:LEU:CA | 1:81:A:LEU:C  | 3        | 3.92          |
| (1,156) | 1:123:A:LEU:N | 1:123:A:LEU:CA | 1:123:A:LEU:C | 1:124:A:GLU:N | 2        | 3.91          |
| (1,152) | 1:121:A:GLU:N | 1:121:A:GLU:CA | 1:121:A:GLU:C | 1:122:A:LEU:N | 15       | 3.9           |
| (1,2)   | 1:4:A:VAL:N   | 1:4:A:VAL:CA   | 1:4:A:VAL:C   | 1:5:A:VAL:N   | 10       | 3.89          |
| (1,7)   | 1:6:A:ILE:C   | 1:7:A:VAL:N    | 1:7:A:VAL:CA  | 1:7:A:VAL:C   | 14       | 3.86          |
| (1,95)  | 1:79:A:ARG:C  | 1:80:A:VAL:N   | 1:80:A:VAL:CA | 1:80:A:VAL:C  | 16       | 3.83          |
| (1,36)  | 1:32:A:VAL:N  | 1:32:A:VAL:CA  | 1:32:A:VAL:C  | 1:33:A:ARG:N  | 7        | 3.83          |
| (1,101) | 1:82:A:VAL:C  | 1:83:A:ILE:N   | 1:83:A:ILE:CA | 1:83:A:ILE:C  | 18       | 3.82          |

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| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,98)  | 1:81:A:LEU:N  | 1:81:A:LEU:CA  | 1:81:A:LEU:C   | 1:82:A:VAL:N  | 17       | 3.79          |
| (1,7)   | 1:6:A:ILE:C   | 1:7:A:VAL:N    | 1:7:A:VAL:CA   | 1:7:A:VAL:C   | 10       | 3.79          |
| (1,4)   | 1:5:A:VAL:N   | 1:5:A:VAL:CA   | 1:5:A:VAL:C    | 1:6:A:ILE:N   | 6        | 3.79          |
| (1,62)  | 1:55:A:VAL:N  | 1:55:A:VAL:CA  | 1:55:A:VAL:C   | 1:56:A:ILE:N  | 18       | 3.76          |
| (1,100) | 1:82:A:VAL:N  | 1:82:A:VAL:CA  | 1:82:A:VAL:C   | 1:83:A:ILE:N  | 11       | 3.75          |
| (1,95)  | 1:79:A:ARG:C  | 1:80:A:VAL:N   | 1:80:A:VAL:CA  | 1:80:A:VAL:C  | 4        | 3.75          |
| (1,7)   | 1:6:A:ILE:C   | 1:7:A:VAL:N    | 1:7:A:VAL:CA   | 1:7:A:VAL:C   | 4        | 3.73          |
| (1,97)  | 1:80:A:VAL:C  | 1:81:A:LEU:N   | 1:81:A:LEU:CA  | 1:81:A:LEU:C  | 14       | 3.72          |
| (1,65)  | 1:56:A:ILE:C  | 1:57:A:PHE:N   | 1:57:A:PHE:CA  | 1:57:A:PHE:C  | 14       | 3.71          |
| (1,134) | 1:108:A:VAL:N | 1:108:A:VAL:CA | 1:108:A:VAL:C  | 1:109:A:THR:N | 1        | 3.69          |
| (1,103) | 1:83:A:ILE:C  | 1:84:A:LYS:N   | 1:84:A:LYS:CA  | 1:84:A:LYS:C  | 6        | 3.69          |
| (1,36)  | 1:32:A:VAL:N  | 1:32:A:VAL:CA  | 1:32:A:VAL:C   | 1:33:A:ARG:N  | 1        | 3.67          |
| (1,2)   | 1:4:A:VAL:N   | 1:4:A:VAL:CA   | 1:4:A:VAL:C    | 1:5:A:VAL:N   | 1        | 3.67          |
| (1,98)  | 1:81:A:LEU:N  | 1:81:A:LEU:CA  | 1:81:A:LEU:C   | 1:82:A:VAL:N  | 18       | 3.62          |
| (1,78)  | 1:66:A:VAL:N  | 1:66:A:VAL:CA  | 1:66:A:VAL:C   | 1:67:A:ARG:N  | 3        | 3.62          |
| (1,74)  | 1:64:A:GLU:N  | 1:64:A:GLU:CA  | 1:64:A:GLU:C   | 1:65:A:VAL:N  | 12       | 3.62          |
| (1,133) | 1:107:A:ARG:C | 1:108:A:VAL:N  | 1:108:A:VAL:CA | 1:108:A:VAL:C | 5        | 3.6           |
| (1,116) | 1:94:A:ARG:N  | 1:94:A:ARG:CA  | 1:94:A:ARG:C   | 1:95:A:PHE:N  | 18       | 3.58          |
| (1,130) | 1:106:A:VAL:N | 1:106:A:VAL:CA | 1:106:A:VAL:C  | 1:107:A:ARG:N | 12       | 3.57          |
| (1,100) | 1:82:A:VAL:N  | 1:82:A:VAL:CA  | 1:82:A:VAL:C   | 1:83:A:ILE:N  | 4        | 3.57          |
| (1,102) | 1:83:A:ILE:N  | 1:83:A:ILE:CA  | 1:83:A:ILE:C   | 1:84:A:LYS:N  | 18       | 3.55          |
| (1,58)  | 1:47:A:ALA:N  | 1:47:A:ALA:CA  | 1:47:A:ALA:C   | 1:48:A:ARG:N  | 10       | 3.51          |
| (1,38)  | 1:33:A:ARG:N  | 1:33:A:ARG:CA  | 1:33:A:ARG:C   | 1:34:A:THR:N  | 13       | 3.51          |
| (1,81)  | 1:67:A:ARG:C  | 1:68:A:ASP:N   | 1:68:A:ASP:CA  | 1:68:A:ASP:C  | 10       | 3.49          |
| (1,130) | 1:106:A:VAL:N | 1:106:A:VAL:CA | 1:106:A:VAL:C  | 1:107:A:ARG:N | 5        | 3.47          |
| (1,35)  | 1:31:A:THR:C  | 1:32:A:VAL:N   | 1:32:A:VAL:CA  | 1:32:A:VAL:C  | 1        | 3.47          |
| (1,28)  | 1:21:A:VAL:N  | 1:21:A:VAL:CA  | 1:21:A:VAL:C   | 1:22:A:VAL:N  | 1        | 3.47          |
| (1,131) | 1:106:A:VAL:C | 1:107:A:ARG:N  | 1:107:A:ARG:CA | 1:107:A:ARG:C | 10       | 3.44          |
| (1,98)  | 1:81:A:LEU:N  | 1:81:A:LEU:CA  | 1:81:A:LEU:C   | 1:82:A:VAL:N  | 5        | 3.44          |
| (1,86)  | 1:70:A:VAL:N  | 1:70:A:VAL:CA  | 1:70:A:VAL:C   | 1:71:A:GLU:N  | 14       | 3.44          |
| (1,84)  | 1:69:A:ILE:N  | 1:69:A:ILE:CA  | 1:69:A:ILE:C   | 1:70:A:VAL:N  | 3        | 3.42          |
| (1,153) | 1:121:A:GLU:C | 1:122:A:LEU:N  | 1:122:A:LEU:CA | 1:122:A:LEU:C | 10       | 3.39          |
| (1,26)  | 1:20:A:GLU:N  | 1:20:A:GLU:CA  | 1:20:A:GLU:C   | 1:21:A:VAL:N  | 13       | 3.38          |
| (1,102) | 1:83:A:ILE:N  | 1:83:A:ILE:CA  | 1:83:A:ILE:C   | 1:84:A:LYS:N  | 11       | 3.37          |
| (1,70)  | 1:62:A:TYR:N  | 1:62:A:TYR:CA  | 1:62:A:TYR:C   | 1:63:A:GLU:N  | 9        | 3.36          |
| (1,103) | 1:83:A:ILE:C  | 1:84:A:LYS:N   | 1:84:A:LYS:CA  | 1:84:A:LYS:C  | 2        | 3.33          |
| (1,56)  | 1:46:A:LYS:N  | 1:46:A:LYS:CA  | 1:46:A:LYS:C   | 1:47:A:ALA:N  | 3        | 3.33          |
| (1,72)  | 1:63:A:GLU:N  | 1:63:A:GLU:CA  | 1:63:A:GLU:C   | 1:64:A:GLU:N  | 13       | 3.32          |
| (1,7)   | 1:6:A:ILE:C   | 1:7:A:VAL:N    | 1:7:A:VAL:CA   | 1:7:A:VAL:C   | 9        | 3.31          |
| (1,77)  | 1:65:A:VAL:C  | 1:66:A:VAL:N   | 1:66:A:VAL:CA  | 1:66:A:VAL:C  | 6        | 3.3           |
| (1,74)  | 1:64:A:GLU:N  | 1:64:A:GLU:CA  | 1:64:A:GLU:C   | 1:65:A:VAL:N  | 6        | 3.3           |
| (1,4)   | 1:5:A:VAL:N   | 1:5:A:VAL:CA   | 1:5:A:VAL:C    | 1:6:A:ILE:N   | 13       | 3.3           |
| (1,108) | 1:90:A:GLU:N  | 1:90:A:GLU:CA  | 1:90:A:GLU:C   | 1:91:A:LEU:N  | 4        | 3.29          |
| (1,104) | 1:84:A:LYS:N  | 1:84:A:LYS:CA  | 1:84:A:LYS:C   | 1:85:A:VAL:N  | 11       | 3.27          |
| (1,44)  | 1:40:A:VAL:N  | 1:40:A:VAL:CA  | 1:40:A:VAL:C   | 1:41:A:LYS:N  | 18       | 3.27          |
| (1,71)  | 1:62:A:TYR:C  | 1:63:A:GLU:N   | 1:63:A:GLU:CA  | 1:63:A:GLU:C  | 15       | 3.26          |
| (1,12)  | 1:13:A:ARG:N  | 1:13:A:ARG:CA  | 1:13:A:ARG:C   | 1:14:A:ILE:N  | 14       | 3.26          |
| (1,2)   | 1:4:A:VAL:N   | 1:4:A:VAL:CA   | 1:4:A:VAL:C    | 1:5:A:VAL:N   | 17       | 3.26          |
| (1,100) | 1:82:A:VAL:N  | 1:82:A:VAL:CA  | 1:82:A:VAL:C   | 1:83:A:ILE:N  | 15       | 3.24          |
| (1,117) | 1:94:A:ARG:C  | 1:95:A:PHE:N   | 1:95:A:PHE:CA  | 1:95:A:PHE:C  | 6        | 3.23          |
| (1,84)  | 1:69:A:ILE:N  | 1:69:A:ILE:CA  | 1:69:A:ILE:C   | 1:70:A:VAL:N  | 5        | 3.23          |

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| Key     | Atom-1        | Atom-2         | Atom-3        | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|---------------|---------------|----------|---------------|
| (1,98)  | 1:81:A:LEU:N  | 1:81:A:LEU:CA  | 1:81:A:LEU:C  | 1:82:A:VAL:N  | 20       | 3.22          |
| (1,71)  | 1:62:A:TYR:C  | 1:63:A:GLU:N   | 1:63:A:GLU:CA | 1:63:A:GLU:C  | 20       | 3.22          |
| (1,60)  | 1:48:A:ARG:N  | 1:48:A:ARG:CA  | 1:48:A:ARG:C  | 1:49:A:LYS:N  | 18       | 3.22          |
| (1,110) | 1:91:A:LEU:N  | 1:91:A:LEU:CA  | 1:91:A:LEU:C  | 1:92:A:LEU:N  | 9        | 3.2           |
| (1,136) | 1:113:A:ASP:N | 1:113:A:ASP:CA | 1:113:A:ASP:C | 1:114:A:GLU:N | 9        | 3.19          |
| (1,152) | 1:121:A:GLU:N | 1:121:A:GLU:CA | 1:121:A:GLU:C | 1:122:A:LEU:N | 1        | 3.18          |
| (1,92)  | 1:73:A:ALA:N  | 1:73:A:ALA:CA  | 1:73:A:ALA:C  | 1:74:A:GLN:N  | 19       | 3.18          |
| (1,110) | 1:91:A:LEU:N  | 1:91:A:LEU:CA  | 1:91:A:LEU:C  | 1:92:A:LEU:N  | 4        | 3.13          |
| (1,105) | 1:84:A:LYS:C  | 1:85:A:VAL:N   | 1:85:A:VAL:CA | 1:85:A:VAL:C  | 2        | 3.13          |
| (1,92)  | 1:73:A:ALA:N  | 1:73:A:ALA:CA  | 1:73:A:ALA:C  | 1:74:A:GLN:N  | 10       | 3.13          |
| (1,100) | 1:82:A:VAL:N  | 1:82:A:VAL:CA  | 1:82:A:VAL:C  | 1:83:A:ILE:N  | 19       | 3.1           |
| (1,95)  | 1:79:A:ARG:C  | 1:80:A:VAL:N   | 1:80:A:VAL:CA | 1:80:A:VAL:C  | 9        | 3.09          |
| (1,7)   | 1:6:A:ILE:C   | 1:7:A:VAL:N    | 1:7:A:VAL:CA  | 1:7:A:VAL:C   | 11       | 3.09          |
| (1,35)  | 1:31:A:THR:C  | 1:32:A:VAL:N   | 1:32:A:VAL:CA | 1:32:A:VAL:C  | 20       | 3.08          |
| (1,116) | 1:94:A:ARG:N  | 1:94:A:ARG:CA  | 1:94:A:ARG:C  | 1:95:A:PHE:N  | 5        | 3.07          |
| (1,48)  | 1:42:A:GLU:N  | 1:42:A:GLU:CA  | 1:42:A:GLU:C  | 1:43:A:GLU:N  | 2        | 3.07          |
| (1,22)  | 1:18:A:LEU:N  | 1:18:A:LEU:CA  | 1:18:A:LEU:C  | 1:19:A:LEU:N  | 20       | 3.07          |
| (1,2)   | 1:4:A:VAL:N   | 1:4:A:VAL:CA   | 1:4:A:VAL:C   | 1:5:A:VAL:N   | 14       | 3.07          |
| (1,74)  | 1:64:A:GLU:N  | 1:64:A:GLU:CA  | 1:64:A:GLU:C  | 1:65:A:VAL:N  | 3        | 3.06          |
| (1,103) | 1:83:A:ILE:C  | 1:84:A:LYS:N   | 1:84:A:LYS:CA | 1:84:A:LYS:C  | 15       | 3.04          |
| (1,146) | 1:118:A:ARG:N | 1:118:A:ARG:CA | 1:118:A:ARG:C | 1:119:A:LEU:N | 18       | 3.03          |
| (1,114) | 1:93:A:GLU:N  | 1:93:A:GLU:CA  | 1:93:A:GLU:C  | 1:94:A:ARG:N  | 2        | 3.03          |
| (1,78)  | 1:66:A:VAL:N  | 1:66:A:VAL:CA  | 1:66:A:VAL:C  | 1:67:A:ARG:N  | 17       | 3.03          |
| (1,114) | 1:93:A:GLU:N  | 1:93:A:GLU:CA  | 1:93:A:GLU:C  | 1:94:A:ARG:N  | 19       | 3.02          |
| (1,104) | 1:84:A:LYS:N  | 1:84:A:LYS:CA  | 1:84:A:LYS:C  | 1:85:A:VAL:N  | 15       | 3.02          |
| (1,103) | 1:83:A:ILE:C  | 1:84:A:LYS:N   | 1:84:A:LYS:CA | 1:84:A:LYS:C  | 3        | 3.02          |
| (1,2)   | 1:4:A:VAL:N   | 1:4:A:VAL:CA   | 1:4:A:VAL:C   | 1:5:A:VAL:N   | 5        | 3.02          |
| (1,95)  | 1:79:A:ARG:C  | 1:80:A:VAL:N   | 1:80:A:VAL:CA | 1:80:A:VAL:C  | 5        | 3.01          |
| (1,72)  | 1:63:A:GLU:N  | 1:63:A:GLU:CA  | 1:63:A:GLU:C  | 1:64:A:GLU:N  | 12       | 2.99          |
| (1,22)  | 1:18:A:LEU:N  | 1:18:A:LEU:CA  | 1:18:A:LEU:C  | 1:19:A:LEU:N  | 16       | 2.99          |
| (1,154) | 1:122:A:LEU:N | 1:122:A:LEU:CA | 1:122:A:LEU:C | 1:123:A:LEU:N | 12       | 2.98          |
| (1,62)  | 1:55:A:VAL:N  | 1:55:A:VAL:CA  | 1:55:A:VAL:C  | 1:56:A:ILE:N  | 7        | 2.98          |
| (1,2)   | 1:4:A:VAL:N   | 1:4:A:VAL:CA   | 1:4:A:VAL:C   | 1:5:A:VAL:N   | 9        | 2.98          |
| (1,98)  | 1:81:A:LEU:N  | 1:81:A:LEU:CA  | 1:81:A:LEU:C  | 1:82:A:VAL:N  | 12       | 2.97          |
| (1,36)  | 1:32:A:VAL:N  | 1:32:A:VAL:CA  | 1:32:A:VAL:C  | 1:33:A:ARG:N  | 12       | 2.96          |
| (1,21)  | 1:17:A:GLU:C  | 1:18:A:LEU:N   | 1:18:A:LEU:CA | 1:18:A:LEU:C  | 6        | 2.93          |
| (1,132) | 1:107:A:ARG:N | 1:107:A:ARG:CA | 1:107:A:ARG:C | 1:108:A:VAL:N | 14       | 2.92          |
| (1,101) | 1:82:A:VAL:C  | 1:83:A:ILE:N   | 1:83:A:ILE:CA | 1:83:A:ILE:C  | 5        | 2.92          |
| (1,101) | 1:82:A:VAL:C  | 1:83:A:ILE:N   | 1:83:A:ILE:CA | 1:83:A:ILE:C  | 8        | 2.91          |
| (1,71)  | 1:62:A:TYR:C  | 1:63:A:GLU:N   | 1:63:A:GLU:CA | 1:63:A:GLU:C  | 16       | 2.91          |
| (1,72)  | 1:63:A:GLU:N  | 1:63:A:GLU:CA  | 1:63:A:GLU:C  | 1:64:A:GLU:N  | 14       | 2.9           |
| (1,59)  | 1:47:A:ALA:C  | 1:48:A:ARG:N   | 1:48:A:ARG:CA | 1:48:A:ARG:C  | 17       | 2.9           |
| (1,130) | 1:106:A:VAL:N | 1:106:A:VAL:CA | 1:106:A:VAL:C | 1:107:A:ARG:N | 7        | 2.86          |
| (1,4)   | 1:5:A:VAL:N   | 1:5:A:VAL:CA   | 1:5:A:VAL:C   | 1:6:A:ILE:N   | 18       | 2.85          |
| (1,97)  | 1:80:A:VAL:C  | 1:81:A:LEU:N   | 1:81:A:LEU:CA | 1:81:A:LEU:C  | 19       | 2.84          |
| (1,7)   | 1:6:A:ILE:C   | 1:7:A:VAL:N    | 1:7:A:VAL:CA  | 1:7:A:VAL:C   | 19       | 2.84          |
| (1,120) | 1:96:A:TYR:N  | 1:96:A:TYR:CA  | 1:96:A:TYR:C  | 1:97:A:GLU:N  | 20       | 2.83          |
| (1,84)  | 1:69:A:ILE:N  | 1:69:A:ILE:CA  | 1:69:A:ILE:C  | 1:70:A:VAL:N  | 18       | 2.81          |
| (1,144) | 1:117:A:LYS:N | 1:117:A:LYS:CA | 1:117:A:LYS:C | 1:118:A:ARG:N | 14       | 2.8           |
| (1,4)   | 1:5:A:VAL:N   | 1:5:A:VAL:CA   | 1:5:A:VAL:C   | 1:6:A:ILE:N   | 7        | 2.79          |
| (1,65)  | 1:56:A:ILE:C  | 1:57:A:PHE:N   | 1:57:A:PHE:CA | 1:57:A:PHE:C  | 18       | 2.77          |

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| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,50)  | 1:43:A:GLU:N  | 1:43:A:GLU:CA  | 1:43:A:GLU:C   | 1:44:A:ILE:N  | 8        | 2.77          |
| (1,36)  | 1:32:A:VAL:N  | 1:32:A:VAL:CA  | 1:32:A:VAL:C   | 1:33:A:ARG:N  | 9        | 2.76          |
| (1,73)  | 1:63:A:GLU:C  | 1:64:A:GLU:N   | 1:64:A:GLU:CA  | 1:64:A:GLU:C  | 13       | 2.75          |
| (1,72)  | 1:63:A:GLU:N  | 1:63:A:GLU:CA  | 1:63:A:GLU:C   | 1:64:A:GLU:N  | 11       | 2.75          |
| (1,144) | 1:117:A:LYS:N | 1:117:A:LYS:CA | 1:117:A:LYS:C  | 1:118:A:ARG:N | 12       | 2.72          |
| (1,132) | 1:107:A:ARG:N | 1:107:A:ARG:CA | 1:107:A:ARG:C  | 1:108:A:VAL:N | 8        | 2.72          |
| (1,152) | 1:121:A:GLU:N | 1:121:A:GLU:CA | 1:121:A:GLU:C  | 1:122:A:LEU:N | 12       | 2.71          |
| (1,134) | 1:108:A:VAL:N | 1:108:A:VAL:CA | 1:108:A:VAL:C  | 1:109:A:THR:N | 4        | 2.7           |
| (1,102) | 1:83:A:ILE:N  | 1:83:A:ILE:CA  | 1:83:A:ILE:C   | 1:84:A:LYS:N  | 20       | 2.7           |
| (1,102) | 1:83:A:ILE:N  | 1:83:A:ILE:CA  | 1:83:A:ILE:C   | 1:84:A:LYS:N  | 15       | 2.69          |
| (1,142) | 1:116:A:LYS:N | 1:116:A:LYS:CA | 1:116:A:LYS:C  | 1:117:A:LYS:N | 10       | 2.68          |
| (1,72)  | 1:63:A:GLU:N  | 1:63:A:GLU:CA  | 1:63:A:GLU:C   | 1:64:A:GLU:N  | 4        | 2.68          |
| (1,133) | 1:107:A:ARG:C | 1:108:A:VAL:N  | 1:108:A:VAL:CA | 1:108:A:VAL:C | 7        | 2.67          |
| (1,116) | 1:94:A:ARG:N  | 1:94:A:ARG:CA  | 1:94:A:ARG:C   | 1:95:A:PHE:N  | 6        | 2.67          |
| (1,76)  | 1:65:A:VAL:N  | 1:65:A:VAL:CA  | 1:65:A:VAL:C   | 1:66:A:VAL:N  | 5        | 2.67          |
| (1,36)  | 1:32:A:VAL:N  | 1:32:A:VAL:CA  | 1:32:A:VAL:C   | 1:33:A:ARG:N  | 6        | 2.67          |
| (1,22)  | 1:18:A:LEU:N  | 1:18:A:LEU:CA  | 1:18:A:LEU:C   | 1:19:A:LEU:N  | 2        | 2.66          |
| (1,2)   | 1:4:A:VAL:N   | 1:4:A:VAL:CA   | 1:4:A:VAL:C    | 1:5:A:VAL:N   | 7        | 2.65          |
| (1,132) | 1:107:A:ARG:N | 1:107:A:ARG:CA | 1:107:A:ARG:C  | 1:108:A:VAL:N | 10       | 2.64          |
| (1,110) | 1:91:A:LEU:N  | 1:91:A:LEU:CA  | 1:91:A:LEU:C   | 1:92:A:LEU:N  | 20       | 2.63          |
| (1,136) | 1:113:A:ASP:N | 1:113:A:ASP:CA | 1:113:A:ASP:C  | 1:114:A:GLU:N | 15       | 2.62          |
| (1,105) | 1:84:A:LYS:C  | 1:85:A:VAL:N   | 1:85:A:VAL:CA  | 1:85:A:VAL:C  | 13       | 2.61          |
| (1,129) | 1:105:A:ASP:C | 1:106:A:VAL:N  | 1:106:A:VAL:CA | 1:106:A:VAL:C | 5        | 2.59          |
| (1,97)  | 1:80:A:VAL:C  | 1:81:A:LEU:N   | 1:81:A:LEU:CA  | 1:81:A:LEU:C  | 10       | 2.59          |
| (1,102) | 1:83:A:ILE:N  | 1:83:A:ILE:CA  | 1:83:A:ILE:C   | 1:84:A:LYS:N  | 2        | 2.58          |
| (1,32)  | 1:23:A:LEU:N  | 1:23:A:LEU:CA  | 1:23:A:LEU:C   | 1:24:A:LYS:N  | 12       | 2.58          |
| (1,36)  | 1:32:A:VAL:N  | 1:32:A:VAL:CA  | 1:32:A:VAL:C   | 1:33:A:ARG:N  | 16       | 2.56          |
| (1,4)   | 1:5:A:VAL:N   | 1:5:A:VAL:CA   | 1:5:A:VAL:C    | 1:6:A:ILE:N   | 16       | 2.56          |
| (1,36)  | 1:32:A:VAL:N  | 1:32:A:VAL:CA  | 1:32:A:VAL:C   | 1:33:A:ARG:N  | 20       | 2.55          |
| (1,96)  | 1:80:A:VAL:N  | 1:80:A:VAL:CA  | 1:80:A:VAL:C   | 1:81:A:LEU:N  | 5        | 2.54          |
| (1,7)   | 1:6:A:ILE:C   | 1:7:A:VAL:N    | 1:7:A:VAL:CA   | 1:7:A:VAL:C   | 7        | 2.53          |
| (1,133) | 1:107:A:ARG:C | 1:108:A:VAL:N  | 1:108:A:VAL:CA | 1:108:A:VAL:C | 14       | 2.52          |
| (1,101) | 1:82:A:VAL:C  | 1:83:A:ILE:N   | 1:83:A:ILE:CA  | 1:83:A:ILE:C  | 4        | 2.52          |
| (1,94)  | 1:74:A:GLN:N  | 1:74:A:GLN:CA  | 1:74:A:GLN:C   | 1:75:A:LYS:N  | 8        | 2.52          |
| (1,102) | 1:83:A:ILE:N  | 1:83:A:ILE:CA  | 1:83:A:ILE:C   | 1:84:A:LYS:N  | 9        | 2.51          |
| (1,73)  | 1:63:A:GLU:C  | 1:64:A:GLU:N   | 1:64:A:GLU:CA  | 1:64:A:GLU:C  | 19       | 2.51          |
| (1,7)   | 1:6:A:ILE:C   | 1:7:A:VAL:N    | 1:7:A:VAL:CA   | 1:7:A:VAL:C   | 1        | 2.51          |
| (1,72)  | 1:63:A:GLU:N  | 1:63:A:GLU:CA  | 1:63:A:GLU:C   | 1:64:A:GLU:N  | 9        | 2.5           |
| (1,22)  | 1:18:A:LEU:N  | 1:18:A:LEU:CA  | 1:18:A:LEU:C   | 1:19:A:LEU:N  | 3        | 2.5           |
| (1,136) | 1:113:A:ASP:N | 1:113:A:ASP:CA | 1:113:A:ASP:C  | 1:114:A:GLU:N | 3        | 2.49          |
| (1,116) | 1:94:A:ARG:N  | 1:94:A:ARG:CA  | 1:94:A:ARG:C   | 1:95:A:PHE:N  | 19       | 2.49          |
| (1,98)  | 1:81:A:LEU:N  | 1:81:A:LEU:CA  | 1:81:A:LEU:C   | 1:82:A:VAL:N  | 10       | 2.49          |
| (1,96)  | 1:80:A:VAL:N  | 1:80:A:VAL:CA  | 1:80:A:VAL:C   | 1:81:A:LEU:N  | 8        | 2.49          |
| (1,117) | 1:94:A:ARG:C  | 1:95:A:PHE:N   | 1:95:A:PHE:CA  | 1:95:A:PHE:C  | 4        | 2.48          |
| (1,106) | 1:85:A:VAL:N  | 1:85:A:VAL:CA  | 1:85:A:VAL:C   | 1:86:A:ALA:N  | 18       | 2.48          |
| (1,2)   | 1:4:A:VAL:N   | 1:4:A:VAL:CA   | 1:4:A:VAL:C    | 1:5:A:VAL:N   | 2        | 2.48          |
| (1,95)  | 1:79:A:ARG:C  | 1:80:A:VAL:N   | 1:80:A:VAL:CA  | 1:80:A:VAL:C  | 17       | 2.47          |
| (1,134) | 1:108:A:VAL:N | 1:108:A:VAL:CA | 1:108:A:VAL:C  | 1:109:A:THR:N | 8        | 2.45          |
| (1,108) | 1:90:A:GLU:N  | 1:90:A:GLU:CA  | 1:90:A:GLU:C   | 1:91:A:LEU:N  | 19       | 2.45          |
| (1,7)   | 1:6:A:ILE:C   | 1:7:A:VAL:N    | 1:7:A:VAL:CA   | 1:7:A:VAL:C   | 16       | 2.45          |
| (1,12)  | 1:13:A:ARG:N  | 1:13:A:ARG:CA  | 1:13:A:ARG:C   | 1:14:A:ILE:N  | 17       | 2.44          |

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| Key     | Atom-1        | Atom-2         | Atom-3        | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|---------------|---------------|----------|---------------|
| (1,78)  | 1:66:A:VAL:N  | 1:66:A:VAL:CA  | 1:66:A:VAL:C  | 1:67:A:ARG:N  | 16       | 2.42          |
| (1,148) | 1:119:A:LEU:N | 1:119:A:LEU:CA | 1:119:A:LEU:C | 1:120:A:LYS:N | 10       | 2.41          |
| (1,116) | 1:94:A:ARG:N  | 1:94:A:ARG:CA  | 1:94:A:ARG:C  | 1:95:A:PHE:N  | 4        | 2.41          |
| (1,101) | 1:82:A:VAL:C  | 1:83:A:ILE:N   | 1:83:A:ILE:CA | 1:83:A:ILE:C  | 6        | 2.41          |
| (1,36)  | 1:32:A:VAL:N  | 1:32:A:VAL:CA  | 1:32:A:VAL:C  | 1:33:A:ARG:N  | 3        | 2.4           |
| (1,20)  | 1:17:A:GLU:N  | 1:17:A:GLU:CA  | 1:17:A:GLU:C  | 1:18:A:LEU:N  | 20       | 2.4           |
| (1,7)   | 1:6:A:ILE:C   | 1:7:A:VAL:N    | 1:7:A:VAL:CA  | 1:7:A:VAL:C   | 8        | 2.39          |
| (1,22)  | 1:18:A:LEU:N  | 1:18:A:LEU:CA  | 1:18:A:LEU:C  | 1:19:A:LEU:N  | 6        | 2.38          |
| (1,75)  | 1:64:A:GLU:C  | 1:65:A:VAL:N   | 1:65:A:VAL:CA | 1:65:A:VAL:C  | 15       | 2.37          |
| (1,130) | 1:106:A:VAL:N | 1:106:A:VAL:CA | 1:106:A:VAL:C | 1:107:A:ARG:N | 3        | 2.36          |
| (1,105) | 1:84:A:LYS:C  | 1:85:A:VAL:N   | 1:85:A:VAL:CA | 1:85:A:VAL:C  | 19       | 2.36          |
| (1,78)  | 1:66:A:VAL:N  | 1:66:A:VAL:CA  | 1:66:A:VAL:C  | 1:67:A:ARG:N  | 2        | 2.35          |
| (1,130) | 1:106:A:VAL:N | 1:106:A:VAL:CA | 1:106:A:VAL:C | 1:107:A:ARG:N | 6        | 2.34          |
| (1,8)   | 1:7:A:VAL:N   | 1:7:A:VAL:CA   | 1:7:A:VAL:C   | 1:8:A:VAL:N   | 10       | 2.34          |
| (1,126) | 1:99:A:LEU:N  | 1:99:A:LEU:CA  | 1:99:A:LEU:C  | 1:100:A:LYS:N | 8        | 2.32          |
| (1,12)  | 1:13:A:ARG:N  | 1:13:A:ARG:CA  | 1:13:A:ARG:C  | 1:14:A:ILE:N  | 19       | 2.32          |
| (1,146) | 1:118:A:ARG:N | 1:118:A:ARG:CA | 1:118:A:ARG:C | 1:119:A:LEU:N | 5        | 2.3           |
| (1,134) | 1:108:A:VAL:N | 1:108:A:VAL:CA | 1:108:A:VAL:C | 1:109:A:THR:N | 17       | 2.3           |
| (1,132) | 1:107:A:ARG:N | 1:107:A:ARG:CA | 1:107:A:ARG:C | 1:108:A:VAL:N | 17       | 2.3           |
| (1,28)  | 1:21:A:VAL:N  | 1:21:A:VAL:CA  | 1:21:A:VAL:C  | 1:22:A:VAL:N  | 6        | 2.29          |
| (1,105) | 1:84:A:LYS:C  | 1:85:A:VAL:N   | 1:85:A:VAL:CA | 1:85:A:VAL:C  | 17       | 2.28          |
| (1,4)   | 1:5:A:VAL:N   | 1:5:A:VAL:CA   | 1:5:A:VAL:C   | 1:6:A:ILE:N   | 11       | 2.28          |
| (1,38)  | 1:33:A:ARG:N  | 1:33:A:ARG:CA  | 1:33:A:ARG:C  | 1:34:A:THR:N  | 19       | 2.27          |
| (1,144) | 1:117:A:LYS:N | 1:117:A:LYS:CA | 1:117:A:LYS:C | 1:118:A:ARG:N | 15       | 2.26          |
| (1,92)  | 1:73:A:ALA:N  | 1:73:A:ALA:CA  | 1:73:A:ALA:C  | 1:74:A:GLN:N  | 17       | 2.25          |
| (1,146) | 1:118:A:ARG:N | 1:118:A:ARG:CA | 1:118:A:ARG:C | 1:119:A:LEU:N | 2        | 2.24          |
| (1,126) | 1:99:A:LEU:N  | 1:99:A:LEU:CA  | 1:99:A:LEU:C  | 1:100:A:LYS:N | 12       | 2.23          |
| (1,113) | 1:92:A:LEU:C  | 1:93:A:GLU:N   | 1:93:A:GLU:CA | 1:93:A:GLU:C  | 4        | 2.23          |
| (1,71)  | 1:62:A:TYR:C  | 1:63:A:GLU:N   | 1:63:A:GLU:CA | 1:63:A:GLU:C  | 3        | 2.23          |
| (1,126) | 1:99:A:LEU:N  | 1:99:A:LEU:CA  | 1:99:A:LEU:C  | 1:100:A:LYS:N | 14       | 2.22          |
| (1,12)  | 1:13:A:ARG:N  | 1:13:A:ARG:CA  | 1:13:A:ARG:C  | 1:14:A:ILE:N  | 1        | 2.21          |
| (1,134) | 1:108:A:VAL:N | 1:108:A:VAL:CA | 1:108:A:VAL:C | 1:109:A:THR:N | 20       | 2.2           |
| (1,97)  | 1:80:A:VAL:C  | 1:81:A:LEU:N   | 1:81:A:LEU:CA | 1:81:A:LEU:C  | 6        | 2.2           |
| (1,86)  | 1:70:A:VAL:N  | 1:70:A:VAL:CA  | 1:70:A:VAL:C  | 1:71:A:GLU:N  | 2        | 2.2           |
| (1,12)  | 1:13:A:ARG:N  | 1:13:A:ARG:CA  | 1:13:A:ARG:C  | 1:14:A:ILE:N  | 11       | 2.2           |
| (1,65)  | 1:56:A:ILE:C  | 1:57:A:PHE:N   | 1:57:A:PHE:CA | 1:57:A:PHE:C  | 6        | 2.19          |
| (1,12)  | 1:13:A:ARG:N  | 1:13:A:ARG:CA  | 1:13:A:ARG:C  | 1:14:A:ILE:N  | 10       | 2.19          |
| (1,140) | 1:115:A:ALA:N | 1:115:A:ALA:CA | 1:115:A:ALA:C | 1:116:A:LYS:N | 9        | 2.18          |
| (1,111) | 1:91:A:LEU:C  | 1:92:A:LEU:N   | 1:92:A:LEU:CA | 1:92:A:LEU:C  | 4        | 2.17          |
| (1,92)  | 1:73:A:ALA:N  | 1:73:A:ALA:CA  | 1:73:A:ALA:C  | 1:74:A:GLN:N  | 1        | 2.16          |
| (1,92)  | 1:73:A:ALA:N  | 1:73:A:ALA:CA  | 1:73:A:ALA:C  | 1:74:A:GLN:N  | 3        | 2.16          |
| (1,64)  | 1:56:A:ILE:N  | 1:56:A:ILE:CA  | 1:56:A:ILE:C  | 1:57:A:PHE:N  | 20       | 2.15          |
| (1,16)  | 1:15:A:LEU:N  | 1:15:A:LEU:CA  | 1:15:A:LEU:C  | 1:16:A:GLU:N  | 1        | 2.13          |
| (1,144) | 1:117:A:LYS:N | 1:117:A:LYS:CA | 1:117:A:LYS:C | 1:118:A:ARG:N | 19       | 2.12          |
| (1,117) | 1:94:A:ARG:C  | 1:95:A:PHE:N   | 1:95:A:PHE:CA | 1:95:A:PHE:C  | 2        | 2.12          |
| (1,73)  | 1:63:A:GLU:C  | 1:64:A:GLU:N   | 1:64:A:GLU:CA | 1:64:A:GLU:C  | 7        | 2.12          |
| (1,136) | 1:113:A:ASP:N | 1:113:A:ASP:CA | 1:113:A:ASP:C | 1:114:A:GLU:N | 4        | 2.11          |
| (1,98)  | 1:81:A:LEU:N  | 1:81:A:LEU:CA  | 1:81:A:LEU:C  | 1:82:A:VAL:N  | 4        | 2.11          |
| (1,22)  | 1:18:A:LEU:N  | 1:18:A:LEU:CA  | 1:18:A:LEU:C  | 1:19:A:LEU:N  | 11       | 2.11          |
| (1,10)  | 1:8:A:VAL:N   | 1:8:A:VAL:CA   | 1:8:A:VAL:C   | 1:9:A:SER:N   | 20       | 2.1           |
| (1,60)  | 1:48:A:ARG:N  | 1:48:A:ARG:CA  | 1:48:A:ARG:C  | 1:49:A:LYS:N  | 3        | 2.09          |

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| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,4)   | 1:5:A:VAL:N   | 1:5:A:VAL:CA   | 1:5:A:VAL:C    | 1:6:A:ILE:N   | 8        | 2.08          |
| (1,1)   | 1:3:A:THR:C   | 1:4:A:VAL:N    | 1:4:A:VAL:CA   | 1:4:A:VAL:C   | 18       | 2.08          |
| (1,76)  | 1:65:A:VAL:N  | 1:65:A:VAL:CA  | 1:65:A:VAL:C   | 1:66:A:VAL:N  | 19       | 2.07          |
| (1,22)  | 1:18:A:LEU:N  | 1:18:A:LEU:CA  | 1:18:A:LEU:C   | 1:19:A:LEU:N  | 9        | 2.07          |
| (1,22)  | 1:18:A:LEU:N  | 1:18:A:LEU:CA  | 1:18:A:LEU:C   | 1:19:A:LEU:N  | 7        | 2.06          |
| (1,129) | 1:105:A:ASP:C | 1:106:A:VAL:N  | 1:106:A:VAL:CA | 1:106:A:VAL:C | 7        | 2.05          |
| (1,116) | 1:94:A:ARG:N  | 1:94:A:ARG:CA  | 1:94:A:ARG:C   | 1:95:A:PHE:N  | 9        | 2.05          |
| (1,1)   | 1:3:A:THR:C   | 1:4:A:VAL:N    | 1:4:A:VAL:CA   | 1:4:A:VAL:C   | 20       | 2.05          |
| (1,151) | 1:120:A:LYS:C | 1:121:A:GLU:N  | 1:121:A:GLU:CA | 1:121:A:GLU:C | 10       | 2.04          |
| (1,112) | 1:92:A:LEU:N  | 1:92:A:LEU:CA  | 1:92:A:LEU:C   | 1:93:A:GLU:N  | 20       | 2.04          |
| (1,105) | 1:84:A:LYS:C  | 1:85:A:VAL:N   | 1:85:A:VAL:CA  | 1:85:A:VAL:C  | 4        | 2.04          |
| (1,7)   | 1:6:A:ILE:C   | 1:7:A:VAL:N    | 1:7:A:VAL:CA   | 1:7:A:VAL:C   | 17       | 2.04          |
| (1,4)   | 1:5:A:VAL:N   | 1:5:A:VAL:CA   | 1:5:A:VAL:C    | 1:6:A:ILE:N   | 19       | 2.04          |
| (1,100) | 1:82:A:VAL:N  | 1:82:A:VAL:CA  | 1:82:A:VAL:C   | 1:83:A:ILE:N  | 6        | 2.03          |
| (1,71)  | 1:62:A:TYR:C  | 1:63:A:GLU:N   | 1:63:A:GLU:CA  | 1:63:A:GLU:C  | 6        | 2.03          |
| (1,20)  | 1:17:A:GLU:N  | 1:17:A:GLU:CA  | 1:17:A:GLU:C   | 1:18:A:LEU:N  | 19       | 2.03          |
| (1,29)  | 1:21:A:VAL:C  | 1:22:A:VAL:N   | 1:22:A:VAL:CA  | 1:22:A:VAL:C  | 5        | 2.02          |
| (1,7)   | 1:6:A:ILE:C   | 1:7:A:VAL:N    | 1:7:A:VAL:CA   | 1:7:A:VAL:C   | 12       | 2.01          |
| (1,130) | 1:106:A:VAL:N | 1:106:A:VAL:CA | 1:106:A:VAL:C  | 1:107:A:ARG:N | 10       | 2.0           |
| (1,97)  | 1:80:A:VAL:C  | 1:81:A:LEU:N   | 1:81:A:LEU:CA  | 1:81:A:LEU:C  | 16       | 2.0           |
| (1,153) | 1:121:A:GLU:C | 1:122:A:LEU:N  | 1:122:A:LEU:CA | 1:122:A:LEU:C | 3        | 1.99          |
| (1,62)  | 1:55:A:VAL:N  | 1:55:A:VAL:CA  | 1:55:A:VAL:C   | 1:56:A:ILE:N  | 8        | 1.99          |
| (1,142) | 1:116:A:LYS:N | 1:116:A:LYS:CA | 1:116:A:LYS:C  | 1:117:A:LYS:N | 19       | 1.98          |
| (1,136) | 1:113:A:ASP:N | 1:113:A:ASP:CA | 1:113:A:ASP:C  | 1:114:A:GLU:N | 2        | 1.98          |
| (1,98)  | 1:81:A:LEU:N  | 1:81:A:LEU:CA  | 1:81:A:LEU:C   | 1:82:A:VAL:N  | 8        | 1.98          |
| (1,74)  | 1:64:A:GLU:N  | 1:64:A:GLU:CA  | 1:64:A:GLU:C   | 1:65:A:VAL:N  | 16       | 1.98          |
| (1,132) | 1:107:A:ARG:N | 1:107:A:ARG:CA | 1:107:A:ARG:C  | 1:108:A:VAL:N | 19       | 1.97          |
| (1,107) | 1:89:A:GLN:C  | 1:90:A:GLU:N   | 1:90:A:GLU:CA  | 1:90:A:GLU:C  | 9        | 1.97          |
| (1,124) | 1:98:A:GLN:N  | 1:98:A:GLN:CA  | 1:98:A:GLN:C   | 1:99:A:LEU:N  | 11       | 1.96          |
| (1,76)  | 1:65:A:VAL:N  | 1:65:A:VAL:CA  | 1:65:A:VAL:C   | 1:66:A:VAL:N  | 10       | 1.95          |
| (1,95)  | 1:79:A:ARG:C  | 1:80:A:VAL:N   | 1:80:A:VAL:CA  | 1:80:A:VAL:C  | 14       | 1.94          |
| (1,65)  | 1:56:A:ILE:C  | 1:57:A:PHE:N   | 1:57:A:PHE:CA  | 1:57:A:PHE:C  | 1        | 1.94          |
| (1,62)  | 1:55:A:VAL:N  | 1:55:A:VAL:CA  | 1:55:A:VAL:C   | 1:56:A:ILE:N  | 3        | 1.94          |
| (1,56)  | 1:46:A:LYS:N  | 1:46:A:LYS:CA  | 1:46:A:LYS:C   | 1:47:A:ALA:N  | 5        | 1.94          |
| (1,54)  | 1:45:A:GLU:N  | 1:45:A:GLU:CA  | 1:45:A:GLU:C   | 1:46:A:LYS:N  | 19       | 1.94          |
| (1,78)  | 1:66:A:VAL:N  | 1:66:A:VAL:CA  | 1:66:A:VAL:C   | 1:67:A:ARG:N  | 10       | 1.93          |
| (1,71)  | 1:62:A:TYR:C  | 1:63:A:GLU:N   | 1:63:A:GLU:CA  | 1:63:A:GLU:C  | 8        | 1.93          |
| (1,60)  | 1:48:A:ARG:N  | 1:48:A:ARG:CA  | 1:48:A:ARG:C   | 1:49:A:LYS:N  | 9        | 1.93          |
| (1,141) | 1:115:A:ALA:C | 1:116:A:LYS:N  | 1:116:A:LYS:CA | 1:116:A:LYS:C | 4        | 1.92          |
| (1,124) | 1:98:A:GLN:N  | 1:98:A:GLN:CA  | 1:98:A:GLN:C   | 1:99:A:LEU:N  | 3        | 1.92          |
| (1,49)  | 1:42:A:GLU:C  | 1:43:A:GLU:N   | 1:43:A:GLU:CA  | 1:43:A:GLU:C  | 13       | 1.92          |
| (1,99)  | 1:81:A:LEU:C  | 1:82:A:VAL:N   | 1:82:A:VAL:CA  | 1:82:A:VAL:C  | 1        | 1.91          |
| (1,51)  | 1:43:A:GLU:C  | 1:44:A:ILE:N   | 1:44:A:ILE:CA  | 1:44:A:ILE:C  | 13       | 1.91          |
| (1,12)  | 1:13:A:ARG:N  | 1:13:A:ARG:CA  | 1:13:A:ARG:C   | 1:14:A:ILE:N  | 18       | 1.91          |
| (1,128) | 1:100:A:LYS:N | 1:100:A:LYS:CA | 1:100:A:LYS:C  | 1:101:A:LYS:N | 14       | 1.9           |
| (1,61)  | 1:54:A:ILE:C  | 1:55:A:VAL:N   | 1:55:A:VAL:CA  | 1:55:A:VAL:C  | 13       | 1.9           |
| (1,12)  | 1:13:A:ARG:N  | 1:13:A:ARG:CA  | 1:13:A:ARG:C   | 1:14:A:ILE:N  | 4        | 1.9           |
| (1,60)  | 1:48:A:ARG:N  | 1:48:A:ARG:CA  | 1:48:A:ARG:C   | 1:49:A:LYS:N  | 10       | 1.88          |
| (1,138) | 1:114:A:GLU:N | 1:114:A:GLU:CA | 1:114:A:GLU:C  | 1:115:A:ALA:N | 10       | 1.87          |
| (1,129) | 1:105:A:ASP:C | 1:106:A:VAL:N  | 1:106:A:VAL:CA | 1:106:A:VAL:C | 9        | 1.87          |
| (1,62)  | 1:55:A:VAL:N  | 1:55:A:VAL:CA  | 1:55:A:VAL:C   | 1:56:A:ILE:N  | 1        | 1.87          |

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| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,154) | 1:122:A:LEU:N | 1:122:A:LEU:CA | 1:122:A:LEU:C  | 1:123:A:LEU:N | 20       | 1.86          |
| (1,48)  | 1:42:A:GLU:N  | 1:42:A:GLU:CA  | 1:42:A:GLU:C   | 1:43:A:GLU:N  | 17       | 1.86          |
| (1,154) | 1:122:A:LEU:N | 1:122:A:LEU:CA | 1:122:A:LEU:C  | 1:123:A:LEU:N | 16       | 1.85          |
| (1,60)  | 1:48:A:ARG:N  | 1:48:A:ARG:CA  | 1:48:A:ARG:C   | 1:49:A:LYS:N  | 5        | 1.85          |
| (1,147) | 1:118:A:ARG:C | 1:119:A:LEU:N  | 1:119:A:LEU:CA | 1:119:A:LEU:C | 15       | 1.84          |
| (1,134) | 1:108:A:VAL:N | 1:108:A:VAL:CA | 1:108:A:VAL:C  | 1:109:A:THR:N | 15       | 1.84          |
| (1,102) | 1:83:A:ILE:N  | 1:83:A:ILE:CA  | 1:83:A:ILE:C   | 1:84:A:LYS:N  | 1        | 1.84          |
| (1,98)  | 1:81:A:LEU:N  | 1:81:A:LEU:CA  | 1:81:A:LEU:C   | 1:82:A:VAL:N  | 1        | 1.84          |
| (1,116) | 1:94:A:ARG:N  | 1:94:A:ARG:CA  | 1:94:A:ARG:C   | 1:95:A:PHE:N  | 17       | 1.83          |
| (1,158) | 1:124:A:GLU:N | 1:124:A:GLU:CA | 1:124:A:GLU:C  | 1:125:A:LYS:N | 12       | 1.82          |
| (1,126) | 1:99:A:LEU:N  | 1:99:A:LEU:CA  | 1:99:A:LEU:C   | 1:100:A:LYS:N | 13       | 1.82          |
| (1,81)  | 1:67:A:ARG:C  | 1:68:A:ASP:N   | 1:68:A:ASP:CA  | 1:68:A:ASP:C  | 4        | 1.81          |
| (1,65)  | 1:56:A:ILE:C  | 1:57:A:PHE:N   | 1:57:A:PHE:CA  | 1:57:A:PHE:C  | 8        | 1.81          |
| (1,105) | 1:84:A:LYS:C  | 1:85:A:VAL:N   | 1:85:A:VAL:CA  | 1:85:A:VAL:C  | 18       | 1.79          |
| (1,62)  | 1:55:A:VAL:N  | 1:55:A:VAL:CA  | 1:55:A:VAL:C   | 1:56:A:ILE:N  | 16       | 1.79          |
| (1,76)  | 1:65:A:VAL:N  | 1:65:A:VAL:CA  | 1:65:A:VAL:C   | 1:66:A:VAL:N  | 16       | 1.78          |
| (1,78)  | 1:66:A:VAL:N  | 1:66:A:VAL:CA  | 1:66:A:VAL:C   | 1:67:A:ARG:N  | 15       | 1.77          |
| (1,26)  | 1:20:A:GLU:N  | 1:20:A:GLU:CA  | 1:20:A:GLU:C   | 1:21:A:VAL:N  | 20       | 1.77          |
| (1,26)  | 1:20:A:GLU:N  | 1:20:A:GLU:CA  | 1:20:A:GLU:C   | 1:21:A:VAL:N  | 19       | 1.76          |
| (1,136) | 1:113:A:ASP:N | 1:113:A:ASP:CA | 1:113:A:ASP:C  | 1:114:A:GLU:N | 5        | 1.75          |
| (1,79)  | 1:66:A:VAL:C  | 1:67:A:ARG:N   | 1:67:A:ARG:CA  | 1:67:A:ARG:C  | 18       | 1.75          |
| (1,76)  | 1:65:A:VAL:N  | 1:65:A:VAL:CA  | 1:65:A:VAL:C   | 1:66:A:VAL:N  | 20       | 1.75          |
| (1,117) | 1:94:A:ARG:C  | 1:95:A:PHE:N   | 1:95:A:PHE:CA  | 1:95:A:PHE:C  | 19       | 1.74          |
| (1,117) | 1:94:A:ARG:C  | 1:95:A:PHE:N   | 1:95:A:PHE:CA  | 1:95:A:PHE:C  | 20       | 1.73          |
| (1,99)  | 1:81:A:LEU:C  | 1:82:A:VAL:N   | 1:82:A:VAL:CA  | 1:82:A:VAL:C  | 8        | 1.73          |
| (1,58)  | 1:47:A:ALA:N  | 1:47:A:ALA:CA  | 1:47:A:ALA:C   | 1:48:A:ARG:N  | 6        | 1.73          |
| (1,138) | 1:114:A:GLU:N | 1:114:A:GLU:CA | 1:114:A:GLU:C  | 1:115:A:ALA:N | 1        | 1.72          |
| (1,120) | 1:96:A:TYR:N  | 1:96:A:TYR:CA  | 1:96:A:TYR:C   | 1:97:A:GLU:N  | 7        | 1.72          |
| (1,97)  | 1:80:A:VAL:C  | 1:81:A:LEU:N   | 1:81:A:LEU:CA  | 1:81:A:LEU:C  | 5        | 1.72          |
| (1,96)  | 1:80:A:VAL:N  | 1:80:A:VAL:CA  | 1:80:A:VAL:C   | 1:81:A:LEU:N  | 1        | 1.71          |
| (1,4)   | 1:5:A:VAL:N   | 1:5:A:VAL:CA   | 1:5:A:VAL:C    | 1:6:A:ILE:N   | 4        | 1.71          |
| (1,133) | 1:107:A:ARG:C | 1:108:A:VAL:N  | 1:108:A:VAL:CA | 1:108:A:VAL:C | 4        | 1.7           |
| (1,64)  | 1:56:A:ILE:N  | 1:56:A:ILE:CA  | 1:56:A:ILE:C   | 1:57:A:PHE:N  | 5        | 1.68          |
| (1,133) | 1:107:A:ARG:C | 1:108:A:VAL:N  | 1:108:A:VAL:CA | 1:108:A:VAL:C | 1        | 1.67          |
| (1,95)  | 1:79:A:ARG:C  | 1:80:A:VAL:N   | 1:80:A:VAL:CA  | 1:80:A:VAL:C  | 20       | 1.67          |
| (1,79)  | 1:66:A:VAL:C  | 1:67:A:ARG:N   | 1:67:A:ARG:CA  | 1:67:A:ARG:C  | 4        | 1.67          |
| (1,116) | 1:94:A:ARG:N  | 1:94:A:ARG:CA  | 1:94:A:ARG:C   | 1:95:A:PHE:N  | 1        | 1.66          |
| (1,82)  | 1:68:A:ASP:N  | 1:68:A:ASP:CA  | 1:68:A:ASP:C   | 1:69:A:ILE:N  | 10       | 1.66          |
| (1,79)  | 1:66:A:VAL:C  | 1:67:A:ARG:N   | 1:67:A:ARG:CA  | 1:67:A:ARG:C  | 5        | 1.66          |
| (1,78)  | 1:66:A:VAL:N  | 1:66:A:VAL:CA  | 1:66:A:VAL:C   | 1:67:A:ARG:N  | 9        | 1.65          |
| (1,72)  | 1:63:A:GLU:N  | 1:63:A:GLU:CA  | 1:63:A:GLU:C   | 1:64:A:GLU:N  | 19       | 1.65          |
| (1,20)  | 1:17:A:GLU:N  | 1:17:A:GLU:CA  | 1:17:A:GLU:C   | 1:18:A:LEU:N  | 14       | 1.65          |
| (1,148) | 1:119:A:LEU:N | 1:119:A:LEU:CA | 1:119:A:LEU:C  | 1:120:A:LYS:N | 5        | 1.64          |
| (1,129) | 1:105:A:ASP:C | 1:106:A:VAL:N  | 1:106:A:VAL:CA | 1:106:A:VAL:C | 16       | 1.64          |
| (1,98)  | 1:81:A:LEU:N  | 1:81:A:LEU:CA  | 1:81:A:LEU:C   | 1:82:A:VAL:N  | 19       | 1.63          |
| (1,136) | 1:113:A:ASP:N | 1:113:A:ASP:CA | 1:113:A:ASP:C  | 1:114:A:GLU:N | 17       | 1.62          |
| (1,126) | 1:99:A:LEU:N  | 1:99:A:LEU:CA  | 1:99:A:LEU:C   | 1:100:A:LYS:N | 10       | 1.62          |
| (1,117) | 1:94:A:ARG:C  | 1:95:A:PHE:N   | 1:95:A:PHE:CA  | 1:95:A:PHE:C  | 12       | 1.62          |
| (1,77)  | 1:65:A:VAL:C  | 1:66:A:VAL:N   | 1:66:A:VAL:CA  | 1:66:A:VAL:C  | 20       | 1.62          |
| (1,132) | 1:107:A:ARG:N | 1:107:A:ARG:CA | 1:107:A:ARG:C  | 1:108:A:VAL:N | 9        | 1.61          |
| (1,20)  | 1:17:A:GLU:N  | 1:17:A:GLU:CA  | 1:17:A:GLU:C   | 1:18:A:LEU:N  | 16       | 1.61          |

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| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,130) | 1:106:A:VAL:N | 1:106:A:VAL:CA | 1:106:A:VAL:C  | 1:107:A:ARG:N | 2        | 1.6           |
| (1,26)  | 1:20:A:GLU:N  | 1:20:A:GLU:CA  | 1:20:A:GLU:C   | 1:21:A:VAL:N  | 3        | 1.6           |
| (1,114) | 1:93:A:GLU:N  | 1:93:A:GLU:CA  | 1:93:A:GLU:C   | 1:94:A:ARG:N  | 10       | 1.59          |
| (1,111) | 1:91:A:LEU:C  | 1:92:A:LEU:N   | 1:92:A:LEU:CA  | 1:92:A:LEU:C  | 20       | 1.59          |
| (1,158) | 1:124:A:GLU:N | 1:124:A:GLU:CA | 1:124:A:GLU:C  | 1:125:A:LYS:N | 18       | 1.57          |
| (1,130) | 1:106:A:VAL:N | 1:106:A:VAL:CA | 1:106:A:VAL:C  | 1:107:A:ARG:N | 8        | 1.57          |
| (1,129) | 1:105:A:ASP:C | 1:106:A:VAL:N  | 1:106:A:VAL:CA | 1:106:A:VAL:C | 1        | 1.57          |
| (1,99)  | 1:81:A:LEU:C  | 1:82:A:VAL:N   | 1:82:A:VAL:CA  | 1:82:A:VAL:C  | 12       | 1.57          |
| (1,97)  | 1:80:A:VAL:C  | 1:81:A:LEU:N   | 1:81:A:LEU:CA  | 1:81:A:LEU:C  | 15       | 1.57          |
| (1,22)  | 1:18:A:LEU:N  | 1:18:A:LEU:CA  | 1:18:A:LEU:C   | 1:19:A:LEU:N  | 19       | 1.57          |
| (1,7)   | 1:6:A:ILE:C   | 1:7:A:VAL:N    | 1:7:A:VAL:CA   | 1:7:A:VAL:C   | 13       | 1.57          |
| (1,151) | 1:120:A:LYS:C | 1:121:A:GLU:N  | 1:121:A:GLU:CA | 1:121:A:GLU:C | 5        | 1.56          |
| (1,73)  | 1:63:A:GLU:C  | 1:64:A:GLU:N   | 1:64:A:GLU:CA  | 1:64:A:GLU:C  | 2        | 1.56          |
| (1,108) | 1:90:A:GLU:N  | 1:90:A:GLU:CA  | 1:90:A:GLU:C   | 1:91:A:LEU:N  | 11       | 1.55          |
| (1,102) | 1:83:A:ILE:N  | 1:83:A:ILE:CA  | 1:83:A:ILE:C   | 1:84:A:LYS:N  | 7        | 1.55          |
| (1,77)  | 1:65:A:VAL:C  | 1:66:A:VAL:N   | 1:66:A:VAL:CA  | 1:66:A:VAL:C  | 18       | 1.54          |
| (1,65)  | 1:56:A:ILE:C  | 1:57:A:PHE:N   | 1:57:A:PHE:CA  | 1:57:A:PHE:C  | 19       | 1.54          |
| (1,41)  | 1:38:A:GLU:C  | 1:39:A:LYS:N   | 1:39:A:LYS:CA  | 1:39:A:LYS:C  | 10       | 1.54          |
| (1,156) | 1:123:A:LEU:N | 1:123:A:LEU:CA | 1:123:A:LEU:C  | 1:124:A:GLU:N | 1        | 1.53          |
| (1,84)  | 1:69:A:ILE:N  | 1:69:A:ILE:CA  | 1:69:A:ILE:C   | 1:70:A:VAL:N  | 17       | 1.53          |
| (1,132) | 1:107:A:ARG:N | 1:107:A:ARG:CA | 1:107:A:ARG:C  | 1:108:A:VAL:N | 5        | 1.52          |
| (1,101) | 1:82:A:VAL:C  | 1:83:A:ILE:N   | 1:83:A:ILE:CA  | 1:83:A:ILE:C  | 2        | 1.52          |
| (1,60)  | 1:48:A:ARG:N  | 1:48:A:ARG:CA  | 1:48:A:ARG:C   | 1:49:A:LYS:N  | 8        | 1.52          |
| (1,26)  | 1:20:A:GLU:N  | 1:20:A:GLU:CA  | 1:20:A:GLU:C   | 1:21:A:VAL:N  | 18       | 1.52          |
| (1,105) | 1:84:A:LYS:C  | 1:85:A:VAL:N   | 1:85:A:VAL:CA  | 1:85:A:VAL:C  | 8        | 1.51          |
| (1,158) | 1:124:A:GLU:N | 1:124:A:GLU:CA | 1:124:A:GLU:C  | 1:125:A:LYS:N | 20       | 1.5           |
| (1,141) | 1:115:A:ALA:C | 1:116:A:LYS:N  | 1:116:A:LYS:CA | 1:116:A:LYS:C | 2        | 1.5           |
| (1,136) | 1:113:A:ASP:N | 1:113:A:ASP:CA | 1:113:A:ASP:C  | 1:114:A:GLU:N | 14       | 1.5           |
| (1,8)   | 1:7:A:VAL:N   | 1:7:A:VAL:CA   | 1:7:A:VAL:C    | 1:8:A:VAL:N   | 9        | 1.5           |
| (1,98)  | 1:81:A:LEU:N  | 1:81:A:LEU:CA  | 1:81:A:LEU:C   | 1:82:A:VAL:N  | 16       | 1.49          |
| (1,86)  | 1:70:A:VAL:N  | 1:70:A:VAL:CA  | 1:70:A:VAL:C   | 1:71:A:GLU:N  | 15       | 1.49          |
| (1,146) | 1:118:A:ARG:N | 1:118:A:ARG:CA | 1:118:A:ARG:C  | 1:119:A:LEU:N | 19       | 1.48          |
| (1,58)  | 1:47:A:ALA:N  | 1:47:A:ALA:CA  | 1:47:A:ALA:C   | 1:48:A:ARG:N  | 3        | 1.47          |
| (1,105) | 1:84:A:LYS:C  | 1:85:A:VAL:N   | 1:85:A:VAL:CA  | 1:85:A:VAL:C  | 6        | 1.46          |
| (1,105) | 1:84:A:LYS:C  | 1:85:A:VAL:N   | 1:85:A:VAL:CA  | 1:85:A:VAL:C  | 9        | 1.45          |
| (1,78)  | 1:66:A:VAL:N  | 1:66:A:VAL:CA  | 1:66:A:VAL:C   | 1:67:A:ARG:N  | 8        | 1.45          |
| (1,59)  | 1:47:A:ALA:C  | 1:48:A:ARG:N   | 1:48:A:ARG:CA  | 1:48:A:ARG:C  | 15       | 1.45          |
| (1,46)  | 1:41:A:LYS:N  | 1:41:A:LYS:CA  | 1:41:A:LYS:C   | 1:42:A:GLU:N  | 19       | 1.45          |
| (1,103) | 1:83:A:ILE:C  | 1:84:A:LYS:N   | 1:84:A:LYS:CA  | 1:84:A:LYS:C  | 4        | 1.43          |
| (1,73)  | 1:63:A:GLU:C  | 1:64:A:GLU:N   | 1:64:A:GLU:CA  | 1:64:A:GLU:C  | 1        | 1.43          |
| (1,36)  | 1:32:A:VAL:N  | 1:32:A:VAL:CA  | 1:32:A:VAL:C   | 1:33:A:ARG:N  | 18       | 1.43          |
| (1,12)  | 1:13:A:ARG:N  | 1:13:A:ARG:CA  | 1:13:A:ARG:C   | 1:14:A:ILE:N  | 13       | 1.43          |
| (1,95)  | 1:79:A:ARG:C  | 1:80:A:VAL:N   | 1:80:A:VAL:CA  | 1:80:A:VAL:C  | 15       | 1.42          |
| (1,78)  | 1:66:A:VAL:N  | 1:66:A:VAL:CA  | 1:66:A:VAL:C   | 1:67:A:ARG:N  | 14       | 1.42          |
| (1,38)  | 1:33:A:ARG:N  | 1:33:A:ARG:CA  | 1:33:A:ARG:C   | 1:34:A:THR:N  | 15       | 1.42          |
| (1,142) | 1:116:A:LYS:N | 1:116:A:LYS:CA | 1:116:A:LYS:C  | 1:117:A:LYS:N | 14       | 1.4           |
| (1,119) | 1:95:A:PHE:C  | 1:96:A:TYR:N   | 1:96:A:TYR:CA  | 1:96:A:TYR:C  | 18       | 1.4           |
| (1,95)  | 1:79:A:ARG:C  | 1:80:A:VAL:N   | 1:80:A:VAL:CA  | 1:80:A:VAL:C  | 6        | 1.4           |
| (1,35)  | 1:31:A:THR:C  | 1:32:A:VAL:N   | 1:32:A:VAL:CA  | 1:32:A:VAL:C  | 13       | 1.4           |
| (1,62)  | 1:55:A:VAL:N  | 1:55:A:VAL:CA  | 1:55:A:VAL:C   | 1:56:A:ILE:N  | 10       | 1.39          |
| (1,12)  | 1:13:A:ARG:N  | 1:13:A:ARG:CA  | 1:13:A:ARG:C   | 1:14:A:ILE:N  | 7        | 1.39          |

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| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,12)  | 1:13:A:ARG:N  | 1:13:A:ARG:CA  | 1:13:A:ARG:C   | 1:14:A:ILE:N  | 20       | 1.39          |
| (1,4)   | 1:5:A:VAL:N   | 1:5:A:VAL:CA   | 1:5:A:VAL:C    | 1:6:A:ILE:N   | 1        | 1.39          |
| (1,114) | 1:93:A:GLU:N  | 1:93:A:GLU:CA  | 1:93:A:GLU:C   | 1:94:A:ARG:N  | 8        | 1.38          |
| (1,77)  | 1:65:A:VAL:C  | 1:66:A:VAL:N   | 1:66:A:VAL:CA  | 1:66:A:VAL:C  | 12       | 1.38          |
| (1,8)   | 1:7:A:VAL:N   | 1:7:A:VAL:CA   | 1:7:A:VAL:C    | 1:8:A:VAL:N   | 4        | 1.38          |
| (1,62)  | 1:55:A:VAL:N  | 1:55:A:VAL:CA  | 1:55:A:VAL:C   | 1:56:A:ILE:N  | 11       | 1.37          |
| (1,128) | 1:100:A:LYS:N | 1:100:A:LYS:CA | 1:100:A:LYS:C  | 1:101:A:LYS:N | 17       | 1.36          |
| (1,92)  | 1:73:A:ALA:N  | 1:73:A:ALA:CA  | 1:73:A:ALA:C   | 1:74:A:GLN:N  | 16       | 1.36          |
| (1,39)  | 1:37:A:LYS:C  | 1:38:A:GLU:N   | 1:38:A:GLU:CA  | 1:38:A:GLU:C  | 6        | 1.36          |
| (1,4)   | 1:5:A:VAL:N   | 1:5:A:VAL:CA   | 1:5:A:VAL:C    | 1:6:A:ILE:N   | 5        | 1.36          |
| (1,119) | 1:95:A:PHE:C  | 1:96:A:TYR:N   | 1:96:A:TYR:CA  | 1:96:A:TYR:C  | 19       | 1.35          |
| (1,17)  | 1:15:A:LEU:C  | 1:16:A:GLU:N   | 1:16:A:GLU:CA  | 1:16:A:GLU:C  | 4        | 1.35          |
| (1,98)  | 1:81:A:LEU:N  | 1:81:A:LEU:CA  | 1:81:A:LEU:C   | 1:82:A:VAL:N  | 11       | 1.34          |
| (1,65)  | 1:56:A:ILE:C  | 1:57:A:PHE:N   | 1:57:A:PHE:CA  | 1:57:A:PHE:C  | 17       | 1.34          |
| (1,135) | 1:112:A:GLU:C | 1:113:A:ASP:N  | 1:113:A:ASP:CA | 1:113:A:ASP:C | 14       | 1.33          |
| (1,100) | 1:82:A:VAL:N  | 1:82:A:VAL:CA  | 1:82:A:VAL:C   | 1:83:A:ILE:N  | 5        | 1.33          |
| (1,88)  | 1:71:A:GLU:N  | 1:71:A:GLU:CA  | 1:71:A:GLU:C   | 1:72:A:TYR:N  | 6        | 1.33          |
| (1,71)  | 1:62:A:TYR:C  | 1:63:A:GLU:N   | 1:63:A:GLU:CA  | 1:63:A:GLU:C  | 11       | 1.33          |
| (1,92)  | 1:73:A:ALA:N  | 1:73:A:ALA:CA  | 1:73:A:ALA:C   | 1:74:A:GLN:N  | 9        | 1.32          |
| (1,92)  | 1:73:A:ALA:N  | 1:73:A:ALA:CA  | 1:73:A:ALA:C   | 1:74:A:GLN:N  | 14       | 1.32          |
| (1,157) | 1:123:A:LEU:C | 1:124:A:GLU:N  | 1:124:A:GLU:CA | 1:124:A:GLU:C | 2        | 1.31          |
| (1,76)  | 1:65:A:VAL:N  | 1:65:A:VAL:CA  | 1:65:A:VAL:C   | 1:66:A:VAL:N  | 8        | 1.3           |
| (1,50)  | 1:43:A:GLU:N  | 1:43:A:GLU:CA  | 1:43:A:GLU:C   | 1:44:A:ILE:N  | 15       | 1.3           |
| (1,152) | 1:121:A:GLU:N | 1:121:A:GLU:CA | 1:121:A:GLU:C  | 1:122:A:LEU:N | 11       | 1.29          |
| (1,116) | 1:94:A:ARG:N  | 1:94:A:ARG:CA  | 1:94:A:ARG:C   | 1:95:A:PHE:N  | 2        | 1.29          |
| (1,81)  | 1:67:A:ARG:C  | 1:68:A:ASP:N   | 1:68:A:ASP:CA  | 1:68:A:ASP:C  | 3        | 1.29          |
| (1,22)  | 1:18:A:LEU:N  | 1:18:A:LEU:CA  | 1:18:A:LEU:C   | 1:19:A:LEU:N  | 10       | 1.29          |
| (1,43)  | 1:39:A:LYS:C  | 1:40:A:VAL:N   | 1:40:A:VAL:CA  | 1:40:A:VAL:C  | 7        | 1.28          |
| (1,12)  | 1:13:A:ARG:N  | 1:13:A:ARG:CA  | 1:13:A:ARG:C   | 1:14:A:ILE:N  | 9        | 1.28          |
| (1,4)   | 1:5:A:VAL:N   | 1:5:A:VAL:CA   | 1:5:A:VAL:C    | 1:6:A:ILE:N   | 3        | 1.28          |
| (1,102) | 1:83:A:ILE:N  | 1:83:A:ILE:CA  | 1:83:A:ILE:C   | 1:84:A:LYS:N  | 8        | 1.27          |
| (1,85)  | 1:69:A:ILE:C  | 1:70:A:VAL:N   | 1:70:A:VAL:CA  | 1:70:A:VAL:C  | 5        | 1.27          |
| (1,85)  | 1:69:A:ILE:C  | 1:70:A:VAL:N   | 1:70:A:VAL:CA  | 1:70:A:VAL:C  | 7        | 1.27          |
| (1,65)  | 1:56:A:ILE:C  | 1:57:A:PHE:N   | 1:57:A:PHE:CA  | 1:57:A:PHE:C  | 4        | 1.27          |
| (1,131) | 1:106:A:VAL:C | 1:107:A:ARG:N  | 1:107:A:ARG:CA | 1:107:A:ARG:C | 1        | 1.26          |
| (1,156) | 1:123:A:LEU:N | 1:123:A:LEU:CA | 1:123:A:LEU:C  | 1:124:A:GLU:N | 9        | 1.25          |
| (1,108) | 1:90:A:GLU:N  | 1:90:A:GLU:CA  | 1:90:A:GLU:C   | 1:91:A:LEU:N  | 10       | 1.25          |
| (1,12)  | 1:13:A:ARG:N  | 1:13:A:ARG:CA  | 1:13:A:ARG:C   | 1:14:A:ILE:N  | 2        | 1.25          |
| (1,158) | 1:124:A:GLU:N | 1:124:A:GLU:CA | 1:124:A:GLU:C  | 1:125:A:LYS:N | 19       | 1.24          |
| (1,72)  | 1:63:A:GLU:N  | 1:63:A:GLU:CA  | 1:63:A:GLU:C   | 1:64:A:GLU:N  | 7        | 1.24          |
| (1,146) | 1:118:A:ARG:N | 1:118:A:ARG:CA | 1:118:A:ARG:C  | 1:119:A:LEU:N | 6        | 1.22          |
| (1,102) | 1:83:A:ILE:N  | 1:83:A:ILE:CA  | 1:83:A:ILE:C   | 1:84:A:LYS:N  | 16       | 1.22          |
| (1,84)  | 1:69:A:ILE:N  | 1:69:A:ILE:CA  | 1:69:A:ILE:C   | 1:70:A:VAL:N  | 7        | 1.22          |
| (1,42)  | 1:39:A:LYS:N  | 1:39:A:LYS:CA  | 1:39:A:LYS:C   | 1:40:A:VAL:N  | 3        | 1.22          |
| (1,131) | 1:106:A:VAL:C | 1:107:A:ARG:N  | 1:107:A:ARG:CA | 1:107:A:ARG:C | 11       | 1.21          |
| (1,128) | 1:100:A:LYS:N | 1:100:A:LYS:CA | 1:100:A:LYS:C  | 1:101:A:LYS:N | 7        | 1.21          |
| (1,20)  | 1:17:A:GLU:N  | 1:17:A:GLU:CA  | 1:17:A:GLU:C   | 1:18:A:LEU:N  | 2        | 1.21          |
| (1,6)   | 1:6:A:ILE:N   | 1:6:A:ILE:CA   | 1:6:A:ILE:C    | 1:7:A:VAL:N   | 20       | 1.21          |
| (1,127) | 1:99:A:LEU:C  | 1:100:A:LYS:N  | 1:100:A:LYS:CA | 1:100:A:LYS:C | 20       | 1.2           |
| (1,158) | 1:124:A:GLU:N | 1:124:A:GLU:CA | 1:124:A:GLU:C  | 1:125:A:LYS:N | 16       | 1.19          |
| (1,135) | 1:112:A:GLU:C | 1:113:A:ASP:N  | 1:113:A:ASP:CA | 1:113:A:ASP:C | 2        | 1.19          |

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| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,134) | 1:108:A:VAL:N | 1:108:A:VAL:CA | 1:108:A:VAL:C  | 1:109:A:THR:N | 3        | 1.19          |
| (1,116) | 1:94:A:ARG:N  | 1:94:A:ARG:CA  | 1:94:A:ARG:C   | 1:95:A:PHE:N  | 7        | 1.19          |
| (1,146) | 1:118:A:ARG:N | 1:118:A:ARG:CA | 1:118:A:ARG:C  | 1:119:A:LEU:N | 11       | 1.18          |
| (1,36)  | 1:32:A:VAL:N  | 1:32:A:VAL:CA  | 1:32:A:VAL:C   | 1:33:A:ARG:N  | 10       | 1.18          |
| (1,133) | 1:107:A:ARG:C | 1:108:A:VAL:N  | 1:108:A:VAL:CA | 1:108:A:VAL:C | 12       | 1.17          |
| (1,119) | 1:95:A:PHE:C  | 1:96:A:TYR:N   | 1:96:A:TYR:CA  | 1:96:A:TYR:C  | 5        | 1.17          |
| (1,119) | 1:95:A:PHE:C  | 1:96:A:TYR:N   | 1:96:A:TYR:CA  | 1:96:A:TYR:C  | 7        | 1.17          |
| (1,78)  | 1:66:A:VAL:N  | 1:66:A:VAL:CA  | 1:66:A:VAL:C   | 1:67:A:ARG:N  | 5        | 1.16          |
| (1,58)  | 1:47:A:ALA:N  | 1:47:A:ALA:CA  | 1:47:A:ALA:C   | 1:48:A:ARG:N  | 4        | 1.16          |
| (1,138) | 1:114:A:GLU:N | 1:114:A:GLU:CA | 1:114:A:GLU:C  | 1:115:A:ALA:N | 18       | 1.15          |
| (1,78)  | 1:66:A:VAL:N  | 1:66:A:VAL:CA  | 1:66:A:VAL:C   | 1:67:A:ARG:N  | 1        | 1.15          |
| (1,73)  | 1:63:A:GLU:C  | 1:64:A:GLU:N   | 1:64:A:GLU:CA  | 1:64:A:GLU:C  | 5        | 1.15          |
| (1,48)  | 1:42:A:GLU:N  | 1:42:A:GLU:CA  | 1:42:A:GLU:C   | 1:43:A:GLU:N  | 13       | 1.15          |
| (1,151) | 1:120:A:LYS:C | 1:121:A:GLU:N  | 1:121:A:GLU:CA | 1:121:A:GLU:C | 14       | 1.14          |
| (1,134) | 1:108:A:VAL:N | 1:108:A:VAL:CA | 1:108:A:VAL:C  | 1:109:A:THR:N | 2        | 1.14          |
| (1,96)  | 1:80:A:VAL:N  | 1:80:A:VAL:CA  | 1:80:A:VAL:C   | 1:81:A:LEU:N  | 15       | 1.14          |
| (1,92)  | 1:73:A:ALA:N  | 1:73:A:ALA:CA  | 1:73:A:ALA:C   | 1:74:A:GLN:N  | 11       | 1.14          |
| (1,77)  | 1:65:A:VAL:C  | 1:66:A:VAL:N   | 1:66:A:VAL:CA  | 1:66:A:VAL:C  | 10       | 1.14          |
| (1,72)  | 1:63:A:GLU:N  | 1:63:A:GLU:CA  | 1:63:A:GLU:C   | 1:64:A:GLU:N  | 2        | 1.14          |
| (1,26)  | 1:20:A:GLU:N  | 1:20:A:GLU:CA  | 1:20:A:GLU:C   | 1:21:A:VAL:N  | 16       | 1.14          |
| (1,119) | 1:95:A:PHE:C  | 1:96:A:TYR:N   | 1:96:A:TYR:CA  | 1:96:A:TYR:C  | 13       | 1.13          |
| (1,105) | 1:84:A:LYS:C  | 1:85:A:VAL:N   | 1:85:A:VAL:CA  | 1:85:A:VAL:C  | 1        | 1.13          |
| (1,12)  | 1:13:A:ARG:N  | 1:13:A:ARG:CA  | 1:13:A:ARG:C   | 1:14:A:ILE:N  | 15       | 1.13          |
| (1,101) | 1:82:A:VAL:C  | 1:83:A:ILE:N   | 1:83:A:ILE:CA  | 1:83:A:ILE:C  | 3        | 1.12          |
| (1,68)  | 1:61:A:ALA:N  | 1:61:A:ALA:CA  | 1:61:A:ALA:C   | 1:62:A:TYR:N  | 2        | 1.12          |
| (1,64)  | 1:56:A:ILE:N  | 1:56:A:ILE:CA  | 1:56:A:ILE:C   | 1:57:A:PHE:N  | 6        | 1.12          |
| (1,60)  | 1:48:A:ARG:N  | 1:48:A:ARG:CA  | 1:48:A:ARG:C   | 1:49:A:LYS:N  | 4        | 1.12          |
| (1,28)  | 1:21:A:VAL:N  | 1:21:A:VAL:CA  | 1:21:A:VAL:C   | 1:22:A:VAL:N  | 15       | 1.12          |
| (1,140) | 1:115:A:ALA:N | 1:115:A:ALA:CA | 1:115:A:ALA:C  | 1:116:A:LYS:N | 15       | 1.11          |
| (1,97)  | 1:80:A:VAL:C  | 1:81:A:LEU:N   | 1:81:A:LEU:CA  | 1:81:A:LEU:C  | 4        | 1.11          |
| (1,102) | 1:83:A:ILE:N  | 1:83:A:ILE:CA  | 1:83:A:ILE:C   | 1:84:A:LYS:N  | 14       | 1.1           |
| (1,101) | 1:82:A:VAL:C  | 1:83:A:ILE:N   | 1:83:A:ILE:CA  | 1:83:A:ILE:C  | 9        | 1.1           |
| (1,58)  | 1:47:A:ALA:N  | 1:47:A:ALA:CA  | 1:47:A:ALA:C   | 1:48:A:ARG:N  | 8        | 1.1           |
| (1,108) | 1:90:A:GLU:N  | 1:90:A:GLU:CA  | 1:90:A:GLU:C   | 1:91:A:LEU:N  | 5        | 1.09          |
| (1,107) | 1:89:A:GLN:C  | 1:90:A:GLU:N   | 1:90:A:GLU:CA  | 1:90:A:GLU:C  | 16       | 1.09          |
| (1,94)  | 1:74:A:GLN:N  | 1:74:A:GLN:CA  | 1:74:A:GLN:C   | 1:75:A:LYS:N  | 11       | 1.09          |
| (1,76)  | 1:65:A:VAL:N  | 1:65:A:VAL:CA  | 1:65:A:VAL:C   | 1:66:A:VAL:N  | 6        | 1.09          |
| (1,62)  | 1:55:A:VAL:N  | 1:55:A:VAL:CA  | 1:55:A:VAL:C   | 1:56:A:ILE:N  | 9        | 1.09          |
| (1,105) | 1:84:A:LYS:C  | 1:85:A:VAL:N   | 1:85:A:VAL:CA  | 1:85:A:VAL:C  | 5        | 1.08          |
| (1,9)   | 1:7:A:VAL:C   | 1:8:A:VAL:N    | 1:8:A:VAL:CA   | 1:8:A:VAL:C   | 10       | 1.07          |
| (1,1)   | 1:3:A:THR:C   | 1:4:A:VAL:N    | 1:4:A:VAL:CA   | 1:4:A:VAL:C   | 19       | 1.07          |
| (1,48)  | 1:42:A:GLU:N  | 1:42:A:GLU:CA  | 1:42:A:GLU:C   | 1:43:A:GLU:N  | 20       | 1.06          |
| (1,35)  | 1:31:A:THR:C  | 1:32:A:VAL:N   | 1:32:A:VAL:CA  | 1:32:A:VAL:C  | 10       | 1.06          |
| (1,55)  | 1:45:A:GLU:C  | 1:46:A:LYS:N   | 1:46:A:LYS:CA  | 1:46:A:LYS:C  | 19       | 1.05          |
| (1,49)  | 1:42:A:GLU:C  | 1:43:A:GLU:N   | 1:43:A:GLU:CA  | 1:43:A:GLU:C  | 19       | 1.05          |
| (1,6)   | 1:6:A:ILE:N   | 1:6:A:ILE:CA   | 1:6:A:ILE:C    | 1:7:A:VAL:N   | 11       | 1.05          |
| (1,141) | 1:115:A:ALA:C | 1:116:A:LYS:N  | 1:116:A:LYS:CA | 1:116:A:LYS:C | 13       | 1.04          |
| (1,131) | 1:106:A:VAL:C | 1:107:A:ARG:N  | 1:107:A:ARG:CA | 1:107:A:ARG:C | 3        | 1.04          |
| (1,130) | 1:106:A:VAL:N | 1:106:A:VAL:CA | 1:106:A:VAL:C  | 1:107:A:ARG:N | 9        | 1.04          |
| (1,119) | 1:95:A:PHE:C  | 1:96:A:TYR:N   | 1:96:A:TYR:CA  | 1:96:A:TYR:C  | 10       | 1.04          |
| (1,78)  | 1:66:A:VAL:N  | 1:66:A:VAL:CA  | 1:66:A:VAL:C   | 1:67:A:ARG:N  | 19       | 1.04          |

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*Continued from previous page...*

| Key     | Atom-1        | Atom-2         | Atom-3        | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|---------------|---------------|----------|---------------|
| (1,63)  | 1:55:A:VAL:C  | 1:56:A:ILE:N   | 1:56:A:ILE:CA | 1:56:A:ILE:C  | 20       | 1.04          |
| (1,11)  | 1:12:A:GLU:C  | 1:13:A:ARG:N   | 1:13:A:ARG:CA | 1:13:A:ARG:C  | 20       | 1.04          |
| (1,104) | 1:84:A:LYS:N  | 1:84:A:LYS:CA  | 1:84:A:LYS:C  | 1:85:A:VAL:N  | 18       | 1.03          |
| (1,97)  | 1:80:A:VAL:C  | 1:81:A:LEU:N   | 1:81:A:LEU:CA | 1:81:A:LEU:C  | 11       | 1.03          |
| (1,73)  | 1:63:A:GLU:C  | 1:64:A:GLU:N   | 1:64:A:GLU:CA | 1:64:A:GLU:C  | 9        | 1.03          |
| (1,39)  | 1:37:A:LYS:C  | 1:38:A:GLU:N   | 1:38:A:GLU:CA | 1:38:A:GLU:C  | 8        | 1.03          |
| (1,36)  | 1:32:A:VAL:N  | 1:32:A:VAL:CA  | 1:32:A:VAL:C  | 1:33:A:ARG:N  | 4        | 1.03          |
| (1,8)   | 1:7:A:VAL:N   | 1:7:A:VAL:CA   | 1:7:A:VAL:C   | 1:8:A:VAL:N   | 6        | 1.03          |
| (1,40)  | 1:38:A:GLU:N  | 1:38:A:GLU:CA  | 1:38:A:GLU:C  | 1:39:A:LYS:N  | 17       | 1.02          |
| (1,124) | 1:98:A:GLN:N  | 1:98:A:GLN:CA  | 1:98:A:GLN:C  | 1:99:A:LEU:N  | 15       | 1.01          |
| (1,93)  | 1:73:A:ALA:C  | 1:74:A:GLN:N   | 1:74:A:GLN:CA | 1:74:A:GLN:C  | 5        | 1.01          |
| (1,146) | 1:118:A:ARG:N | 1:118:A:ARG:CA | 1:118:A:ARG:C | 1:119:A:LEU:N | 4        | 1.0           |
| (1,12)  | 1:13:A:ARG:N  | 1:13:A:ARG:CA  | 1:13:A:ARG:C  | 1:14:A:ILE:N  | 3        | 1.0           |