



# Full wwPDB NMR Structure Validation Report ⓘ

Mar 25, 2026 – 11:49 PM UTC

PDB ID : 2LE0 / pdb\_00002le0  
BMRB ID : 17687  
Title : PARP BRCT Domain  
Authors : Mueller, G.; Loeffler, P.; Cuneo, M.; Derose, E.; London, R.  
Deposited on : 2011-06-03

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

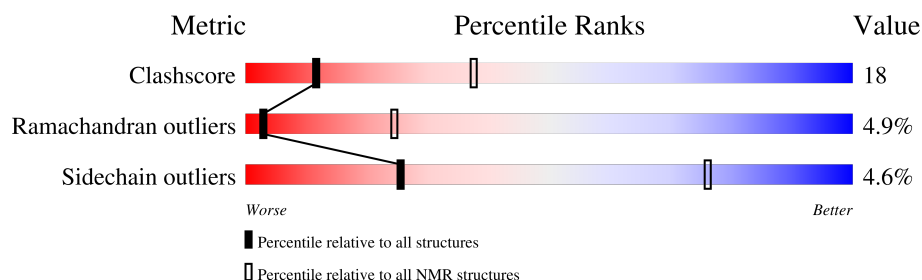
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 82%.

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     | 106    |                  |

## 2 Ensemble composition and analysis

This entry contains 10 models. Model 2 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:97 (96)         | 0.73              | 2            |

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

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

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

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

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1665 atoms, of which 853 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Poly [ADP-ribose] polymerase 1.

| Mol | Chain | Residues | Atoms |     |     |     |     |   | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|-------|
| 1   | A     | 106      | Total | C   | H   | N   | O   | S | 0     |
|     |       |          | 1665  | 504 | 853 | 147 | 154 | 7 |       |

There are 7 discrepancies between the modelled and reference sequences:

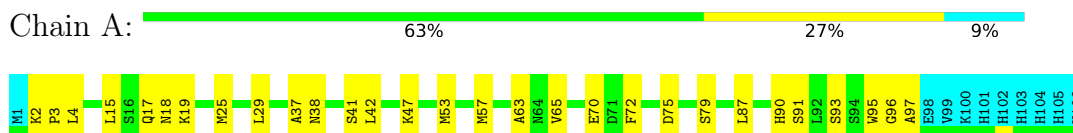
| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| A     | 1       | MET      | -      | initiating methionine | UNP P27008 |
| A     | 101     | HIS      | -      | expression tag        | UNP P27008 |
| A     | 102     | HIS      | -      | expression tag        | UNP P27008 |
| A     | 103     | HIS      | -      | expression tag        | UNP P27008 |
| A     | 104     | HIS      | -      | expression tag        | UNP P27008 |
| A     | 105     | HIS      | -      | expression tag        | UNP P27008 |
| A     | 106     | HIS      | -      | expression tag        | UNP P27008 |

## 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: Poly [ADP-ribose] polymerase 1

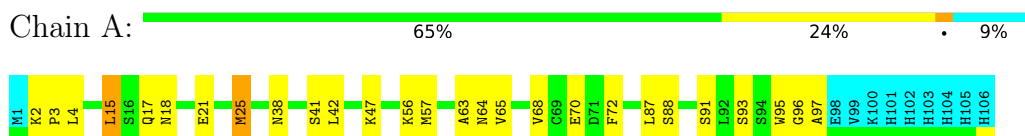


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

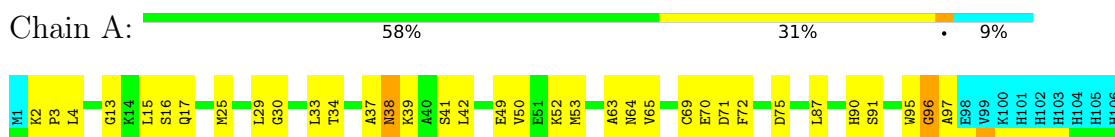
#### 4.2.1 Score per residue for model 1

- Molecule 1: Poly [ADP-ribose] polymerase 1



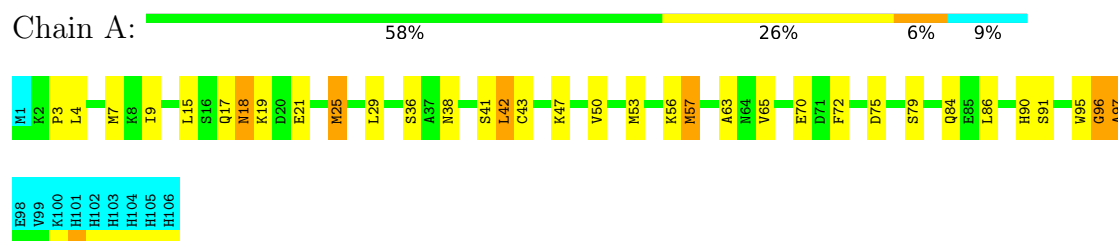
#### 4.2.2 Score per residue for model 2 (medoid)

- Molecule 1: Poly [ADP-ribose] polymerase 1



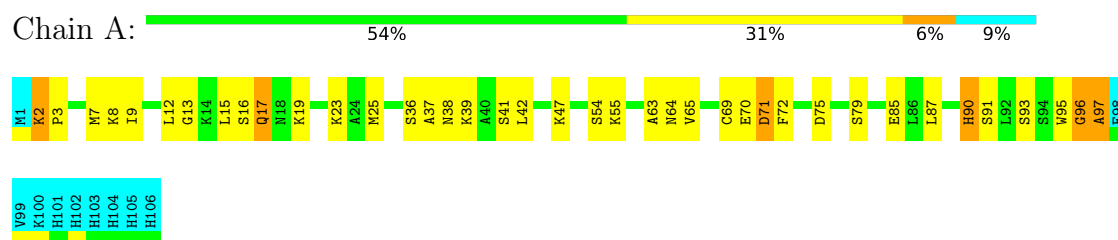
### 4.2.3 Score per residue for model 3

- Molecule 1: Poly [ADP-ribose] polymerase 1



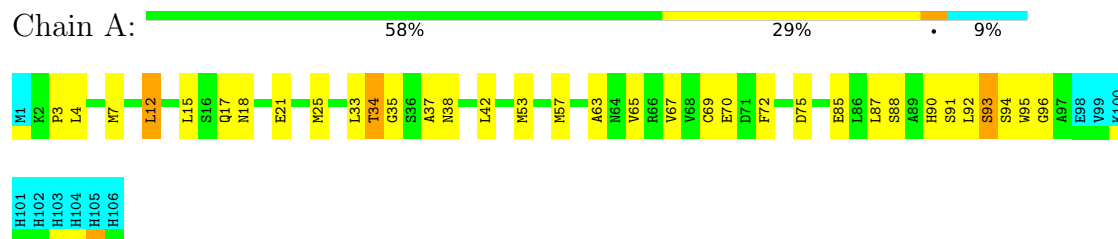
### 4.2.4 Score per residue for model 4

- Molecule 1: Poly [ADP-ribose] polymerase 1



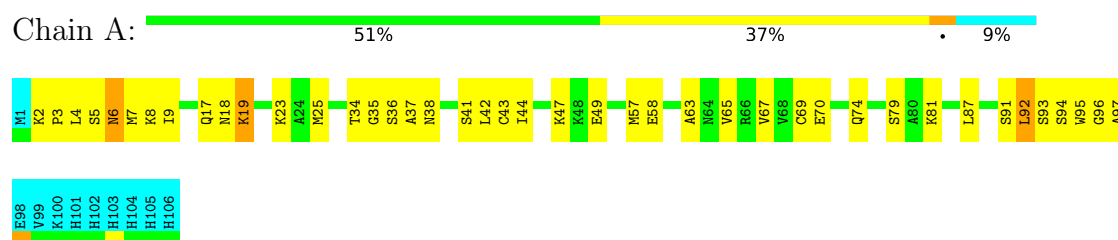
### 4.2.5 Score per residue for model 5

- Molecule 1: Poly [ADP-ribose] polymerase 1



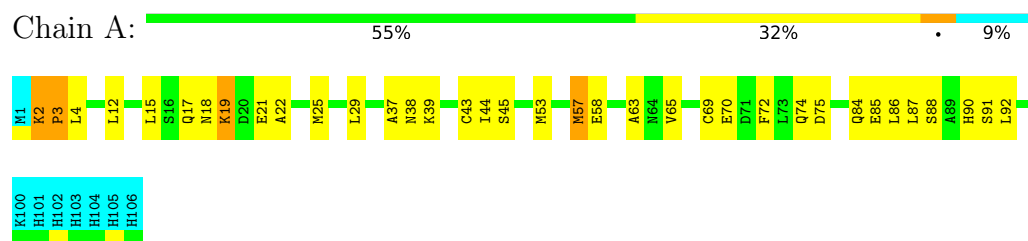
### 4.2.6 Score per residue for model 6

- Molecule 1: Poly [ADP-ribose] polymerase 1



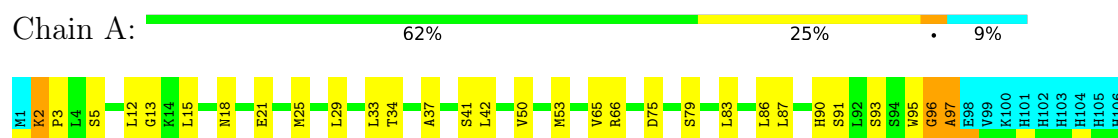
### 4.2.7 Score per residue for model 7

- Molecule 1: Poly [ADP-ribose] polymerase 1



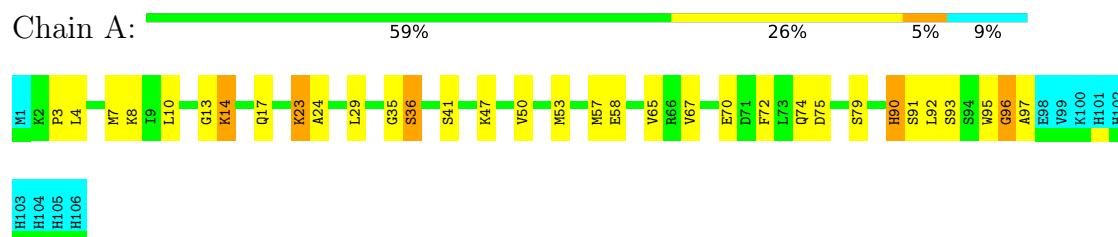
### 4.2.8 Score per residue for model 8

- Molecule 1: Poly [ADP-ribose] polymerase 1



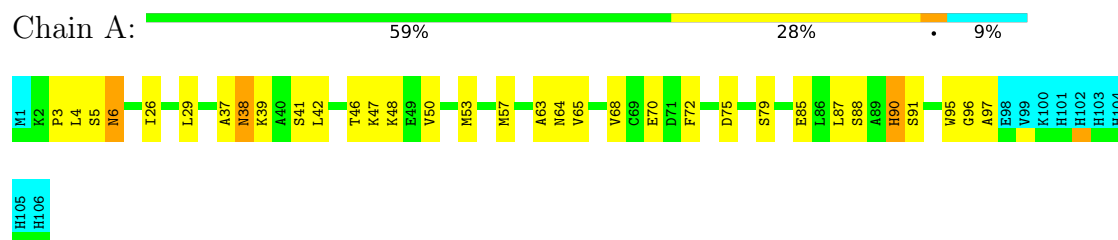
### 4.2.9 Score per residue for model 9

- Molecule 1: Poly [ADP-ribose] polymerase 1



### 4.2.10 Score per residue for model 10

- Molecule 1: Poly [ADP-ribose] polymerase 1



## 5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 10 were deposited, based on the following criterion: *structures with the lowest energy*.

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

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

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

|                                              |                |
|----------------------------------------------|----------------|
| Chemical shift file(s)                       | working_cs.cif |
| Number of chemical shift lists               | 1              |
| Total number of shifts                       | 1095           |
| Number of shifts mapped to atoms             | 1095           |
| Number of unparsed shifts                    | 0              |
| Number of shifts with mapping errors         | 0              |
| Number of shifts with mapping warnings       | 0              |
| Assignment completeness (well-defined parts) | 82%            |



## 6 Model quality

### 6.1 Standard geometry

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     | 0.59±0.01    | 0±0/723 ( 0.0± 0.0%) | 1.00±0.01   | 0±0/964 ( 0.1± 0.1%) |
| All | All   | 0.59         | 0/7230 ( 0.0%)       | 1.00        | 5/9640 ( 0.1%)       |

There are no bond-length outliers.

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

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) | Models |       |
|-----|-------|-----|------|----------|-------|-------------|----------|--------|-------|
|     |       |     |      |          |       |             |          | Worst  | Total |
| 1   | A     | 36  | SER  | CB-CA-C  | -5.88 | 109.77      | 116.54   | 3      | 1     |
| 1   | A     | 30  | GLY  | N-CA-C   | -5.49 | 107.21      | 114.95   | 2      | 1     |
| 1   | A     | 90  | HIS  | CA-CB-CG | -5.25 | 108.55      | 113.80   | 4      | 3     |

There are no chirality outliers.

There are no planarity outliers.

### 6.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes |
|-----|-------|-------|----------|----------|---------|
| 1   | A     | 718   | 766      | 765      | 26±3    |
| All | All   | 7180  | 7660     | 7650     | 262     |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 18.

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

| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:4:LEU:HD12  | 1:A:29:LEU:HD12 | 0.83     | 1.50        | 3      | 5     |
| 1:A:7:MET:HE3   | 1:A:41:SER:OG   | 0.76     | 1.80        | 9      | 4     |
| 1:A:50:VAL:O    | 1:A:53:MET:SD   | 0.72     | 2.47        | 10     | 1     |
| 1:A:87:LEU:HD12 | 1:A:87:LEU:C    | 0.69     | 2.13        | 1      | 4     |
| 1:A:15:LEU:H    | 1:A:15:LEU:HD23 | 0.66     | 1.48        | 1      | 3     |
| 1:A:17:GLN:NE2  | 1:A:74:GLN:NE2  | 0.63     | 2.45        | 9      | 2     |
| 1:A:69:CYS:SG   | 1:A:70:GLU:N    | 0.62     | 2.73        | 4      | 4     |
| 1:A:65:VAL:O    | 1:A:95:TRP:NE1  | 0.61     | 2.32        | 5      | 10    |
| 1:A:91:SER:O    | 1:A:93:SER:N    | 0.61     | 2.33        | 9      | 2     |
| 1:A:96:GLY:O    | 1:A:97:ALA:HB3  | 0.60     | 1.97        | 9      | 5     |
| 1:A:15:LEU:H    | 1:A:15:LEU:CD2  | 0.59     | 2.11        | 1      | 1     |
| 1:A:41:SER:C    | 1:A:42:LEU:HD12 | 0.59     | 2.23        | 10     | 4     |
| 1:A:53:MET:CE   | 1:A:57:MET:HE2  | 0.59     | 2.28        | 10     | 4     |
| 1:A:91:SER:C    | 1:A:93:SER:H    | 0.58     | 2.06        | 5      | 3     |
| 1:A:85:GLU:N    | 1:A:85:GLU:OE1  | 0.58     | 2.36        | 4      | 1     |
| 1:A:70:GLU:H    | 1:A:70:GLU:CD   | 0.57     | 2.08        | 1      | 1     |
| 1:A:75:ASP:OD2  | 1:A:90:HIS:NE2  | 0.57     | 2.38        | 7      | 7     |
| 1:A:91:SER:C    | 1:A:93:SER:N    | 0.56     | 2.62        | 6      | 3     |
| 1:A:93:SER:OG   | 1:A:95:TRP:CD2  | 0.56     | 2.58        | 4      | 3     |
| 1:A:38:ASN:ND2  | 1:A:63:ALA:O    | 0.56     | 2.39        | 5      | 8     |
| 1:A:70:GLU:O    | 1:A:74:GLN:NE2  | 0.55     | 2.39        | 6      | 1     |
| 1:A:12:LEU:HD23 | 1:A:12:LEU:O    | 0.55     | 2.01        | 8      | 1     |
| 1:A:15:LEU:HD23 | 1:A:15:LEU:N    | 0.54     | 2.18        | 1      | 3     |
| 1:A:50:VAL:O    | 1:A:53:MET:HE2  | 0.54     | 2.02        | 3      | 4     |
| 1:A:2:LYS:N     | 1:A:3:PRO:CD    | 0.54     | 2.71        | 1      | 3     |
| 1:A:70:GLU:C    | 1:A:72:PHE:N    | 0.53     | 2.64        | 7      | 6     |
| 1:A:42:LEU:HD23 | 1:A:68:VAL:HG11 | 0.53     | 1.80        | 10     | 2     |
| 1:A:96:GLY:O    | 1:A:97:ALA:CB   | 0.53     | 2.57        | 3      | 3     |
| 1:A:15:LEU:CD2  | 1:A:15:LEU:N    | 0.53     | 2.71        | 1      | 2     |
| 1:A:67:VAL:O    | 1:A:91:SER:O    | 0.53     | 2.26        | 9      | 3     |
| 1:A:12:LEU:O    | 1:A:12:LEU:HD13 | 0.53     | 2.03        | 5      | 1     |
| 1:A:25:MET:HE1  | 1:A:74:GLN:NE2  | 0.53     | 2.18        | 7      | 1     |
| 1:A:7:MET:HE1   | 1:A:42:LEU:HD12 | 0.52     | 1.81        | 6      | 3     |
| 1:A:12:LEU:CD1  | 1:A:43:CYS:SG   | 0.52     | 2.98        | 7      | 1     |
| 1:A:2:LYS:H     | 1:A:3:PRO:CD    | 0.52     | 2.18        | 7      | 1     |
| 1:A:37:ALA:C    | 1:A:39:LYS:H    | 0.51     | 2.13        | 10     | 4     |
| 1:A:4:LEU:HD22  | 1:A:9:ILE:HD11  | 0.51     | 1.82        | 3      | 1     |
| 1:A:87:LEU:C    | 1:A:87:LEU:CD1  | 0.51     | 2.84        | 1      | 3     |
| 1:A:33:LEU:O    | 1:A:34:THR:OG1  | 0.51     | 2.26        | 2      | 3     |
| 1:A:25:MET:SD   | 1:A:25:MET:C    | 0.51     | 2.94        | 2      | 5     |
| 1:A:95:TRP:C    | 1:A:95:TRP:CD1  | 0.51     | 2.88        | 4      | 6     |
| 1:A:93:SER:OG   | 1:A:95:TRP:CE3  | 0.51     | 2.63        | 6      | 2     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:42:LEU:HD13 | 1:A:43:CYS:N    | 0.50     | 2.22        | 3      | 1     |
| 1:A:72:PHE:CD1  | 1:A:72:PHE:C    | 0.50     | 2.90        | 2      | 7     |
| 1:A:85:GLU:O    | 1:A:88:SER:OG   | 0.50     | 2.28        | 5      | 3     |
| 1:A:7:MET:HE2   | 1:A:9:ILE:HD11  | 0.50     | 1.82        | 4      | 1     |
| 1:A:18:ASN:HD22 | 1:A:21:GLU:CD   | 0.50     | 2.15        | 3      | 4     |
| 1:A:18:ASN:HD21 | 1:A:21:GLU:CD   | 0.49     | 2.14        | 8      | 1     |
| 1:A:87:LEU:O    | 1:A:91:SER:OG   | 0.48     | 2.31        | 2      | 3     |
| 1:A:17:GLN:NE2  | 1:A:70:GLU:CD   | 0.48     | 2.71        | 2      | 1     |
| 1:A:5:SER:O     | 1:A:6:ASN:CB    | 0.48     | 2.61        | 6      | 2     |
| 1:A:53:MET:HE3  | 1:A:57:MET:HE2  | 0.48     | 1.85        | 10     | 1     |
| 1:A:70:GLU:O    | 1:A:72:PHE:N    | 0.48     | 2.47        | 2      | 4     |
| 1:A:42:LEU:C    | 1:A:42:LEU:CD1  | 0.48     | 2.87        | 3      | 1     |
| 1:A:79:SER:OG   | 1:A:81:LYS:CD   | 0.48     | 2.62        | 6      | 1     |
| 1:A:86:LEU:O    | 1:A:90:HIS:CD2  | 0.48     | 2.67        | 3      | 3     |
| 1:A:17:GLN:N    | 1:A:70:GLU:OE2  | 0.48     | 2.47        | 5      | 1     |
| 1:A:43:CYS:SG   | 1:A:44:ILE:N    | 0.48     | 2.87        | 6      | 2     |
| 1:A:47:LYS:O    | 1:A:50:VAL:N    | 0.47     | 2.47        | 10     | 1     |
| 1:A:8:LYS:O     | 1:A:41:SER:OG   | 0.47     | 2.32        | 9      | 3     |
| 1:A:70:GLU:OE1  | 1:A:70:GLU:N    | 0.47     | 2.46        | 10     | 1     |
| 1:A:43:CYS:SG   | 1:A:65:VAL:HG11 | 0.47     | 2.49        | 3      | 1     |
| 1:A:75:ASP:O    | 1:A:79:SER:N    | 0.47     | 2.48        | 10     | 5     |
| 1:A:15:LEU:N    | 1:A:15:LEU:CD2  | 0.47     | 2.77        | 5      | 1     |
| 1:A:15:LEU:HD11 | 1:A:70:GLU:OE2  | 0.47     | 2.09        | 7      | 1     |
| 1:A:87:LEU:O    | 1:A:91:SER:CB   | 0.47     | 2.63        | 4      | 3     |
| 1:A:46:THR:CG2  | 1:A:70:GLU:OE1  | 0.47     | 2.63        | 10     | 1     |
| 1:A:47:LYS:O    | 1:A:48:LYS:C    | 0.47     | 2.58        | 10     | 1     |
| 1:A:17:GLN:CD   | 1:A:70:GLU:OE2  | 0.47     | 2.58        | 3      | 2     |
| 1:A:35:GLY:O    | 1:A:36:SER:C    | 0.46     | 2.59        | 9      | 1     |
| 1:A:18:ASN:ND2  | 1:A:21:GLU:OE2  | 0.46     | 2.48        | 7      | 2     |
| 1:A:4:LEU:CD2   | 1:A:4:LEU:N     | 0.46     | 2.78        | 1      | 1     |
| 1:A:17:GLN:CG   | 1:A:70:GLU:OE2  | 0.46     | 2.63        | 3      | 1     |
| 1:A:47:LYS:C    | 1:A:49:GLU:N    | 0.46     | 2.71        | 6      | 1     |
| 1:A:70:GLU:C    | 1:A:72:PHE:H    | 0.45     | 2.20        | 2      | 2     |
| 1:A:12:LEU:O    | 1:A:13:GLY:C    | 0.45     | 2.58        | 4      | 1     |
| 1:A:90:HIS:O    | 1:A:91:SER:C    | 0.45     | 2.60        | 4      | 1     |
| 1:A:92:LEU:O    | 1:A:93:SER:O    | 0.45     | 2.34        | 5      | 1     |
| 1:A:13:GLY:O    | 1:A:14:LYS:O    | 0.45     | 2.34        | 9      | 1     |
| 1:A:95:TRP:CD1  | 1:A:95:TRP:C    | 0.45     | 2.95        | 1      | 1     |
| 1:A:25:MET:SD   | 1:A:25:MET:O    | 0.45     | 2.75        | 8      | 3     |
| 1:A:34:THR:CG2  | 1:A:35:GLY:N    | 0.45     | 2.80        | 5      | 1     |
| 1:A:33:LEU:C    | 1:A:34:THR:HG1  | 0.45     | 2.19        | 8      | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:17:GLN:NE2  | 1:A:70:GLU:OE2  | 0.45     | 2.50        | 3      | 1     |
| 1:A:84:GLN:N    | 1:A:84:GLN:CD   | 0.45     | 2.75        | 3      | 2     |
| 1:A:15:LEU:HD11 | 1:A:70:GLU:CD   | 0.44     | 2.37        | 2      | 1     |
| 1:A:64:ASN:OD1  | 1:A:97:ALA:N    | 0.44     | 2.50        | 10     | 2     |
| 1:A:5:SER:O     | 1:A:6:ASN:CG    | 0.44     | 2.61        | 10     | 2     |
| 1:A:5:SER:O     | 1:A:6:ASN:ND2   | 0.44     | 2.50        | 10     | 1     |
| 1:A:91:SER:OG   | 1:A:93:SER:O    | 0.44     | 2.36        | 1      | 2     |
| 1:A:66:ARG:NH1  | 1:A:87:LEU:HD22 | 0.44     | 2.28        | 8      | 1     |
| 1:A:34:THR:OG1  | 1:A:35:GLY:N    | 0.44     | 2.51        | 6      | 1     |
| 1:A:19:LYS:HD3  | 1:A:23:LYS:HZ1  | 0.44     | 1.71        | 6      | 1     |
| 1:A:49:GLU:O    | 1:A:52:LYS:CG   | 0.43     | 2.66        | 2      | 1     |
| 1:A:17:GLN:NE2  | 1:A:70:GLU:CG   | 0.43     | 2.81        | 3      | 1     |
| 1:A:5:SER:C     | 1:A:6:ASN:CG    | 0.43     | 2.86        | 10     | 2     |
| 1:A:4:LEU:HD12  | 1:A:29:LEU:CD1  | 0.43     | 2.34        | 10     | 2     |
| 1:A:4:LEU:HD22  | 1:A:4:LEU:N     | 0.43     | 2.27        | 6      | 1     |
| 1:A:16:SER:O    | 1:A:17:GLN:O    | 0.43     | 2.37        | 4      | 1     |
| 1:A:4:LEU:HD12  | 1:A:9:ILE:HD11  | 0.43     | 1.90        | 6      | 1     |
| 1:A:5:SER:OG    | 1:A:29:LEU:O    | 0.43     | 2.37        | 8      | 1     |
| 1:A:4:LEU:N     | 1:A:4:LEU:HD22  | 0.43     | 2.29        | 1      | 1     |
| 1:A:47:LYS:C    | 1:A:49:GLU:H    | 0.43     | 2.22        | 6      | 1     |
| 1:A:93:SER:OG   | 1:A:94:SER:N    | 0.43     | 2.51        | 6      | 1     |
| 1:A:4:LEU:N     | 1:A:4:LEU:CD2   | 0.42     | 2.82        | 6      | 1     |
| 1:A:33:LEU:C    | 1:A:34:THR:OG1  | 0.42     | 2.62        | 8      | 1     |
| 1:A:42:LEU:HD21 | 1:A:66:ARG:HH21 | 0.42     | 1.74        | 8      | 1     |
| 1:A:87:LEU:O    | 1:A:91:SER:N    | 0.42     | 2.52        | 10     | 1     |
| 1:A:4:LEU:CD1   | 1:A:29:LEU:HD12 | 0.42     | 2.35        | 3      | 1     |
| 1:A:23:LYS:NZ   | 1:A:23:LYS:CB   | 0.42     | 2.82        | 9      | 1     |
| 1:A:5:SER:O     | 1:A:6:ASN:OD1   | 0.42     | 2.38        | 6      | 1     |
| 1:A:87:LEU:HD12 | 1:A:87:LEU:O    | 0.42     | 2.15        | 5      | 1     |
| 1:A:4:LEU:HD12  | 1:A:4:LEU:N     | 0.42     | 2.30        | 5      | 1     |
| 1:A:2:LYS:H     | 1:A:3:PRO:HD2   | 0.42     | 1.74        | 7      | 1     |
| 1:A:23:LYS:CG   | 1:A:24:ALA:N    | 0.42     | 2.83        | 9      | 1     |
| 1:A:37:ALA:O    | 1:A:39:LYS:N    | 0.41     | 2.53        | 10     | 1     |
| 1:A:70:GLU:CD   | 1:A:70:GLU:N    | 0.41     | 2.77        | 1      | 1     |
| 1:A:37:ALA:C    | 1:A:39:LYS:N    | 0.41     | 2.78        | 2      | 2     |
| 1:A:21:GLU:CG   | 1:A:22:ALA:N    | 0.41     | 2.84        | 7      | 1     |
| 1:A:87:LEU:HD12 | 1:A:88:SER:N    | 0.41     | 2.30        | 1      | 1     |
| 1:A:15:LEU:HD21 | 1:A:17:GLN:O    | 0.41     | 2.15        | 1      | 1     |
| 1:A:42:LEU:CD1  | 1:A:43:CYS:O    | 0.41     | 2.69        | 3      | 1     |
| 1:A:83:LEU:HD12 | 1:A:83:LEU:H    | 0.41     | 1.75        | 8      | 1     |
| 1:A:54:SER:OG   | 1:A:55:LYS:N    | 0.41     | 2.54        | 4      | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:4:LEU:HD13  | 1:A:7:MET:SD    | 0.41     | 2.56        | 6      | 1     |
| 1:A:12:LEU:HD23 | 1:A:12:LEU:C    | 0.41     | 2.41        | 8      | 1     |
| 1:A:66:ARG:HH12 | 1:A:87:LEU:HD22 | 0.40     | 1.75        | 8      | 1     |
| 1:A:70:GLU:O    | 1:A:71:ASP:C    | 0.40     | 2.64        | 4      | 1     |
| 1:A:91:SER:O    | 1:A:92:LEU:C    | 0.40     | 2.64        | 6      | 1     |
| 1:A:45:SER:O    | 1:A:92:LEU:CD1  | 0.40     | 2.70        | 7      | 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     | 96/106 (91%)   | 84±2 (87±2%) | 7±2 (8±2%) | 5±1 (5±1%) | 3           | 24 |
| All | All   | 960/1060 (91%) | 839 (87%)    | 74 (8%)    | 47 (5%)    | 3           | 24 |

All 19 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     | 96  | GLY  | 9              |
| 1   | A     | 3   | PRO  | 8              |
| 1   | A     | 97  | ALA  | 4              |
| 1   | A     | 19  | LYS  | 3              |
| 1   | A     | 37  | ALA  | 3              |
| 1   | A     | 13  | GLY  | 2              |
| 1   | A     | 38  | ASN  | 2              |
| 1   | A     | 71  | ASP  | 2              |
| 1   | A     | 18  | ASN  | 2              |
| 1   | A     | 6   | ASN  | 2              |
| 1   | A     | 92  | LEU  | 2              |
| 1   | A     | 16  | SER  | 1              |
| 1   | A     | 91  | SER  | 1              |
| 1   | A     | 17  | GLN  | 1              |
| 1   | A     | 93  | SER  | 1              |
| 1   | A     | 94  | SER  | 1              |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 2   | LYS  | 1              |
| 1   | A     | 14  | LYS  | 1              |
| 1   | A     | 36  | SER  | 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     | 81/91 (89%)   | 77±2 (95±3%) | 4±2 (5±3%) | 25          | 76 |
| All | All   | 810/910 (89%) | 773 (95%)    | 37 (5%)    | 25          | 76 |

All 17 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     | 57  | MET  | 5              |
| 1   | A     | 25  | MET  | 4              |
| 1   | A     | 47  | LYS  | 4              |
| 1   | A     | 15  | LEU  | 3              |
| 1   | A     | 2   | LYS  | 3              |
| 1   | A     | 58  | GLU  | 3              |
| 1   | A     | 56  | LYS  | 2              |
| 1   | A     | 23  | LYS  | 2              |
| 1   | A     | 36  | SER  | 2              |
| 1   | A     | 19  | LYS  | 2              |
| 1   | A     | 42  | LEU  | 1              |
| 1   | A     | 64  | ASN  | 1              |
| 1   | A     | 12  | LEU  | 1              |
| 1   | A     | 34  | THR  | 1              |
| 1   | A     | 69  | CYS  | 1              |
| 1   | A     | 10  | LEU  | 1              |
| 1   | A     | 26  | ILE  | 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 82% for the well-defined parts and 77% for the entire structure.

### 7.1 Chemical shift list 1

File name: working\_cs.cif

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

#### 7.1.1 Bookkeeping

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

|                                         |      |
|-----------------------------------------|------|
| Total number of shifts                  | 1095 |
| Number of shifts mapped to atoms        | 1095 |
| Number of unparsed shifts               | 0    |
| Number of shifts with mapping errors    | 0    |
| Number of shifts with mapping warnings  | 0    |
| Number of shift outliers (ShiftChecker) | 1    |

#### 7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

| Nucleus                | # values | Correction $\pm$ precision, ppm | Suggested action           |
|------------------------|----------|---------------------------------|----------------------------|
| $^{13}\text{C}_\alpha$ | 98       | $-0.10 \pm 0.11$                | None needed ( $< 0.5$ ppm) |
| $^{13}\text{C}_\beta$  | 93       | $-0.01 \pm 0.11$                | None needed ( $< 0.5$ ppm) |
| $^{13}\text{C}'$       | 0        | —                               | None (insufficient data)   |
| $^{15}\text{N}$        | 90       | $0.27 \pm 0.39$                 | 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 82%, i.e. 1041 atoms were assigned a chemical shift out of a possible 1268. 0 out of 18 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total         | $^1\text{H}$  | $^{13}\text{C}$ | $^{15}\text{N}$ |
|-----------|---------------|---------------|-----------------|-----------------|
| Backbone  | 352/483 (73%) | 174/196 (89%) | 93/192 (48%)    | 85/95 (89%)     |
| Sidechain | 671/755 (89%) | 453/492 (92%) | 211/238 (89%)   | 7/25 (28%)      |

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|          | <b>Total</b>    | <b><sup>1</sup>H</b> | <b><sup>13</sup>C</b> | <b><sup>15</sup>N</b> |
|----------|-----------------|----------------------|-----------------------|-----------------------|
| Aromatic | 18/30 (60%)     | 9/15 (60%)           | 8/12 (67%)            | 1/3 (33%)             |
| Overall  | 1041/1268 (82%) | 636/703 (90%)        | 312/442 (71%)         | 93/123 (76%)          |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 77%, i.e. 1095 atoms were assigned a chemical shift out of a possible 1424. 0 out of 19 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | <b>Total</b>    | <b><sup>1</sup>H</b> | <b><sup>13</sup>C</b> | <b><sup>15</sup>N</b> |
|-----------|-----------------|----------------------|-----------------------|-----------------------|
| Backbone  | 371/533 (70%)   | 183/216 (85%)        | 98/212 (46%)          | 90/105 (86%)          |
| Sidechain | 706/813 (87%)   | 477/530 (90%)        | 222/257 (86%)         | 7/26 (27%)            |
| Aromatic  | 18/78 (23%)     | 9/39 (23%)           | 8/24 (33%)            | 1/15 (7%)             |
| Overall   | 1095/1424 (77%) | 669/785 (85%)        | 328/493 (67%)         | 98/146 (67%)          |

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

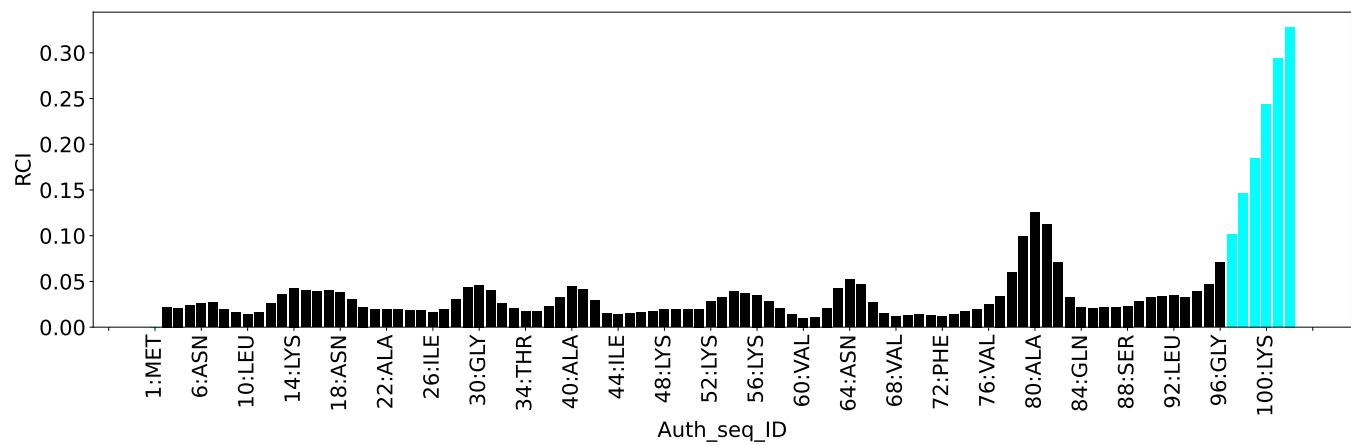
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

| List Id | Chain | Res | Type | Atom | Shift, ppm | Expected range, ppm | Z-score |
|---------|-------|-----|------|------|------------|---------------------|---------|
| 1       | A     | 61  | LYS  | HB3  | -0.15      | 0.46 – 3.04         | -7.4    |

#### 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                                | 1631  |
| Intra-residue ( $ i-j =0$ )                              | 449   |
| Sequential ( $ i-j =1$ )                                 | 447   |
| Medium range ( $ i-j >1$ and $ i-j <5$ )                 | 330   |
| Long range ( $ i-j \geq 5$ )                             | 405   |
| Inter-chain                                              | 0     |
| Hydrogen bond restraints                                 | 0     |
| Disulfide bond restraints                                | 0     |
| Total dihedral-angle restraints                          | 387   |
| Number of unmapped restraints                            | 0     |
| Number of restraints per residue                         | 19.0  |
| Number of long range restraints per residue <sup>1</sup> | 3.8   |

<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)  | 13.4                                   | 0.2     |
| 0.2-0.5 (Medium) | 25.0                                   | 0.5     |
| >0.5 (Large)     | 70.4                                   | 9.49    |

### 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)   | 2.1                                    | 9.78    |
| 10.0-20.0 (Medium) | 1.2                                    | 19.01   |
| >20.0 (Large)      | 0.8                                    | 48.28   |

## 9 Distance violation analysis ⓘ

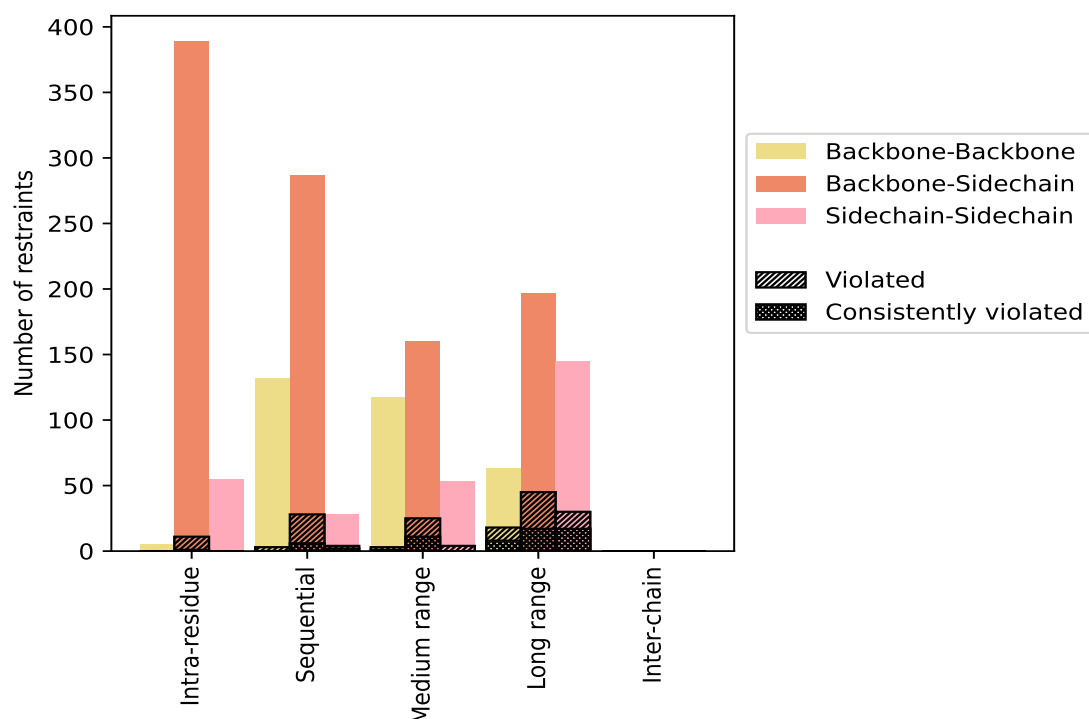
### 9.1 Summary of distance violations ⓘ

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>449</b>  | <b>27.5</b>    | <b>11</b>             | <b>2.4</b>     | <b>0.7</b>     | <b>1</b>                           | <b>0.2</b>     | <b>0.1</b>     |
| Backbone-Backbone                                                           | 5           | 0.3            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 389         | 23.9           | 11                    | 2.8            | 0.7            | 1                                  | 0.3            | 0.1            |
| Sidechain-Sidechain                                                         | 55          | 3.4            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| <b>Sequential (<math> i-j =1</math>)</b>                                    | <b>447</b>  | <b>27.4</b>    | <b>35</b>             | <b>7.8</b>     | <b>2.1</b>     | <b>8</b>                           | <b>1.8</b>     | <b>0.5</b>     |
| Backbone-Backbone                                                           | 132         | 8.1            | 3                     | 2.3            | 0.2            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 287         | 17.6           | 28                    | 9.8            | 1.7            | 6                                  | 2.1            | 0.4            |
| Sidechain-Sidechain                                                         | 28          | 1.7            | 4                     | 14.3           | 0.2            | 2                                  | 7.1            | 0.1            |
| <b>Medium range (<math> i-j &gt;1</math> &amp; <math> i-j &lt;5</math>)</b> | <b>330</b>  | <b>20.2</b>    | <b>32</b>             | <b>9.7</b>     | <b>2.0</b>     | <b>12</b>                          | <b>3.6</b>     | <b>0.7</b>     |
| Backbone-Backbone                                                           | 117         | 7.2            | 3                     | 2.6            | 0.2            | 1                                  | 0.9            | 0.1            |
| Backbone-Sidechain                                                          | 160         | 9.8            | 25                    | 15.6           | 1.5            | 11                                 | 6.9            | 0.7            |
| Sidechain-Sidechain                                                         | 53          | 3.2            | 4                     | 7.5            | 0.2            | 0                                  | 0.0            | 0.0            |
| <b>Long range (<math> i-j \geq 5</math>)</b>                                | <b>405</b>  | <b>24.8</b>    | <b>93</b>             | <b>23.0</b>    | <b>5.7</b>     | <b>42</b>                          | <b>10.4</b>    | <b>2.6</b>     |
| Backbone-Backbone                                                           | 63          | 3.9            | 18                    | 28.6           | 1.1            | 8                                  | 12.7           | 0.5            |
| Backbone-Sidechain                                                          | 197         | 12.1           | 45                    | 22.8           | 2.8            | 17                                 | 8.6            | 1.0            |
| Sidechain-Sidechain                                                         | 145         | 8.9            | 30                    | 20.7           | 1.8            | 17                                 | 11.7           | 1.0            |
| <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>1631</b> | <b>100.0</b>   | <b>171</b>            | <b>10.5</b>    | <b>10.5</b>    | <b>63</b>                          | <b>3.9</b>     | <b>3.9</b>     |
| Backbone-Backbone                                                           | 317         | 19.4           | 24                    | 7.6            | 1.5            | 9                                  | 2.8            | 0.6            |
| Backbone-Sidechain                                                          | 1033        | 63.3           | 109                   | 10.6           | 6.7            | 35                                 | 3.4            | 2.1            |
| Sidechain-Sidechain                                                         | 281         | 17.2           | 38                    | 13.5           | 2.3            | 19                                 | 6.8            | 1.2            |

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

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



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

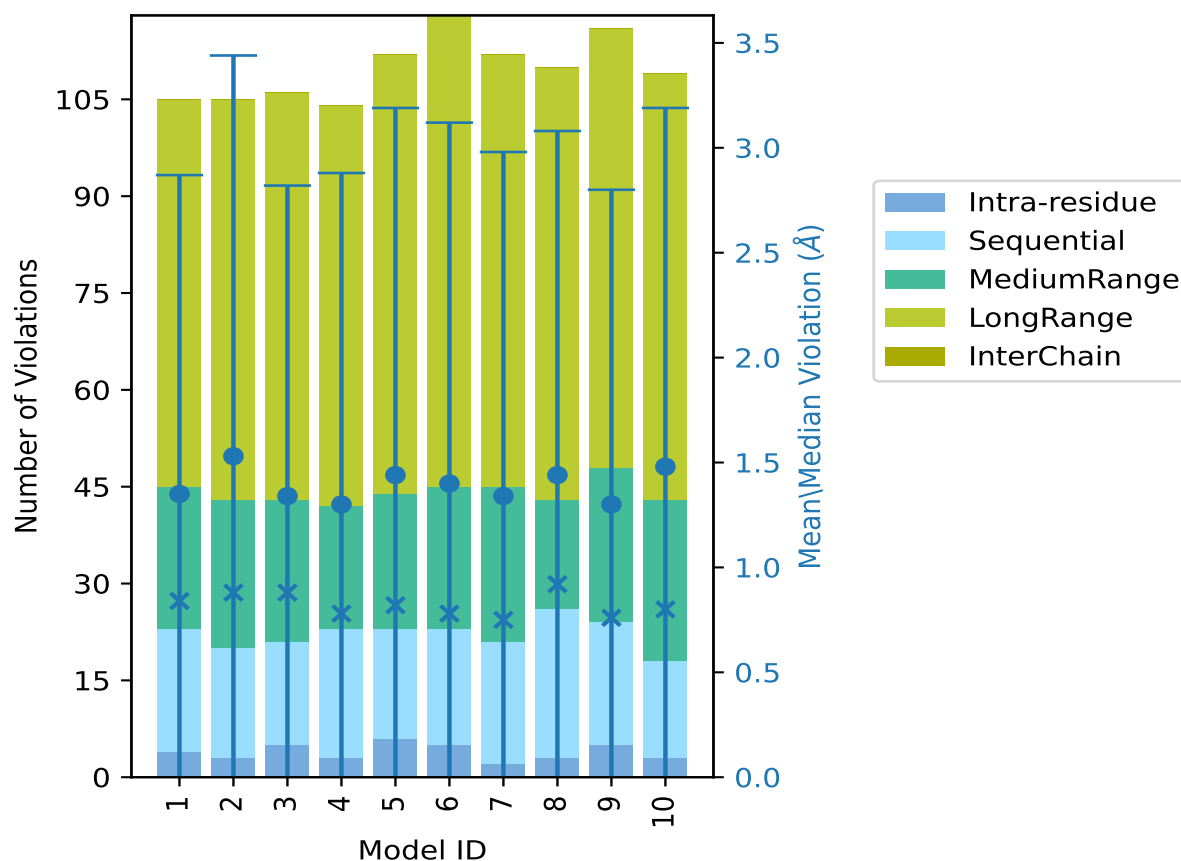
## 9.2 Distance violation statistics for each model [i](#)

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

| Model ID | Number of violations |                 |                 |                 |                 |       | Mean (Å) | Max (Å) | SD <sup>6</sup> (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
|          | IR <sup>1</sup>      | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total |          |         |                     |            |
| 1        | 4                    | 19              | 22              | 60              | 0               | 105   | 1.35     | 8.4     | 1.52                | 0.84       |
| 2        | 3                    | 17              | 23              | 62              | 0               | 105   | 1.53     | 9.49    | 1.91                | 0.88       |
| 3        | 5                    | 16              | 22              | 63              | 0               | 106   | 1.34     | 7.25    | 1.48                | 0.88       |
| 4        | 3                    | 20              | 19              | 62              | 0               | 104   | 1.3      | 8.74    | 1.58                | 0.78       |
| 5        | 6                    | 17              | 21              | 68              | 0               | 112   | 1.44     | 8.98    | 1.75                | 0.82       |
| 6        | 5                    | 18              | 22              | 73              | 0               | 118   | 1.4      | 9.21    | 1.72                | 0.78       |
| 7        | 2                    | 19              | 24              | 67              | 0               | 112   | 1.34     | 8.64    | 1.64                | 0.75       |
| 8        | 3                    | 23              | 17              | 67              | 0               | 110   | 1.44     | 9.01    | 1.64                | 0.92       |
| 9        | 5                    | 19              | 24              | 68              | 0               | 116   | 1.3      | 7.81    | 1.5                 | 0.76       |
| 10       | 3                    | 15              | 25              | 66              | 0               | 109   | 1.48     | 8.5     | 1.71                | 0.8        |

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

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



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

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

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1460(IR:438, SQ:412, MR:298, LR:312, 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>       | %    |
| 4                             | 6               | 4               | 11              | 0               | 25    | 1                        | 10.0 |
| 0                             | 4               | 2               | 6               | 0               | 12    | 2                        | 20.0 |
| 4                             | 5               | 0               | 9               | 0               | 18    | 3                        | 30.0 |

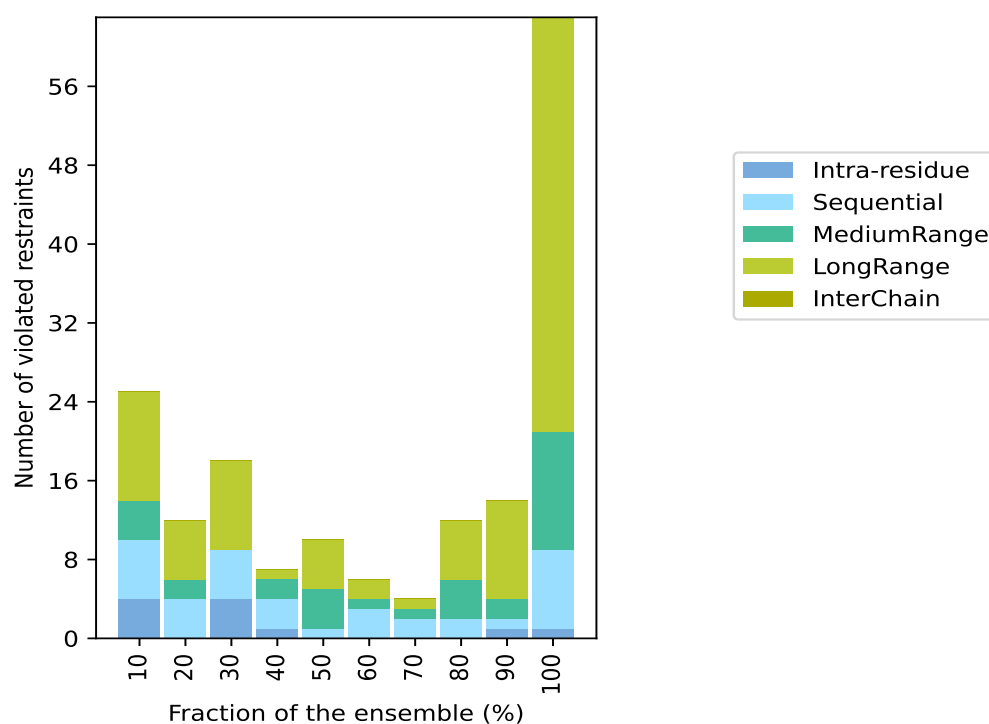
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| Number of violated restraints |                 |                 |                 |                 |       | Fraction of the ensemble |       |
|-------------------------------|-----------------|-----------------|-----------------|-----------------|-------|--------------------------|-------|
| IR <sup>1</sup>               | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total | Count <sup>6</sup>       | %     |
| 1                             | 3               | 2               | 1               | 0               | 7     | 4                        | 40.0  |
| 0                             | 1               | 4               | 5               | 0               | 10    | 5                        | 50.0  |
| 0                             | 3               | 1               | 2               | 0               | 6     | 6                        | 60.0  |
| 0                             | 2               | 1               | 1               | 0               | 4     | 7                        | 70.0  |
| 0                             | 2               | 4               | 6               | 0               | 12    | 8                        | 80.0  |
| 1                             | 1               | 2               | 10              | 0               | 14    | 9                        | 90.0  |
| 1                             | 8               | 12              | 42              | 0               | 63    | 10                       | 100.0 |

<sup>1</sup>Intra-residue restraints, <sup>2</sup>Sequential restraints, <sup>3</sup>Medium range restraints, <sup>4</sup>Long range restraints, <sup>5</sup>Inter-chain restraints, <sup>6</sup> Number of models with violations

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



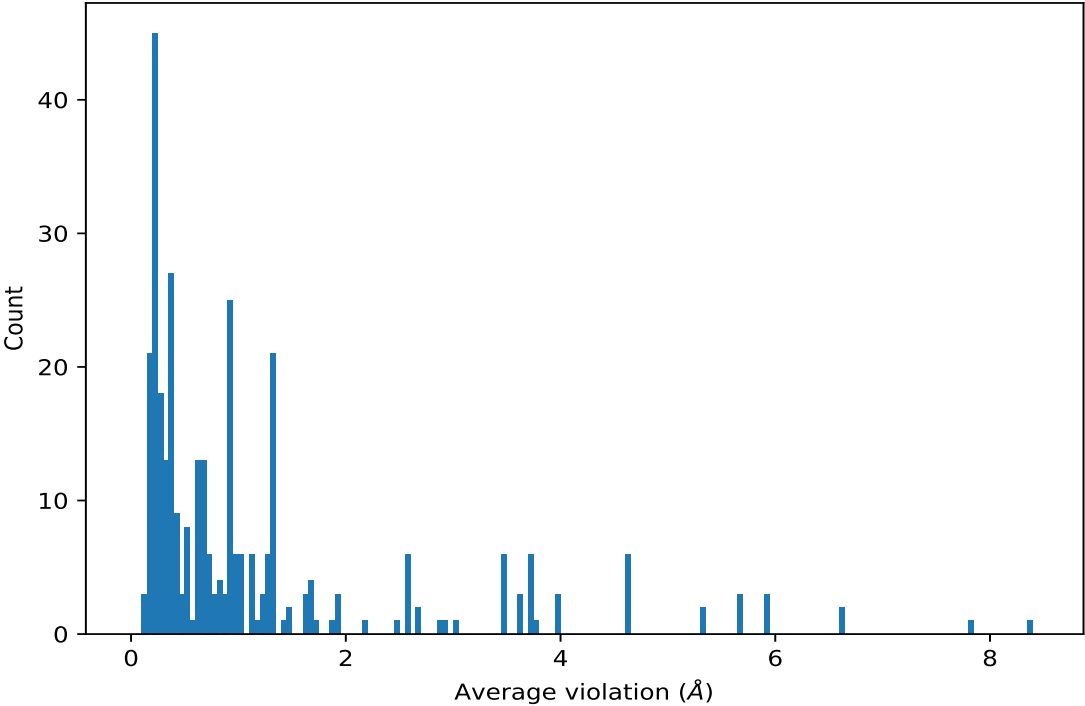
## 9.4 Most violated distance restraints in the ensemble [i](#)

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

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



in the ensemble



9.4.2 Table: Most violated distance restraints ⓘ

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

| Key      | Atom-1         | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1211) | 1:5:A:SER:H    | 1:84:A:GLN:HE22 | 10                  | 8.36     | 0.95                | 8.62       |
| (1,1212) | 1:5:A:SER:H    | 1:84:A:GLN:HE21 | 10                  | 7.84     | 0.51                | 7.82       |
| (1,1321) | 1:5:A:SER:H    | 1:84:A:GLN:HE21 | 10                  | 6.61     | 0.56                | 6.63       |
| (1,1321) | 1:5:A:SER:H    | 1:84:A:GLN:HE22 | 10                  | 6.61     | 0.56                | 6.63       |
| (1,1232) | 1:4:A:LEU:HD11 | 1:84:A:GLN:HE22 | 10                  | 5.93     | 0.88                | 6.0        |
| (1,1232) | 1:4:A:LEU:HD12 | 1:84:A:GLN:HE22 | 10                  | 5.93     | 0.88                | 6.0        |
| (1,1232) | 1:4:A:LEU:HD13 | 1:84:A:GLN:HE22 | 10                  | 5.93     | 0.88                | 6.0        |
| (1,1235) | 1:4:A:LEU:HD11 | 1:84:A:GLN:HE21 | 10                  | 5.68     | 1.04                | 5.68       |
| (1,1235) | 1:4:A:LEU:HD12 | 1:84:A:GLN:HE21 | 10                  | 5.68     | 1.04                | 5.68       |
| (1,1235) | 1:4:A:LEU:HD13 | 1:84:A:GLN:HE21 | 10                  | 5.68     | 1.04                | 5.68       |
| (1,1317) | 1:4:A:LEU:H    | 1:84:A:GLN:HE21 | 10                  | 5.3      | 0.54                | 5.3        |
| (1,1317) | 1:4:A:LEU:H    | 1:84:A:GLN:HE22 | 10                  | 5.3      | 0.54                | 5.3        |
| (1,1318) | 1:4:A:LEU:HD11 | 1:84:A:GLN:HE21 | 10                  | 4.61     | 0.84                | 4.69       |
| (1,1318) | 1:4:A:LEU:HD11 | 1:84:A:GLN:HE22 | 10                  | 4.61     | 0.84                | 4.69       |
| (1,1318) | 1:4:A:LEU:HD12 | 1:84:A:GLN:HE21 | 10                  | 4.61     | 0.84                | 4.69       |

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| Key      | Atom-1         | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1318) | 1:4:A:LEU:HD12 | 1:84:A:GLN:HE22 | 10                  | 4.61     | 0.84                | 4.69       |
| (1,1318) | 1:4:A:LEU:HD13 | 1:84:A:GLN:HE21 | 10                  | 4.61     | 0.84                | 4.69       |
| (1,1318) | 1:4:A:LEU:HD13 | 1:84:A:GLN:HE22 | 10                  | 4.61     | 0.84                | 4.69       |
| (1,1229) | 1:4:A:LEU:HD21 | 1:84:A:GLN:HE22 | 10                  | 3.98     | 1.07                | 3.92       |
| (1,1229) | 1:4:A:LEU:HD22 | 1:84:A:GLN:HE22 | 10                  | 3.98     | 1.07                | 3.92       |
| (1,1229) | 1:4:A:LEU:HD23 | 1:84:A:GLN:HE22 | 10                  | 3.98     | 1.07                | 3.92       |
| (1,170)  | 1:89:A:ALA:H   | 1:92:A:LEU:HB2  | 10                  | 3.77     | 0.61                | 4.11       |
| (1,1319) | 1:4:A:LEU:HD21 | 1:84:A:GLN:HE21 | 10                  | 3.72     | 0.86                | 3.5        |
| (1,1319) | 1:4:A:LEU:HD21 | 1:84:A:GLN:HE22 | 10                  | 3.72     | 0.86                | 3.5        |
| (1,1319) | 1:4:A:LEU:HD22 | 1:84:A:GLN:HE21 | 10                  | 3.72     | 0.86                | 3.5        |
| (1,1319) | 1:4:A:LEU:HD22 | 1:84:A:GLN:HE22 | 10                  | 3.72     | 0.86                | 3.5        |
| (1,1319) | 1:4:A:LEU:HD23 | 1:84:A:GLN:HE21 | 10                  | 3.72     | 0.86                | 3.5        |
| (1,1319) | 1:4:A:LEU:HD23 | 1:84:A:GLN:HE22 | 10                  | 3.72     | 0.86                | 3.5        |
| (1,1234) | 1:4:A:LEU:HD21 | 1:84:A:GLN:HE21 | 10                  | 3.64     | 0.91                | 3.4        |
| (1,1234) | 1:4:A:LEU:HD22 | 1:84:A:GLN:HE21 | 10                  | 3.64     | 0.91                | 3.4        |
| (1,1234) | 1:4:A:LEU:HD23 | 1:84:A:GLN:HE21 | 10                  | 3.64     | 0.91                | 3.4        |
| (1,315)  | 1:7:A:MET:HE1  | 1:84:A:GLN:HE21 | 10                  | 3.48     | 0.68                | 3.38       |
| (1,315)  | 1:7:A:MET:HE2  | 1:84:A:GLN:HE21 | 10                  | 3.48     | 0.68                | 3.38       |
| (1,315)  | 1:7:A:MET:HE3  | 1:84:A:GLN:HE21 | 10                  | 3.48     | 0.68                | 3.38       |
| (1,309)  | 1:7:A:MET:HE1  | 1:84:A:GLN:HE22 | 10                  | 3.48     | 0.78                | 3.33       |
| (1,309)  | 1:7:A:MET:HE2  | 1:84:A:GLN:HE22 | 10                  | 3.48     | 0.78                | 3.33       |
| (1,309)  | 1:7:A:MET:HE3  | 1:84:A:GLN:HE22 | 10                  | 3.48     | 0.78                | 3.33       |
| (1,1085) | 1:6:A:ASN:HA   | 1:32:A:LYS:H    | 10                  | 3.0      | 0.21                | 3.02       |
| (1,284)  | 1:72:A:PHE:HB2 | 1:87:A:LEU:HB2  | 10                  | 2.93     | 0.77                | 2.66       |
| (1,902)  | 1:72:A:PHE:HB3 | 1:87:A:LEU:H    | 10                  | 2.85     | 0.24                | 2.96       |
| (1,1413) | 1:23:A:LYS:HE2 | 1:27:A:GLU:H    | 10                  | 2.68     | 0.46                | 2.79       |
| (1,1413) | 1:23:A:LYS:HE3 | 1:27:A:GLU:H    | 10                  | 2.68     | 0.46                | 2.79       |
| (1,1327) | 1:7:A:MET:HE1  | 1:84:A:GLN:HE21 | 10                  | 2.55     | 0.64                | 2.42       |
| (1,1327) | 1:7:A:MET:HE1  | 1:84:A:GLN:HE22 | 10                  | 2.55     | 0.64                | 2.42       |
| (1,1327) | 1:7:A:MET:HE2  | 1:84:A:GLN:HE21 | 10                  | 2.55     | 0.64                | 2.42       |
| (1,1327) | 1:7:A:MET:HE2  | 1:84:A:GLN:HE22 | 10                  | 2.55     | 0.64                | 2.42       |
| (1,1327) | 1:7:A:MET:HE3  | 1:84:A:GLN:HE21 | 10                  | 2.55     | 0.64                | 2.42       |
| (1,1327) | 1:7:A:MET:HE3  | 1:84:A:GLN:HE22 | 10                  | 2.55     | 0.64                | 2.42       |
| (1,331)  | 1:72:A:PHE:HB3 | 1:87:A:LEU:HA   | 10                  | 2.45     | 0.31                | 2.46       |
| (1,285)  | 1:72:A:PHE:HB2 | 1:87:A:LEU:HB3  | 10                  | 2.19     | 0.59                | 1.94       |
| (1,282)  | 1:72:A:PHE:HB2 | 1:86:A:LEU:HB2  | 10                  | 1.92     | 0.21                | 1.91       |
| (1,739)  | 1:16:A:SER:H   | 1:45:A:SER:H    | 10                  | 1.89     | 0.54                | 1.9        |
| (1,901)  | 1:72:A:PHE:HB2 | 1:87:A:LEU:H    | 10                  | 1.7      | 0.24                | 1.69       |
| (1,369)  | 1:76:A:VAL:HA  | 1:83:A:LEU:HA   | 10                  | 1.68     | 0.27                | 1.67       |
| (1,1543) | 1:72:A:PHE:HB2 | 1:87:A:LEU:HB2  | 10                  | 1.68     | 0.58                | 1.44       |
| (1,1543) | 1:72:A:PHE:HB2 | 1:87:A:LEU:HB3  | 10                  | 1.68     | 0.58                | 1.44       |
| (1,1222) | 1:5:A:SER:H    | 1:7:A:MET:HB3   | 10                  | 1.66     | 0.19                | 1.63       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,155)  | 1:68:A:VAL:H    | 1:92:A:LEU:HD21 | 10                  | 1.63     | 0.32                | 1.68       |
| (1,155)  | 1:68:A:VAL:H    | 1:92:A:LEU:HD22 | 10                  | 1.63     | 0.32                | 1.68       |
| (1,155)  | 1:68:A:VAL:H    | 1:92:A:LEU:HD23 | 10                  | 1.63     | 0.32                | 1.68       |
| (1,1111) | 1:7:A:MET:HB3   | 1:32:A:LYS:H    | 10                  | 1.47     | 0.18                | 1.52       |
| (1,773)  | 1:15:A:LEU:HA   | 1:45:A:SER:H    | 10                  | 1.45     | 0.52                | 1.34       |
| (1,1177) | 1:52:A:LYS:HE2  | 1:54:A:SER:H    | 10                  | 1.44     | 0.38                | 1.52       |
| (1,1178) | 1:52:A:LYS:HE3  | 1:54:A:SER:H    | 10                  | 1.34     | 0.26                | 1.33       |
| (1,118)  | 1:57:A:MET:HE1  | 1:92:A:LEU:HD11 | 10                  | 1.33     | 0.25                | 1.31       |
| (1,118)  | 1:57:A:MET:HE1  | 1:92:A:LEU:HD12 | 10                  | 1.33     | 0.25                | 1.31       |
| (1,118)  | 1:57:A:MET:HE1  | 1:92:A:LEU:HD13 | 10                  | 1.33     | 0.25                | 1.31       |
| (1,118)  | 1:57:A:MET:HE2  | 1:92:A:LEU:HD11 | 10                  | 1.33     | 0.25                | 1.31       |
| (1,118)  | 1:57:A:MET:HE2  | 1:92:A:LEU:HD12 | 10                  | 1.33     | 0.25                | 1.31       |
| (1,118)  | 1:57:A:MET:HE2  | 1:92:A:LEU:HD13 | 10                  | 1.33     | 0.25                | 1.31       |
| (1,118)  | 1:57:A:MET:HE3  | 1:92:A:LEU:HD11 | 10                  | 1.33     | 0.25                | 1.31       |
| (1,118)  | 1:57:A:MET:HE3  | 1:92:A:LEU:HD12 | 10                  | 1.33     | 0.25                | 1.31       |
| (1,118)  | 1:57:A:MET:HE3  | 1:92:A:LEU:HD13 | 10                  | 1.33     | 0.25                | 1.31       |
| (1,119)  | 1:57:A:MET:HE1  | 1:92:A:LEU:HD11 | 10                  | 1.33     | 0.25                | 1.31       |
| (1,119)  | 1:57:A:MET:HE1  | 1:92:A:LEU:HD12 | 10                  | 1.33     | 0.25                | 1.31       |
| (1,119)  | 1:57:A:MET:HE1  | 1:92:A:LEU:HD13 | 10                  | 1.33     | 0.25                | 1.31       |
| (1,119)  | 1:57:A:MET:HE2  | 1:92:A:LEU:HD11 | 10                  | 1.33     | 0.25                | 1.31       |
| (1,119)  | 1:57:A:MET:HE2  | 1:92:A:LEU:HD12 | 10                  | 1.33     | 0.25                | 1.31       |
| (1,119)  | 1:57:A:MET:HE2  | 1:92:A:LEU:HD13 | 10                  | 1.33     | 0.25                | 1.31       |
| (1,119)  | 1:57:A:MET:HE3  | 1:92:A:LEU:HD11 | 10                  | 1.33     | 0.25                | 1.31       |
| (1,119)  | 1:57:A:MET:HE3  | 1:92:A:LEU:HD12 | 10                  | 1.33     | 0.25                | 1.31       |
| (1,119)  | 1:57:A:MET:HE3  | 1:92:A:LEU:HD13 | 10                  | 1.33     | 0.25                | 1.31       |
| (1,1134) | 1:91:A:SER:H    | 1:92:A:LEU:HB2  | 10                  | 1.28     | 0.48                | 1.52       |
| (1,1223) | 1:5:A:SER:H     | 1:7:A:MET:HE1   | 10                  | 1.27     | 0.2                 | 1.31       |
| (1,1223) | 1:5:A:SER:H     | 1:7:A:MET:HE2   | 10                  | 1.27     | 0.2                 | 1.31       |
| (1,1223) | 1:5:A:SER:H     | 1:7:A:MET:HE3   | 10                  | 1.27     | 0.2                 | 1.31       |
| (1,1109) | 1:7:A:MET:HG2   | 1:32:A:LYS:H    | 10                  | 1.25     | 0.3                 | 1.28       |
| (1,1300) | 1:28:A:LYS:HG3  | 1:30:A:GLY:H    | 10                  | 1.24     | 0.09                | 1.27       |
| (1,1108) | 1:49:A:GLU:HB3  | 1:54:A:SER:H    | 10                  | 1.22     | 0.33                | 1.19       |
| (1,227)  | 1:4:A:LEU:HB3   | 1:30:A:GLY:HA2  | 10                  | 1.19     | 0.24                | 1.23       |
| (1,614)  | 1:67:A:VAL:H    | 1:96:A:GLY:H    | 10                  | 1.14     | 0.18                | 1.13       |
| (1,1259) | 1:38:A:ASN:HD22 | 1:96:A:GLY:H    | 10                  | 1.11     | 0.28                | 1.18       |
| (1,1069) | 1:5:A:SER:H     | 1:32:A:LYS:H    | 10                  | 1.04     | 0.27                | 1.08       |
| (1,1125) | 1:83:A:LEU:HG   | 1:84:A:GLN:H    | 10                  | 1.01     | 0.39                | 0.96       |
| (1,82)   | 1:28:A:LYS:HG3  | 1:29:A:LEU:HG   | 10                  | 1.0      | 0.23                | 1.06       |
| (1,408)  | 1:72:A:PHE:HA   | 1:87:A:LEU:HA   | 10                  | 0.98     | 0.21                | 0.98       |
| (1,802)  | 1:53:A:MET:HE1  | 1:58:A:GLU:H    | 10                  | 0.96     | 0.14                | 0.94       |
| (1,802)  | 1:53:A:MET:HE2  | 1:58:A:GLU:H    | 10                  | 0.96     | 0.14                | 0.94       |
| (1,802)  | 1:53:A:MET:HE3  | 1:58:A:GLU:H    | 10                  | 0.96     | 0.14                | 0.94       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,480)  | 1:49:A:GLU:HB2  | 1:57:A:MET:HG3  | 10                  | 0.93     | 0.17                | 1.01       |
| (1,1607) | 1:91:A:SER:HB2  | 1:92:A:LEU:HD11 | 10                  | 0.91     | 0.2                 | 1.01       |
| (1,1607) | 1:91:A:SER:HB2  | 1:92:A:LEU:HD12 | 10                  | 0.91     | 0.2                 | 1.01       |
| (1,1607) | 1:91:A:SER:HB2  | 1:92:A:LEU:HD13 | 10                  | 0.91     | 0.2                 | 1.01       |
| (1,1607) | 1:91:A:SER:HB3  | 1:92:A:LEU:HD11 | 10                  | 0.91     | 0.2                 | 1.01       |
| (1,1607) | 1:91:A:SER:HB3  | 1:92:A:LEU:HD12 | 10                  | 0.91     | 0.2                 | 1.01       |
| (1,1607) | 1:91:A:SER:HB3  | 1:92:A:LEU:HD13 | 10                  | 0.91     | 0.2                 | 1.01       |
| (1,108)  | 1:9:A:ILE:HA    | 1:10:A:LEU:HD11 | 10                  | 0.76     | 0.07                | 0.79       |
| (1,108)  | 1:9:A:ILE:HA    | 1:10:A:LEU:HD12 | 10                  | 0.76     | 0.07                | 0.79       |
| (1,108)  | 1:9:A:ILE:HA    | 1:10:A:LEU:HD13 | 10                  | 0.76     | 0.07                | 0.79       |
| (1,600)  | 1:65:A:VAL:HG21 | 1:66:A:ARG:H    | 10                  | 0.69     | 0.06                | 0.68       |
| (1,600)  | 1:65:A:VAL:HG22 | 1:66:A:ARG:H    | 10                  | 0.69     | 0.06                | 0.68       |
| (1,600)  | 1:65:A:VAL:HG23 | 1:66:A:ARG:H    | 10                  | 0.69     | 0.06                | 0.68       |
| (1,43)   | 1:63:A:ALA:HA   | 1:65:A:VAL:HG11 | 10                  | 0.68     | 0.07                | 0.69       |
| (1,43)   | 1:63:A:ALA:HA   | 1:65:A:VAL:HG12 | 10                  | 0.68     | 0.07                | 0.69       |
| (1,43)   | 1:63:A:ALA:HA   | 1:65:A:VAL:HG13 | 10                  | 0.68     | 0.07                | 0.69       |
| (1,44)   | 1:63:A:ALA:HA   | 1:65:A:VAL:HG11 | 10                  | 0.68     | 0.07                | 0.69       |
| (1,44)   | 1:63:A:ALA:HA   | 1:65:A:VAL:HG12 | 10                  | 0.68     | 0.07                | 0.69       |
| (1,44)   | 1:63:A:ALA:HA   | 1:65:A:VAL:HG13 | 10                  | 0.68     | 0.07                | 0.69       |
| (1,224)  | 1:4:A:LEU:HB2   | 1:30:A:GLY:HA2  | 10                  | 0.66     | 0.09                | 0.67       |
| (1,582)  | 1:10:A:LEU:H    | 1:42:A:LEU:HD21 | 10                  | 0.65     | 0.22                | 0.6        |
| (1,582)  | 1:10:A:LEU:H    | 1:42:A:LEU:HD22 | 10                  | 0.65     | 0.22                | 0.6        |
| (1,582)  | 1:10:A:LEU:H    | 1:42:A:LEU:HD23 | 10                  | 0.65     | 0.22                | 0.6        |
| (1,1093) | 1:90:A:HIS:HB3  | 1:91:A:SER:H    | 10                  | 0.64     | 0.28                | 0.59       |
| (1,1264) | 1:94:A:SER:HA   | 1:96:A:GLY:H    | 10                  | 0.61     | 0.18                | 0.56       |
| (1,665)  | 1:65:A:VAL:HG11 | 1:97:A:ALA:H    | 10                  | 0.52     | 0.19                | 0.48       |
| (1,665)  | 1:65:A:VAL:HG12 | 1:97:A:ALA:H    | 10                  | 0.52     | 0.19                | 0.48       |
| (1,665)  | 1:65:A:VAL:HG13 | 1:97:A:ALA:H    | 10                  | 0.52     | 0.19                | 0.48       |
| (1,281)  | 1:72:A:PHE:HB2  | 1:86:A:LEU:HB3  | 10                  | 0.5      | 0.15                | 0.5        |
| (1,648)  | 1:65:A:VAL:HB   | 1:67:A:VAL:H    | 10                  | 0.43     | 0.12                | 0.42       |
| (1,943)  | 1:75:A:ASP:H    | 1:76:A:VAL:HB   | 10                  | 0.42     | 0.03                | 0.42       |
| (1,320)  | 1:53:A:MET:HE1  | 1:57:A:MET:HA   | 10                  | 0.38     | 0.05                | 0.38       |
| (1,320)  | 1:53:A:MET:HE2  | 1:57:A:MET:HA   | 10                  | 0.38     | 0.05                | 0.38       |
| (1,320)  | 1:53:A:MET:HE3  | 1:57:A:MET:HA   | 10                  | 0.38     | 0.05                | 0.38       |
| (1,607)  | 1:66:A:ARG:H    | 1:97:A:ALA:H    | 10                  | 0.36     | 0.11                | 0.36       |
| (1,935)  | 1:76:A:VAL:H    | 1:76:A:VAL:HB   | 10                  | 0.33     | 0.0                 | 0.33       |
| (1,1414) | 1:23:A:LYS:HE2  | 1:27:A:GLU:HG3  | 9                   | 1.91     | 0.29                | 1.91       |
| (1,1414) | 1:23:A:LYS:HE3  | 1:27:A:GLU:HG3  | 9                   | 1.91     | 0.29                | 1.91       |
| (1,765)  | 1:38:A:ASN:HD22 | 1:98:A:GLU:H    | 9                   | 1.26     | 0.61                | 1.18       |
| (1,865)  | 1:18:A:ASN:HD22 | 1:20:A:ASP:H    | 9                   | 0.86     | 0.15                | 0.91       |
| (1,769)  | 1:15:A:LEU:HA   | 1:70:A:GLU:H    | 9                   | 0.82     | 0.28                | 0.73       |
| (1,156)  | 1:68:A:VAL:H    | 1:92:A:LEU:HD21 | 9                   | 0.7      | 0.26                | 0.71       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,156)  | 1:68:A:VAL:H    | 1:92:A:LEU:HD22 | 9                   | 0.7      | 0.26                | 0.71       |
| (1,156)  | 1:68:A:VAL:H    | 1:92:A:LEU:HD23 | 9                   | 0.7      | 0.26                | 0.71       |
| (1,157)  | 1:68:A:VAL:H    | 1:92:A:LEU:HD21 | 9                   | 0.7      | 0.26                | 0.71       |
| (1,157)  | 1:68:A:VAL:H    | 1:92:A:LEU:HD22 | 9                   | 0.7      | 0.26                | 0.71       |
| (1,157)  | 1:68:A:VAL:H    | 1:92:A:LEU:HD23 | 9                   | 0.7      | 0.26                | 0.71       |
| (1,634)  | 1:69:A:CYS:HB2  | 1:92:A:LEU:H    | 9                   | 0.64     | 0.41                | 0.79       |
| (1,756)  | 1:34:A:THR:H    | 1:40:A:ALA:H    | 9                   | 0.64     | 0.22                | 0.59       |
| (1,649)  | 1:9:A:ILE:H     | 1:33:A:LEU:HG   | 9                   | 0.49     | 0.21                | 0.4        |
| (1,481)  | 1:49:A:GLU:HB3  | 1:57:A:MET:HG3  | 9                   | 0.47     | 0.13                | 0.48       |
| (1,109)  | 1:28:A:LYS:HG3  | 1:29:A:LEU:HA   | 9                   | 0.42     | 0.14                | 0.44       |
| (1,1344) | 1:9:A:ILE:HG12  | 1:32:A:LYS:HB3  | 9                   | 0.28     | 0.09                | 0.31       |
| (1,1344) | 1:9:A:ILE:HG13  | 1:32:A:LYS:HB3  | 9                   | 0.28     | 0.09                | 0.31       |
| (1,983)  | 1:11:A:THR:H    | 1:43:A:CYS:HA   | 9                   | 0.25     | 0.08                | 0.25       |
| (1,1028) | 1:23:A:LYS:H    | 1:23:A:LYS:HB3  | 9                   | 0.24     | 0.02                | 0.24       |
| (1,1623) | 1:99:A:VAL:H    | 1:100:A:LYS:HD2 | 8                   | 1.33     | 0.7                 | 1.3        |
| (1,1623) | 1:99:A:VAL:H    | 1:100:A:LYS:HD3 | 8                   | 1.33     | 0.7                 | 1.3        |
| (1,1060) | 1:6:A:ASN:H     | 1:32:A:LYS:H    | 8                   | 1.13     | 0.23                | 1.19       |
| (1,619)  | 1:38:A:ASN:HD21 | 1:97:A:ALA:H    | 8                   | 0.57     | 0.28                | 0.52       |
| (1,1062) | 1:7:A:MET:H     | 1:32:A:LYS:H    | 8                   | 0.46     | 0.14                | 0.5        |
| (1,1384) | 1:18:A:ASN:HD21 | 1:20:A:ASP:H    | 8                   | 0.39     | 0.09                | 0.4        |
| (1,1384) | 1:18:A:ASN:HD22 | 1:20:A:ASP:H    | 8                   | 0.39     | 0.09                | 0.4        |
| (1,683)  | 1:12:A:LEU:H    | 1:43:A:CYS:HA   | 8                   | 0.36     | 0.15                | 0.38       |
| (1,1166) | 1:4:A:LEU:H     | 1:30:A:GLY:HA3  | 8                   | 0.29     | 0.15                | 0.28       |
| (1,1606) | 1:91:A:SER:HB2  | 1:92:A:LEU:HG   | 8                   | 0.23     | 0.07                | 0.22       |
| (1,1606) | 1:91:A:SER:HB3  | 1:92:A:LEU:HG   | 8                   | 0.23     | 0.07                | 0.22       |
| (1,1051) | 1:63:A:ALA:H    | 1:65:A:VAL:HG11 | 8                   | 0.22     | 0.09                | 0.23       |
| (1,1051) | 1:63:A:ALA:H    | 1:65:A:VAL:HG12 | 8                   | 0.22     | 0.09                | 0.23       |
| (1,1051) | 1:63:A:ALA:H    | 1:65:A:VAL:HG13 | 8                   | 0.22     | 0.09                | 0.23       |
| (1,1052) | 1:63:A:ALA:H    | 1:65:A:VAL:HG11 | 8                   | 0.22     | 0.09                | 0.23       |
| (1,1052) | 1:63:A:ALA:H    | 1:65:A:VAL:HG12 | 8                   | 0.22     | 0.09                | 0.23       |
| (1,1052) | 1:63:A:ALA:H    | 1:65:A:VAL:HG13 | 8                   | 0.22     | 0.09                | 0.23       |
| (1,590)  | 1:42:A:LEU:HA   | 1:44:A:ILE:H    | 8                   | 0.18     | 0.05                | 0.18       |
| (1,790)  | 1:50:A:VAL:H    | 1:57:A:MET:HG3  | 8                   | 0.17     | 0.05                | 0.18       |
| (1,1507) | 1:58:A:GLU:HG2  | 1:59:A:GLU:H    | 7                   | 0.85     | 0.03                | 0.85       |
| (1,1507) | 1:58:A:GLU:HG3  | 1:59:A:GLU:H    | 7                   | 0.85     | 0.03                | 0.85       |
| (1,476)  | 1:69:A:CYS:HB3  | 1:71:A:ASP:HA   | 7                   | 0.81     | 0.41                | 1.04       |
| (1,621)  | 1:38:A:ASN:HD22 | 1:97:A:ALA:H    | 7                   | 0.39     | 0.15                | 0.4        |
| (1,1293) | 1:30:A:GLY:H    | 1:31:A:GLY:H    | 7                   | 0.12     | 0.01                | 0.11       |
| (1,1048) | 1:4:A:LEU:HD11  | 1:7:A:MET:H     | 6                   | 1.11     | 0.24                | 1.23       |
| (1,1048) | 1:4:A:LEU:HD12  | 1:7:A:MET:H     | 6                   | 1.11     | 0.24                | 1.23       |
| (1,1048) | 1:4:A:LEU:HD13  | 1:7:A:MET:H     | 6                   | 1.11     | 0.24                | 1.23       |
| (1,1447) | 1:45:A:SER:HB2  | 1:46:A:THR:H    | 6                   | 0.28     | 0.08                | 0.29       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1447) | 1:45:A:SER:HB3  | 1:46:A:THR:H    | 6                   | 0.28     | 0.08                | 0.29       |
| (1,768)  | 1:11:A:THR:HA   | 1:45:A:SER:H    | 6                   | 0.27     | 0.11                | 0.24       |
| (1,310)  | 1:53:A:MET:HE1  | 1:61:A:LYS:H    | 6                   | 0.25     | 0.12                | 0.21       |
| (1,310)  | 1:53:A:MET:HE2  | 1:61:A:LYS:H    | 6                   | 0.25     | 0.12                | 0.21       |
| (1,310)  | 1:53:A:MET:HE3  | 1:61:A:LYS:H    | 6                   | 0.25     | 0.12                | 0.21       |
| (1,783)  | 1:57:A:MET:HG3  | 1:58:A:GLU:H    | 6                   | 0.16     | 0.02                | 0.15       |
| (1,784)  | 1:57:A:MET:HG2  | 1:58:A:GLU:H    | 6                   | 0.12     | 0.01                | 0.11       |
| (1,446)  | 1:4:A:LEU:HD11  | 1:7:A:MET:HB2   | 5                   | 0.5      | 0.14                | 0.48       |
| (1,446)  | 1:4:A:LEU:HD12  | 1:7:A:MET:HB2   | 5                   | 0.5      | 0.14                | 0.48       |
| (1,446)  | 1:4:A:LEU:HD13  | 1:7:A:MET:HB2   | 5                   | 0.5      | 0.14                | 0.48       |
| (1,1446) | 1:45:A:SER:H    | 1:70:A:GLU:HG2  | 5                   | 0.41     | 0.16                | 0.39       |
| (1,1446) | 1:45:A:SER:H    | 1:70:A:GLU:HG3  | 5                   | 0.41     | 0.16                | 0.39       |
| (1,1396) | 1:19:A:LYS:HD2  | 1:21:A:GLU:H    | 5                   | 0.41     | 0.24                | 0.36       |
| (1,1396) | 1:19:A:LYS:HD3  | 1:21:A:GLU:H    | 5                   | 0.41     | 0.24                | 0.36       |
| (1,353)  | 1:7:A:MET:HE1   | 1:42:A:LEU:HD21 | 5                   | 0.37     | 0.02                | 0.37       |
| (1,353)  | 1:7:A:MET:HE1   | 1:42:A:LEU:HD22 | 5                   | 0.37     | 0.02                | 0.37       |
| (1,353)  | 1:7:A:MET:HE1   | 1:42:A:LEU:HD23 | 5                   | 0.37     | 0.02                | 0.37       |
| (1,353)  | 1:7:A:MET:HE2   | 1:42:A:LEU:HD21 | 5                   | 0.37     | 0.02                | 0.37       |
| (1,353)  | 1:7:A:MET:HE2   | 1:42:A:LEU:HD22 | 5                   | 0.37     | 0.02                | 0.37       |
| (1,353)  | 1:7:A:MET:HE2   | 1:42:A:LEU:HD23 | 5                   | 0.37     | 0.02                | 0.37       |
| (1,353)  | 1:7:A:MET:HE3   | 1:42:A:LEU:HD21 | 5                   | 0.37     | 0.02                | 0.37       |
| (1,353)  | 1:7:A:MET:HE3   | 1:42:A:LEU:HD22 | 5                   | 0.37     | 0.02                | 0.37       |
| (1,353)  | 1:7:A:MET:HE3   | 1:42:A:LEU:HD23 | 5                   | 0.37     | 0.02                | 0.37       |
| (1,736)  | 1:15:A:LEU:HD11 | 1:22:A:ALA:H    | 5                   | 0.31     | 0.16                | 0.29       |
| (1,736)  | 1:15:A:LEU:HD12 | 1:22:A:ALA:H    | 5                   | 0.31     | 0.16                | 0.29       |
| (1,736)  | 1:15:A:LEU:HD13 | 1:22:A:ALA:H    | 5                   | 0.31     | 0.16                | 0.29       |
| (1,737)  | 1:15:A:LEU:HD11 | 1:22:A:ALA:H    | 5                   | 0.31     | 0.16                | 0.29       |
| (1,737)  | 1:15:A:LEU:HD12 | 1:22:A:ALA:H    | 5                   | 0.31     | 0.16                | 0.29       |
| (1,737)  | 1:15:A:LEU:HD13 | 1:22:A:ALA:H    | 5                   | 0.31     | 0.16                | 0.29       |
| (1,304)  | 1:50:A:VAL:H    | 1:53:A:MET:HE1  | 5                   | 0.29     | 0.2                 | 0.23       |
| (1,304)  | 1:50:A:VAL:H    | 1:53:A:MET:HE2  | 5                   | 0.29     | 0.2                 | 0.23       |
| (1,304)  | 1:50:A:VAL:H    | 1:53:A:MET:HE3  | 5                   | 0.29     | 0.2                 | 0.23       |
| (1,1301) | 1:4:A:LEU:HB3   | 1:30:A:GLY:H    | 5                   | 0.22     | 0.13                | 0.17       |
| (1,907)  | 1:72:A:PHE:HB2  | 1:76:A:VAL:H    | 5                   | 0.22     | 0.04                | 0.21       |
| (1,129)  | 1:42:A:LEU:HD11 | 1:43:A:CYS:H    | 5                   | 0.17     | 0.07                | 0.13       |
| (1,129)  | 1:42:A:LEU:HD12 | 1:43:A:CYS:H    | 5                   | 0.17     | 0.07                | 0.13       |
| (1,129)  | 1:42:A:LEU:HD13 | 1:43:A:CYS:H    | 5                   | 0.17     | 0.07                | 0.13       |
| (1,1540) | 1:70:A:GLU:HG2  | 1:71:A:ASP:HA   | 4                   | 0.82     | 0.03                | 0.83       |
| (1,1540) | 1:70:A:GLU:HG3  | 1:71:A:ASP:HA   | 4                   | 0.82     | 0.03                | 0.83       |
| (1,347)  | 1:25:A:MET:HE1  | 1:29:A:LEU:HD21 | 4                   | 0.6      | 0.23                | 0.6        |
| (1,347)  | 1:25:A:MET:HE1  | 1:29:A:LEU:HD22 | 4                   | 0.6      | 0.23                | 0.6        |
| (1,347)  | 1:25:A:MET:HE1  | 1:29:A:LEU:HD23 | 4                   | 0.6      | 0.23                | 0.6        |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,347)  | 1:25:A:MET:HE2  | 1:29:A:LEU:HD21 | 4                   | 0.6      | 0.23                | 0.6        |
| (1,347)  | 1:25:A:MET:HE2  | 1:29:A:LEU:HD22 | 4                   | 0.6      | 0.23                | 0.6        |
| (1,347)  | 1:25:A:MET:HE2  | 1:29:A:LEU:HD23 | 4                   | 0.6      | 0.23                | 0.6        |
| (1,347)  | 1:25:A:MET:HE3  | 1:29:A:LEU:HD21 | 4                   | 0.6      | 0.23                | 0.6        |
| (1,347)  | 1:25:A:MET:HE3  | 1:29:A:LEU:HD22 | 4                   | 0.6      | 0.23                | 0.6        |
| (1,347)  | 1:25:A:MET:HE3  | 1:29:A:LEU:HD23 | 4                   | 0.6      | 0.23                | 0.6        |
| (1,1485) | 1:52:A:LYS:HD2  | 1:54:A:SER:H    | 4                   | 0.33     | 0.08                | 0.35       |
| (1,1485) | 1:52:A:LYS:HD3  | 1:54:A:SER:H    | 4                   | 0.33     | 0.08                | 0.35       |
| (1,799)  | 1:70:A:GLU:H    | 1:70:A:GLU:HB3  | 4                   | 0.3      | 0.02                | 0.3        |
| (1,900)  | 1:45:A:SER:HB3  | 1:68:A:VAL:H    | 4                   | 0.24     | 0.08                | 0.24       |
| (1,1252) | 1:92:A:LEU:HD11 | 1:93:A:SER:H    | 4                   | 0.18     | 0.08                | 0.18       |
| (1,1252) | 1:92:A:LEU:HD12 | 1:93:A:SER:H    | 4                   | 0.18     | 0.08                | 0.18       |
| (1,1252) | 1:92:A:LEU:HD13 | 1:93:A:SER:H    | 4                   | 0.18     | 0.08                | 0.18       |
| (1,1426) | 1:28:A:LYS:HD2  | 1:29:A:LEU:H    | 4                   | 0.16     | 0.04                | 0.14       |
| (1,1426) | 1:28:A:LYS:HD3  | 1:29:A:LEU:H    | 4                   | 0.16     | 0.04                | 0.14       |
| (1,1116) | 1:73:A:LEU:H    | 1:74:A:GLN:HG2  | 3                   | 1.21     | 0.02                | 1.23       |
| (1,1550) | 1:74:A:GLN:HA   | 1:74:A:GLN:HE21 | 3                   | 0.95     | 0.23                | 0.8        |
| (1,1550) | 1:74:A:GLN:HA   | 1:74:A:GLN:HE22 | 3                   | 0.95     | 0.23                | 0.8        |
| (1,85)   | 1:9:A:ILE:HD11  | 1:42:A:LEU:HD21 | 3                   | 0.9      | 0.64                | 0.92       |
| (1,85)   | 1:9:A:ILE:HD11  | 1:42:A:LEU:HD22 | 3                   | 0.9      | 0.64                | 0.92       |
| (1,85)   | 1:9:A:ILE:HD11  | 1:42:A:LEU:HD23 | 3                   | 0.9      | 0.64                | 0.92       |
| (1,85)   | 1:9:A:ILE:HD12  | 1:42:A:LEU:HD21 | 3                   | 0.9      | 0.64                | 0.92       |
| (1,85)   | 1:9:A:ILE:HD12  | 1:42:A:LEU:HD22 | 3                   | 0.9      | 0.64                | 0.92       |
| (1,85)   | 1:9:A:ILE:HD12  | 1:42:A:LEU:HD23 | 3                   | 0.9      | 0.64                | 0.92       |
| (1,85)   | 1:9:A:ILE:HD13  | 1:42:A:LEU:HD21 | 3                   | 0.9      | 0.64                | 0.92       |
| (1,85)   | 1:9:A:ILE:HD13  | 1:42:A:LEU:HD22 | 3                   | 0.9      | 0.64                | 0.92       |
| (1,85)   | 1:9:A:ILE:HD13  | 1:42:A:LEU:HD23 | 3                   | 0.9      | 0.64                | 0.92       |
| (1,86)   | 1:9:A:ILE:HD11  | 1:42:A:LEU:HD21 | 3                   | 0.9      | 0.64                | 0.92       |
| (1,86)   | 1:9:A:ILE:HD11  | 1:42:A:LEU:HD22 | 3                   | 0.9      | 0.64                | 0.92       |
| (1,86)   | 1:9:A:ILE:HD11  | 1:42:A:LEU:HD23 | 3                   | 0.9      | 0.64                | 0.92       |
| (1,86)   | 1:9:A:ILE:HD12  | 1:42:A:LEU:HD21 | 3                   | 0.9      | 0.64                | 0.92       |
| (1,86)   | 1:9:A:ILE:HD12  | 1:42:A:LEU:HD22 | 3                   | 0.9      | 0.64                | 0.92       |
| (1,86)   | 1:9:A:ILE:HD12  | 1:42:A:LEU:HD23 | 3                   | 0.9      | 0.64                | 0.92       |
| (1,86)   | 1:9:A:ILE:HD13  | 1:42:A:LEU:HD21 | 3                   | 0.9      | 0.64                | 0.92       |
| (1,86)   | 1:9:A:ILE:HD13  | 1:42:A:LEU:HD22 | 3                   | 0.9      | 0.64                | 0.92       |
| (1,86)   | 1:9:A:ILE:HD13  | 1:42:A:LEU:HD23 | 3                   | 0.9      | 0.64                | 0.92       |
| (1,1119) | 1:74:A:GLN:H    | 1:74:A:GLN:HG2  | 3                   | 0.5      | 0.06                | 0.53       |
| (1,1395) | 1:19:A:LYS:HD2  | 1:20:A:ASP:HA   | 3                   | 0.42     | 0.23                | 0.41       |
| (1,1395) | 1:19:A:LYS:HD3  | 1:20:A:ASP:HA   | 3                   | 0.42     | 0.23                | 0.41       |
| (1,288)  | 1:53:A:MET:HE1  | 1:61:A:LYS:HE3  | 3                   | 0.33     | 0.07                | 0.34       |
| (1,288)  | 1:53:A:MET:HE2  | 1:61:A:LYS:HE3  | 3                   | 0.33     | 0.07                | 0.34       |
| (1,288)  | 1:53:A:MET:HE3  | 1:61:A:LYS:HE3  | 3                   | 0.33     | 0.07                | 0.34       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,926)  | 1:74:A:GLN:HG2  | 1:75:A:ASP:H    | 3                   | 0.26     | 0.06                | 0.29       |
| (1,291)  | 1:9:A:ILE:HG21  | 1:42:A:LEU:HD21 | 3                   | 0.24     | 0.13                | 0.19       |
| (1,291)  | 1:9:A:ILE:HG21  | 1:42:A:LEU:HD22 | 3                   | 0.24     | 0.13                | 0.19       |
| (1,291)  | 1:9:A:ILE:HG21  | 1:42:A:LEU:HD23 | 3                   | 0.24     | 0.13                | 0.19       |
| (1,291)  | 1:9:A:ILE:HG22  | 1:42:A:LEU:HD21 | 3                   | 0.24     | 0.13                | 0.19       |
| (1,291)  | 1:9:A:ILE:HG22  | 1:42:A:LEU:HD22 | 3                   | 0.24     | 0.13                | 0.19       |
| (1,291)  | 1:9:A:ILE:HG22  | 1:42:A:LEU:HD23 | 3                   | 0.24     | 0.13                | 0.19       |
| (1,291)  | 1:9:A:ILE:HG23  | 1:42:A:LEU:HD21 | 3                   | 0.24     | 0.13                | 0.19       |
| (1,291)  | 1:9:A:ILE:HG23  | 1:42:A:LEU:HD22 | 3                   | 0.24     | 0.13                | 0.19       |
| (1,291)  | 1:9:A:ILE:HG23  | 1:42:A:LEU:HD23 | 3                   | 0.24     | 0.13                | 0.19       |
| (1,292)  | 1:9:A:ILE:HG21  | 1:42:A:LEU:HD21 | 3                   | 0.24     | 0.13                | 0.19       |
| (1,292)  | 1:9:A:ILE:HG21  | 1:42:A:LEU:HD22 | 3                   | 0.24     | 0.13                | 0.19       |
| (1,292)  | 1:9:A:ILE:HG21  | 1:42:A:LEU:HD23 | 3                   | 0.24     | 0.13                | 0.19       |
| (1,292)  | 1:9:A:ILE:HG22  | 1:42:A:LEU:HD21 | 3                   | 0.24     | 0.13                | 0.19       |
| (1,292)  | 1:9:A:ILE:HG22  | 1:42:A:LEU:HD22 | 3                   | 0.24     | 0.13                | 0.19       |
| (1,292)  | 1:9:A:ILE:HG22  | 1:42:A:LEU:HD23 | 3                   | 0.24     | 0.13                | 0.19       |
| (1,292)  | 1:9:A:ILE:HG23  | 1:42:A:LEU:HD21 | 3                   | 0.24     | 0.13                | 0.19       |
| (1,292)  | 1:9:A:ILE:HG23  | 1:42:A:LEU:HD22 | 3                   | 0.24     | 0.13                | 0.19       |
| (1,292)  | 1:9:A:ILE:HG23  | 1:42:A:LEU:HD23 | 3                   | 0.24     | 0.13                | 0.19       |
| (1,1047) | 1:10:A:LEU:HD11 | 1:34:A:THR:H    | 3                   | 0.23     | 0.07                | 0.25       |
| (1,1047) | 1:10:A:LEU:HD12 | 1:34:A:THR:H    | 3                   | 0.23     | 0.07                | 0.25       |
| (1,1047) | 1:10:A:LEU:HD13 | 1:34:A:THR:H    | 3                   | 0.23     | 0.07                | 0.25       |
| (1,179)  | 1:15:A:LEU:HA   | 1:46:A:THR:HG21 | 3                   | 0.2      | 0.1                 | 0.16       |
| (1,179)  | 1:15:A:LEU:HA   | 1:46:A:THR:HG22 | 3                   | 0.2      | 0.1                 | 0.16       |
| (1,179)  | 1:15:A:LEU:HA   | 1:46:A:THR:HG23 | 3                   | 0.2      | 0.1                 | 0.16       |
| (1,180)  | 1:15:A:LEU:HA   | 1:46:A:THR:HG21 | 3                   | 0.2      | 0.1                 | 0.16       |
| (1,180)  | 1:15:A:LEU:HA   | 1:46:A:THR:HG22 | 3                   | 0.2      | 0.1                 | 0.16       |
| (1,180)  | 1:15:A:LEU:HA   | 1:46:A:THR:HG23 | 3                   | 0.2      | 0.1                 | 0.16       |
| (1,601)  | 1:15:A:LEU:H    | 1:15:A:LEU:HD21 | 3                   | 0.18     | 0.05                | 0.17       |
| (1,601)  | 1:15:A:LEU:H    | 1:15:A:LEU:HD22 | 3                   | 0.18     | 0.05                | 0.17       |
| (1,601)  | 1:15:A:LEU:H    | 1:15:A:LEU:HD23 | 3                   | 0.18     | 0.05                | 0.17       |
| (1,602)  | 1:15:A:LEU:H    | 1:15:A:LEU:HD21 | 3                   | 0.18     | 0.05                | 0.17       |
| (1,602)  | 1:15:A:LEU:H    | 1:15:A:LEU:HD22 | 3                   | 0.18     | 0.05                | 0.17       |
| (1,602)  | 1:15:A:LEU:H    | 1:15:A:LEU:HD23 | 3                   | 0.18     | 0.05                | 0.17       |
| (1,1127) | 1:28:A:LYS:HD2  | 1:29:A:LEU:H    | 3                   | 0.17     | 0.05                | 0.18       |
| (1,1215) | 1:5:A:SER:H     | 1:31:A:GLY:HA2  | 3                   | 0.16     | 0.04                | 0.17       |
| (1,1034) | 1:33:A:LEU:HG   | 1:34:A:THR:H    | 3                   | 0.12     | 0.01                | 0.11       |
| (1,287)  | 1:53:A:MET:HE1  | 1:61:A:LYS:HE2  | 2                   | 1.04     | 0.34                | 1.04       |
| (1,287)  | 1:53:A:MET:HE2  | 1:61:A:LYS:HE2  | 2                   | 1.04     | 0.34                | 1.04       |
| (1,287)  | 1:53:A:MET:HE3  | 1:61:A:LYS:HE2  | 2                   | 1.04     | 0.34                | 1.04       |
| (1,930)  | 1:68:A:VAL:H    | 1:92:A:LEU:HG   | 2                   | 0.37     | 0.22                | 0.37       |
| (1,296)  | 1:53:A:MET:HE1  | 1:54:A:SER:H    | 2                   | 0.36     | 0.18                | 0.36       |

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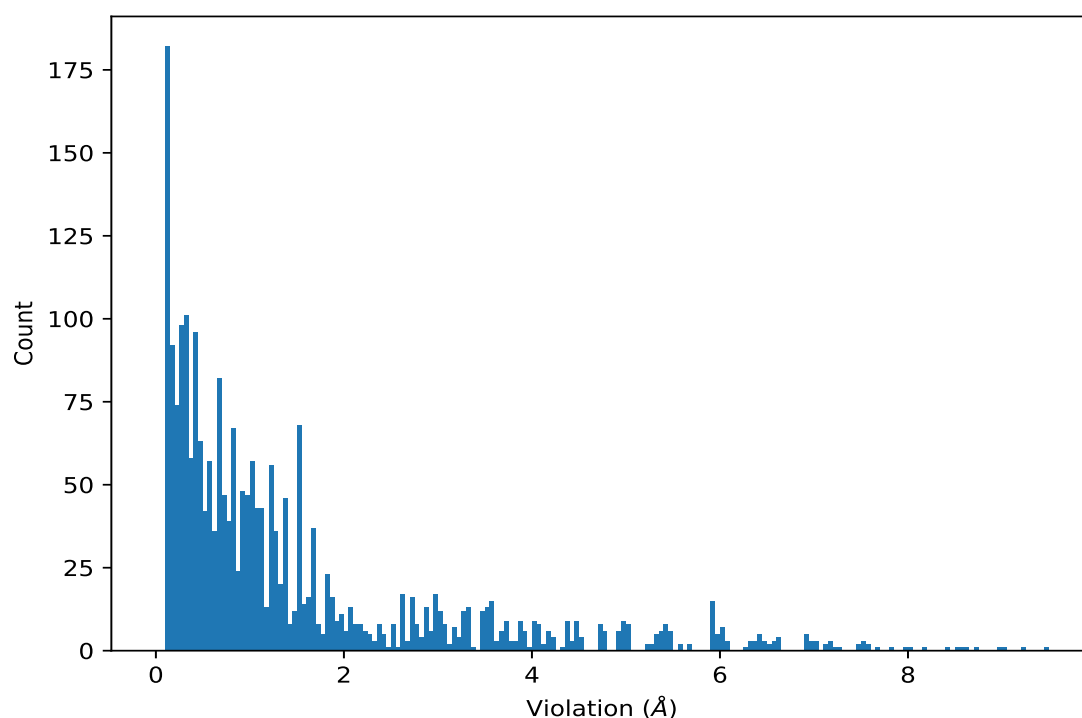
| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,296)  | 1:53:A:MET:HE2  | 1:54:A:SER:H    | 2                   | 0.36     | 0.18                | 0.36       |
| (1,296)  | 1:53:A:MET:HE3  | 1:54:A:SER:H    | 2                   | 0.36     | 0.18                | 0.36       |
| (1,1136) | 1:41:A:SER:H    | 1:42:A:LEU:HD21 | 2                   | 0.35     | 0.06                | 0.35       |
| (1,1136) | 1:41:A:SER:H    | 1:42:A:LEU:HD22 | 2                   | 0.35     | 0.06                | 0.35       |
| (1,1136) | 1:41:A:SER:H    | 1:42:A:LEU:HD23 | 2                   | 0.35     | 0.06                | 0.35       |
| (1,1137) | 1:41:A:SER:H    | 1:42:A:LEU:HD21 | 2                   | 0.35     | 0.06                | 0.35       |
| (1,1137) | 1:41:A:SER:H    | 1:42:A:LEU:HD22 | 2                   | 0.35     | 0.06                | 0.35       |
| (1,1137) | 1:41:A:SER:H    | 1:42:A:LEU:HD23 | 2                   | 0.35     | 0.06                | 0.35       |
| (1,837)  | 1:12:A:LEU:HD21 | 1:61:A:LYS:H    | 2                   | 0.29     | 0.18                | 0.29       |
| (1,837)  | 1:12:A:LEU:HD22 | 1:61:A:LYS:H    | 2                   | 0.29     | 0.18                | 0.29       |
| (1,837)  | 1:12:A:LEU:HD23 | 1:61:A:LYS:H    | 2                   | 0.29     | 0.18                | 0.29       |
| (1,1276) | 1:4:A:LEU:HG    | 1:31:A:GLY:H    | 2                   | 0.26     | 0.1                 | 0.26       |
| (1,505)  | 1:22:A:ALA:HA   | 1:25:A:MET:HA   | 2                   | 0.24     | 0.04                | 0.24       |
| (1,1346) | 1:12:A:LEU:H    | 1:45:A:SER:HB2  | 2                   | 0.22     | 0.04                | 0.22       |
| (1,1346) | 1:12:A:LEU:H    | 1:45:A:SER:HB3  | 2                   | 0.22     | 0.04                | 0.22       |
| (1,893)  | 1:79:A:SER:HB2  | 1:81:A:LYS:H    | 2                   | 0.21     | 0.02                | 0.21       |
| (1,1419) | 1:25:A:MET:HG2  | 1:74:A:GLN:HE21 | 2                   | 0.2      | 0.09                | 0.2        |
| (1,1419) | 1:25:A:MET:HG2  | 1:74:A:GLN:HE22 | 2                   | 0.2      | 0.09                | 0.2        |
| (1,1617) | 1:97:A:ALA:HA   | 1:98:A:GLU:HB2  | 2                   | 0.16     | 0.02                | 0.16       |
| (1,1617) | 1:97:A:ALA:HA   | 1:98:A:GLU:HB3  | 2                   | 0.16     | 0.02                | 0.16       |

<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) |
|----------|-------------|-----------------|----------|---------------|
| (1,1211) | 1:5:A:SER:H | 1:84:A:GLN:HE22 | 2        | 9.49          |
| (1,1211) | 1:5:A:SER:H | 1:84:A:GLN:HE22 | 6        | 9.21          |
| (1,1211) | 1:5:A:SER:H | 1:84:A:GLN:HE22 | 8        | 9.01          |
| (1,1211) | 1:5:A:SER:H | 1:84:A:GLN:HE22 | 5        | 8.98          |
| (1,1211) | 1:5:A:SER:H | 1:84:A:GLN:HE22 | 4        | 8.74          |
| (1,1212) | 1:5:A:SER:H | 1:84:A:GLN:HE21 | 7        | 8.64          |
| (1,1212) | 1:5:A:SER:H | 1:84:A:GLN:HE21 | 2        | 8.56          |
| (1,1211) | 1:5:A:SER:H | 1:84:A:GLN:HE22 | 10       | 8.5           |
| (1,1211) | 1:5:A:SER:H | 1:84:A:GLN:HE22 | 1        | 8.4           |
| (1,1212) | 1:5:A:SER:H | 1:84:A:GLN:HE21 | 6        | 8.15          |
| (1,1212) | 1:5:A:SER:H | 1:84:A:GLN:HE21 | 8        | 8.04          |
| (1,1212) | 1:5:A:SER:H | 1:84:A:GLN:HE21 | 5        | 7.96          |
| (1,1211) | 1:5:A:SER:H | 1:84:A:GLN:HE22 | 9        | 7.81          |
| (1,1212) | 1:5:A:SER:H | 1:84:A:GLN:HE21 | 10       | 7.68          |
| (1,1212) | 1:5:A:SER:H | 1:84:A:GLN:HE21 | 4        | 7.57          |
| (1,1212) | 1:5:A:SER:H | 1:84:A:GLN:HE21 | 1        | 7.56          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,1232) | 1:4:A:LEU:HD11 | 1:84:A:GLN:HE22 | 2        | 7.52          |
| (1,1232) | 1:4:A:LEU:HD12 | 1:84:A:GLN:HE22 | 2        | 7.52          |
| (1,1232) | 1:4:A:LEU:HD13 | 1:84:A:GLN:HE22 | 2        | 7.52          |
| (1,1321) | 1:5:A:SER:H    | 1:84:A:GLN:HE21 | 2        | 7.45          |
| (1,1321) | 1:5:A:SER:H    | 1:84:A:GLN:HE22 | 2        | 7.45          |
| (1,1212) | 1:5:A:SER:H    | 1:84:A:GLN:HE21 | 3        | 7.25          |
| (1,1211) | 1:5:A:SER:H    | 1:84:A:GLN:HE22 | 7        | 7.22          |
| (1,1235) | 1:4:A:LEU:HD11 | 1:84:A:GLN:HE21 | 7        | 7.19          |
| (1,1235) | 1:4:A:LEU:HD12 | 1:84:A:GLN:HE21 | 7        | 7.19          |
| (1,1235) | 1:4:A:LEU:HD13 | 1:84:A:GLN:HE21 | 7        | 7.19          |
| (1,1321) | 1:5:A:SER:H    | 1:84:A:GLN:HE21 | 6        | 7.13          |
| (1,1321) | 1:5:A:SER:H    | 1:84:A:GLN:HE22 | 6        | 7.13          |
| (1,1235) | 1:4:A:LEU:HD11 | 1:84:A:GLN:HE21 | 2        | 7.02          |
| (1,1235) | 1:4:A:LEU:HD12 | 1:84:A:GLN:HE21 | 2        | 7.02          |
| (1,1235) | 1:4:A:LEU:HD13 | 1:84:A:GLN:HE21 | 2        | 7.02          |
| (1,1321) | 1:5:A:SER:H    | 1:84:A:GLN:HE21 | 8        | 6.99          |
| (1,1321) | 1:5:A:SER:H    | 1:84:A:GLN:HE22 | 8        | 6.99          |
| (1,1212) | 1:5:A:SER:H    | 1:84:A:GLN:HE21 | 9        | 6.98          |
| (1,1321) | 1:5:A:SER:H    | 1:84:A:GLN:HE21 | 5        | 6.94          |
| (1,1321) | 1:5:A:SER:H    | 1:84:A:GLN:HE22 | 5        | 6.94          |
| (1,1232) | 1:4:A:LEU:HD11 | 1:84:A:GLN:HE22 | 10       | 6.91          |
| (1,1232) | 1:4:A:LEU:HD12 | 1:84:A:GLN:HE22 | 10       | 6.91          |
| (1,1232) | 1:4:A:LEU:HD13 | 1:84:A:GLN:HE22 | 10       | 6.91          |
| (1,1321) | 1:5:A:SER:H    | 1:84:A:GLN:HE21 | 4        | 6.64          |
| (1,1321) | 1:5:A:SER:H    | 1:84:A:GLN:HE22 | 4        | 6.64          |
| (1,1321) | 1:5:A:SER:H    | 1:84:A:GLN:HE21 | 10       | 6.62          |
| (1,1321) | 1:5:A:SER:H    | 1:84:A:GLN:HE22 | 10       | 6.62          |
| (1,1235) | 1:4:A:LEU:HD11 | 1:84:A:GLN:HE21 | 10       | 6.56          |
| (1,1235) | 1:4:A:LEU:HD12 | 1:84:A:GLN:HE21 | 10       | 6.56          |
| (1,1235) | 1:4:A:LEU:HD13 | 1:84:A:GLN:HE21 | 10       | 6.56          |
| (1,1321) | 1:5:A:SER:H    | 1:84:A:GLN:HE21 | 1        | 6.52          |
| (1,1321) | 1:5:A:SER:H    | 1:84:A:GLN:HE22 | 1        | 6.52          |
| (1,1229) | 1:4:A:LEU:HD21 | 1:84:A:GLN:HE22 | 5        | 6.49          |
| (1,1229) | 1:4:A:LEU:HD22 | 1:84:A:GLN:HE22 | 5        | 6.49          |
| (1,1229) | 1:4:A:LEU:HD23 | 1:84:A:GLN:HE22 | 5        | 6.49          |
| (1,1232) | 1:4:A:LEU:HD11 | 1:84:A:GLN:HE22 | 7        | 6.44          |
| (1,1232) | 1:4:A:LEU:HD12 | 1:84:A:GLN:HE22 | 7        | 6.44          |
| (1,1232) | 1:4:A:LEU:HD13 | 1:84:A:GLN:HE22 | 7        | 6.44          |
| (1,1321) | 1:5:A:SER:H    | 1:84:A:GLN:HE21 | 7        | 6.4           |
| (1,1321) | 1:5:A:SER:H    | 1:84:A:GLN:HE22 | 7        | 6.4           |
| (1,1235) | 1:4:A:LEU:HD11 | 1:84:A:GLN:HE21 | 3        | 6.38          |
| (1,1235) | 1:4:A:LEU:HD12 | 1:84:A:GLN:HE21 | 3        | 6.38          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,1235) | 1:4:A:LEU:HD13 | 1:84:A:GLN:HE21 | 3        | 6.38          |
| (1,1232) | 1:4:A:LEU:HD11 | 1:84:A:GLN:HE22 | 9        | 6.33          |
| (1,1232) | 1:4:A:LEU:HD12 | 1:84:A:GLN:HE22 | 9        | 6.33          |
| (1,1232) | 1:4:A:LEU:HD13 | 1:84:A:GLN:HE22 | 9        | 6.33          |
| (1,1211) | 1:5:A:SER:H    | 1:84:A:GLN:HE22 | 3        | 6.27          |
| (1,1232) | 1:4:A:LEU:HD11 | 1:84:A:GLN:HE22 | 3        | 6.1           |
| (1,1232) | 1:4:A:LEU:HD12 | 1:84:A:GLN:HE22 | 3        | 6.1           |
| (1,1232) | 1:4:A:LEU:HD13 | 1:84:A:GLN:HE22 | 3        | 6.1           |
| (1,1317) | 1:4:A:LEU:H    | 1:84:A:GLN:HE21 | 6        | 6.05          |
| (1,1317) | 1:4:A:LEU:H    | 1:84:A:GLN:HE22 | 6        | 6.05          |
| (1,1234) | 1:4:A:LEU:HD21 | 1:84:A:GLN:HE21 | 5        | 6.03          |
| (1,1234) | 1:4:A:LEU:HD22 | 1:84:A:GLN:HE21 | 5        | 6.03          |
| (1,1234) | 1:4:A:LEU:HD23 | 1:84:A:GLN:HE21 | 5        | 6.03          |
| (1,1321) | 1:5:A:SER:H    | 1:84:A:GLN:HE21 | 9        | 6.0           |
| (1,1321) | 1:5:A:SER:H    | 1:84:A:GLN:HE22 | 9        | 6.0           |
| (1,1235) | 1:4:A:LEU:HD11 | 1:84:A:GLN:HE21 | 9        | 5.98          |
| (1,1235) | 1:4:A:LEU:HD12 | 1:84:A:GLN:HE21 | 9        | 5.98          |
| (1,1235) | 1:4:A:LEU:HD13 | 1:84:A:GLN:HE21 | 9        | 5.98          |
| (1,1317) | 1:4:A:LEU:H    | 1:84:A:GLN:HE21 | 2        | 5.95          |
| (1,1317) | 1:4:A:LEU:H    | 1:84:A:GLN:HE22 | 2        | 5.95          |
| (1,1318) | 1:4:A:LEU:HD11 | 1:84:A:GLN:HE21 | 2        | 5.92          |
| (1,1318) | 1:4:A:LEU:HD11 | 1:84:A:GLN:HE22 | 2        | 5.92          |
| (1,1318) | 1:4:A:LEU:HD12 | 1:84:A:GLN:HE21 | 2        | 5.92          |
| (1,1318) | 1:4:A:LEU:HD12 | 1:84:A:GLN:HE22 | 2        | 5.92          |
| (1,1318) | 1:4:A:LEU:HD13 | 1:84:A:GLN:HE21 | 2        | 5.92          |
| (1,1318) | 1:4:A:LEU:HD13 | 1:84:A:GLN:HE22 | 2        | 5.92          |
| (1,1319) | 1:4:A:LEU:HD21 | 1:84:A:GLN:HE21 | 5        | 5.91          |
| (1,1319) | 1:4:A:LEU:HD21 | 1:84:A:GLN:HE22 | 5        | 5.91          |
| (1,1319) | 1:4:A:LEU:HD22 | 1:84:A:GLN:HE21 | 5        | 5.91          |
| (1,1319) | 1:4:A:LEU:HD22 | 1:84:A:GLN:HE22 | 5        | 5.91          |
| (1,1319) | 1:4:A:LEU:HD23 | 1:84:A:GLN:HE21 | 5        | 5.91          |
| (1,1319) | 1:4:A:LEU:HD23 | 1:84:A:GLN:HE22 | 5        | 5.91          |
| (1,1232) | 1:4:A:LEU:HD11 | 1:84:A:GLN:HE22 | 6        | 5.9           |
| (1,1232) | 1:4:A:LEU:HD12 | 1:84:A:GLN:HE22 | 6        | 5.9           |
| (1,1232) | 1:4:A:LEU:HD13 | 1:84:A:GLN:HE22 | 6        | 5.9           |
| (1,1317) | 1:4:A:LEU:H    | 1:84:A:GLN:HE21 | 8        | 5.67          |
| (1,1317) | 1:4:A:LEU:H    | 1:84:A:GLN:HE22 | 8        | 5.67          |
| (1,1317) | 1:4:A:LEU:H    | 1:84:A:GLN:HE21 | 5        | 5.58          |
| (1,1317) | 1:4:A:LEU:H    | 1:84:A:GLN:HE22 | 5        | 5.58          |
| (1,1318) | 1:4:A:LEU:HD11 | 1:84:A:GLN:HE21 | 7        | 5.49          |
| (1,1318) | 1:4:A:LEU:HD11 | 1:84:A:GLN:HE22 | 7        | 5.49          |
| (1,1318) | 1:4:A:LEU:HD12 | 1:84:A:GLN:HE21 | 7        | 5.49          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,1318) | 1:4:A:LEU:HD12 | 1:84:A:GLN:HE22 | 7        | 5.49          |
| (1,1318) | 1:4:A:LEU:HD13 | 1:84:A:GLN:HE21 | 7        | 5.49          |
| (1,1318) | 1:4:A:LEU:HD13 | 1:84:A:GLN:HE22 | 7        | 5.49          |
| (1,1318) | 1:4:A:LEU:HD11 | 1:84:A:GLN:HE21 | 10       | 5.44          |
| (1,1318) | 1:4:A:LEU:HD11 | 1:84:A:GLN:HE22 | 10       | 5.44          |
| (1,1318) | 1:4:A:LEU:HD12 | 1:84:A:GLN:HE21 | 10       | 5.44          |
| (1,1318) | 1:4:A:LEU:HD12 | 1:84:A:GLN:HE22 | 10       | 5.44          |
| (1,1318) | 1:4:A:LEU:HD13 | 1:84:A:GLN:HE21 | 10       | 5.44          |
| (1,1318) | 1:4:A:LEU:HD13 | 1:84:A:GLN:HE22 | 10       | 5.44          |
| (1,1321) | 1:5:A:SER:H    | 1:84:A:GLN:HE21 | 3        | 5.41          |
| (1,1321) | 1:5:A:SER:H    | 1:84:A:GLN:HE22 | 3        | 5.41          |
| (1,1235) | 1:4:A:LEU:HD11 | 1:84:A:GLN:HE21 | 6        | 5.37          |
| (1,1235) | 1:4:A:LEU:HD12 | 1:84:A:GLN:HE21 | 6        | 5.37          |
| (1,1235) | 1:4:A:LEU:HD13 | 1:84:A:GLN:HE21 | 6        | 5.37          |
| (1,1232) | 1:4:A:LEU:HD11 | 1:84:A:GLN:HE22 | 8        | 5.36          |
| (1,1232) | 1:4:A:LEU:HD12 | 1:84:A:GLN:HE22 | 8        | 5.36          |
| (1,1232) | 1:4:A:LEU:HD13 | 1:84:A:GLN:HE22 | 8        | 5.36          |
| (1,1317) | 1:4:A:LEU:H    | 1:84:A:GLN:HE21 | 4        | 5.32          |
| (1,1317) | 1:4:A:LEU:H    | 1:84:A:GLN:HE22 | 4        | 5.32          |
| (1,1232) | 1:4:A:LEU:HD11 | 1:84:A:GLN:HE22 | 5        | 5.31          |
| (1,1232) | 1:4:A:LEU:HD12 | 1:84:A:GLN:HE22 | 5        | 5.31          |
| (1,1232) | 1:4:A:LEU:HD13 | 1:84:A:GLN:HE22 | 5        | 5.31          |
| (1,1317) | 1:4:A:LEU:H    | 1:84:A:GLN:HE21 | 1        | 5.28          |
| (1,1317) | 1:4:A:LEU:H    | 1:84:A:GLN:HE22 | 1        | 5.28          |
| (1,1317) | 1:4:A:LEU:H    | 1:84:A:GLN:HE21 | 10       | 5.24          |
| (1,1317) | 1:4:A:LEU:H    | 1:84:A:GLN:HE22 | 10       | 5.24          |
| (1,1317) | 1:4:A:LEU:H    | 1:84:A:GLN:HE21 | 7        | 5.02          |
| (1,1317) | 1:4:A:LEU:H    | 1:84:A:GLN:HE22 | 7        | 5.02          |
| (1,1318) | 1:4:A:LEU:HD11 | 1:84:A:GLN:HE21 | 3        | 5.01          |
| (1,1318) | 1:4:A:LEU:HD11 | 1:84:A:GLN:HE22 | 3        | 5.01          |
| (1,1318) | 1:4:A:LEU:HD12 | 1:84:A:GLN:HE21 | 3        | 5.01          |
| (1,1318) | 1:4:A:LEU:HD12 | 1:84:A:GLN:HE22 | 3        | 5.01          |
| (1,1318) | 1:4:A:LEU:HD13 | 1:84:A:GLN:HE21 | 3        | 5.01          |
| (1,1318) | 1:4:A:LEU:HD13 | 1:84:A:GLN:HE22 | 3        | 5.01          |
| (1,1235) | 1:4:A:LEU:HD11 | 1:84:A:GLN:HE21 | 8        | 4.98          |
| (1,1235) | 1:4:A:LEU:HD12 | 1:84:A:GLN:HE21 | 8        | 4.98          |
| (1,1235) | 1:4:A:LEU:HD13 | 1:84:A:GLN:HE21 | 8        | 4.98          |
| (1,1229) | 1:4:A:LEU:HD21 | 1:84:A:GLN:HE22 | 6        | 4.97          |
| (1,1229) | 1:4:A:LEU:HD22 | 1:84:A:GLN:HE22 | 6        | 4.97          |
| (1,1229) | 1:4:A:LEU:HD23 | 1:84:A:GLN:HE22 | 6        | 4.97          |
| (1,1232) | 1:4:A:LEU:HD11 | 1:84:A:GLN:HE22 | 4        | 4.95          |
| (1,1232) | 1:4:A:LEU:HD12 | 1:84:A:GLN:HE22 | 4        | 4.95          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,1232) | 1:4:A:LEU:HD13 | 1:84:A:GLN:HE22 | 4        | 4.95          |
| (1,1318) | 1:4:A:LEU:HD11 | 1:84:A:GLN:HE21 | 9        | 4.93          |
| (1,1318) | 1:4:A:LEU:HD11 | 1:84:A:GLN:HE22 | 9        | 4.93          |
| (1,1318) | 1:4:A:LEU:HD12 | 1:84:A:GLN:HE21 | 9        | 4.93          |
| (1,1318) | 1:4:A:LEU:HD12 | 1:84:A:GLN:HE22 | 9        | 4.93          |
| (1,1318) | 1:4:A:LEU:HD13 | 1:84:A:GLN:HE21 | 9        | 4.93          |
| (1,1318) | 1:4:A:LEU:HD13 | 1:84:A:GLN:HE22 | 9        | 4.93          |
| (1,309)  | 1:7:A:MET:HE1  | 1:84:A:GLN:HE22 | 2        | 4.79          |
| (1,309)  | 1:7:A:MET:HE2  | 1:84:A:GLN:HE22 | 2        | 4.79          |
| (1,309)  | 1:7:A:MET:HE3  | 1:84:A:GLN:HE22 | 2        | 4.79          |
| (1,309)  | 1:7:A:MET:HE1  | 1:84:A:GLN:HE22 | 6        | 4.76          |
| (1,309)  | 1:7:A:MET:HE2  | 1:84:A:GLN:HE22 | 6        | 4.76          |
| (1,309)  | 1:7:A:MET:HE3  | 1:84:A:GLN:HE22 | 6        | 4.76          |
| (1,1317) | 1:4:A:LEU:H    | 1:84:A:GLN:HE21 | 9        | 4.71          |
| (1,1317) | 1:4:A:LEU:H    | 1:84:A:GLN:HE22 | 9        | 4.71          |
| (1,1235) | 1:4:A:LEU:HD11 | 1:84:A:GLN:HE21 | 5        | 4.7           |
| (1,1235) | 1:4:A:LEU:HD12 | 1:84:A:GLN:HE21 | 5        | 4.7           |
| (1,1235) | 1:4:A:LEU:HD13 | 1:84:A:GLN:HE21 | 5        | 4.7           |
| (1,315)  | 1:7:A:MET:HE1  | 1:84:A:GLN:HE21 | 2        | 4.7           |
| (1,315)  | 1:7:A:MET:HE2  | 1:84:A:GLN:HE21 | 2        | 4.7           |
| (1,315)  | 1:7:A:MET:HE3  | 1:84:A:GLN:HE21 | 2        | 4.7           |
| (1,315)  | 1:7:A:MET:HE1  | 1:84:A:GLN:HE21 | 6        | 4.53          |
| (1,315)  | 1:7:A:MET:HE2  | 1:84:A:GLN:HE21 | 6        | 4.53          |
| (1,315)  | 1:7:A:MET:HE3  | 1:84:A:GLN:HE21 | 6        | 4.53          |
| (1,284)  | 1:72:A:PHE:HB2 | 1:87:A:LEU:HB2  | 10       | 4.53          |
| (1,1232) | 1:4:A:LEU:HD11 | 1:84:A:GLN:HE22 | 1        | 4.48          |
| (1,1232) | 1:4:A:LEU:HD12 | 1:84:A:GLN:HE22 | 1        | 4.48          |
| (1,1232) | 1:4:A:LEU:HD13 | 1:84:A:GLN:HE22 | 1        | 4.48          |
| (1,1318) | 1:4:A:LEU:HD11 | 1:84:A:GLN:HE21 | 6        | 4.45          |
| (1,1318) | 1:4:A:LEU:HD11 | 1:84:A:GLN:HE22 | 6        | 4.45          |
| (1,1318) | 1:4:A:LEU:HD12 | 1:84:A:GLN:HE21 | 6        | 4.45          |
| (1,1318) | 1:4:A:LEU:HD12 | 1:84:A:GLN:HE22 | 6        | 4.45          |
| (1,1318) | 1:4:A:LEU:HD13 | 1:84:A:GLN:HE21 | 6        | 4.45          |
| (1,1318) | 1:4:A:LEU:HD13 | 1:84:A:GLN:HE22 | 6        | 4.45          |
| (1,1229) | 1:4:A:LEU:HD21 | 1:84:A:GLN:HE22 | 8        | 4.4           |
| (1,1229) | 1:4:A:LEU:HD22 | 1:84:A:GLN:HE22 | 8        | 4.4           |
| (1,1229) | 1:4:A:LEU:HD23 | 1:84:A:GLN:HE22 | 8        | 4.4           |
| (1,1235) | 1:4:A:LEU:HD11 | 1:84:A:GLN:HE21 | 4        | 4.39          |
| (1,1235) | 1:4:A:LEU:HD12 | 1:84:A:GLN:HE21 | 4        | 4.39          |
| (1,1235) | 1:4:A:LEU:HD13 | 1:84:A:GLN:HE21 | 4        | 4.39          |
| (1,1319) | 1:4:A:LEU:HD21 | 1:84:A:GLN:HE21 | 6        | 4.38          |
| (1,1319) | 1:4:A:LEU:HD21 | 1:84:A:GLN:HE22 | 6        | 4.38          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,1319) | 1:4:A:LEU:HD22 | 1:84:A:GLN:HE21 | 6        | 4.38          |
| (1,1319) | 1:4:A:LEU:HD22 | 1:84:A:GLN:HE22 | 6        | 4.38          |
| (1,1319) | 1:4:A:LEU:HD23 | 1:84:A:GLN:HE21 | 6        | 4.38          |
| (1,1319) | 1:4:A:LEU:HD23 | 1:84:A:GLN:HE22 | 6        | 4.38          |
| (1,170)  | 1:89:A:ALA:H   | 1:92:A:LEU:HB2  | 4        | 4.31          |
| (1,170)  | 1:89:A:ALA:H   | 1:92:A:LEU:HB2  | 2        | 4.23          |
| (1,1235) | 1:4:A:LEU:HD11 | 1:84:A:GLN:HE21 | 1        | 4.21          |
| (1,1235) | 1:4:A:LEU:HD12 | 1:84:A:GLN:HE21 | 1        | 4.21          |
| (1,1235) | 1:4:A:LEU:HD13 | 1:84:A:GLN:HE21 | 1        | 4.21          |
| (1,1317) | 1:4:A:LEU:H    | 1:84:A:GLN:HE21 | 3        | 4.18          |
| (1,1317) | 1:4:A:LEU:H    | 1:84:A:GLN:HE22 | 3        | 4.18          |
| (1,1234) | 1:4:A:LEU:HD21 | 1:84:A:GLN:HE21 | 6        | 4.18          |
| (1,1234) | 1:4:A:LEU:HD22 | 1:84:A:GLN:HE21 | 6        | 4.18          |
| (1,1234) | 1:4:A:LEU:HD23 | 1:84:A:GLN:HE21 | 6        | 4.18          |
| (1,170)  | 1:89:A:ALA:H   | 1:92:A:LEU:HB2  | 1        | 4.16          |
| (1,170)  | 1:89:A:ALA:H   | 1:92:A:LEU:HB2  | 3        | 4.14          |
| (1,170)  | 1:89:A:ALA:H   | 1:92:A:LEU:HB2  | 8        | 4.13          |
| (1,170)  | 1:89:A:ALA:H   | 1:92:A:LEU:HB2  | 7        | 4.09          |
| (1,170)  | 1:89:A:ALA:H   | 1:92:A:LEU:HB2  | 10       | 4.09          |
| (1,1318) | 1:4:A:LEU:HD11 | 1:84:A:GLN:HE21 | 8        | 4.05          |
| (1,1318) | 1:4:A:LEU:HD11 | 1:84:A:GLN:HE22 | 8        | 4.05          |
| (1,1318) | 1:4:A:LEU:HD12 | 1:84:A:GLN:HE21 | 8        | 4.05          |
| (1,1318) | 1:4:A:LEU:HD12 | 1:84:A:GLN:HE22 | 8        | 4.05          |
| (1,1318) | 1:4:A:LEU:HD13 | 1:84:A:GLN:HE21 | 8        | 4.05          |
| (1,1318) | 1:4:A:LEU:HD13 | 1:84:A:GLN:HE22 | 8        | 4.05          |
| (1,1229) | 1:4:A:LEU:HD21 | 1:84:A:GLN:HE22 | 4        | 4.03          |
| (1,1229) | 1:4:A:LEU:HD22 | 1:84:A:GLN:HE22 | 4        | 4.03          |
| (1,1229) | 1:4:A:LEU:HD23 | 1:84:A:GLN:HE22 | 4        | 4.03          |
| (1,1229) | 1:4:A:LEU:HD21 | 1:84:A:GLN:HE22 | 2        | 4.02          |
| (1,1229) | 1:4:A:LEU:HD22 | 1:84:A:GLN:HE22 | 2        | 4.02          |
| (1,1229) | 1:4:A:LEU:HD23 | 1:84:A:GLN:HE22 | 2        | 4.02          |
| (1,309)  | 1:7:A:MET:HE1  | 1:84:A:GLN:HE22 | 5        | 4.0           |
| (1,309)  | 1:7:A:MET:HE2  | 1:84:A:GLN:HE22 | 5        | 4.0           |
| (1,309)  | 1:7:A:MET:HE3  | 1:84:A:GLN:HE22 | 5        | 4.0           |
| (1,284)  | 1:72:A:PHE:HB2 | 1:87:A:LEU:HB2  | 9        | 3.97          |
| (1,1319) | 1:4:A:LEU:HD21 | 1:84:A:GLN:HE21 | 8        | 3.94          |
| (1,1319) | 1:4:A:LEU:HD21 | 1:84:A:GLN:HE22 | 8        | 3.94          |
| (1,1319) | 1:4:A:LEU:HD22 | 1:84:A:GLN:HE21 | 8        | 3.94          |
| (1,1319) | 1:4:A:LEU:HD22 | 1:84:A:GLN:HE22 | 8        | 3.94          |
| (1,1319) | 1:4:A:LEU:HD23 | 1:84:A:GLN:HE21 | 8        | 3.94          |
| (1,1319) | 1:4:A:LEU:HD23 | 1:84:A:GLN:HE22 | 8        | 3.94          |
| (1,315)  | 1:7:A:MET:HE1  | 1:84:A:GLN:HE21 | 5        | 3.89          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,315)  | 1:7:A:MET:HE2  | 1:84:A:GLN:HE21 | 5        | 3.89          |
| (1,315)  | 1:7:A:MET:HE3  | 1:84:A:GLN:HE21 | 5        | 3.89          |
| (1,1318) | 1:4:A:LEU:HD11 | 1:84:A:GLN:HE21 | 5        | 3.88          |
| (1,1318) | 1:4:A:LEU:HD11 | 1:84:A:GLN:HE22 | 5        | 3.88          |
| (1,1318) | 1:4:A:LEU:HD12 | 1:84:A:GLN:HE21 | 5        | 3.88          |
| (1,1318) | 1:4:A:LEU:HD12 | 1:84:A:GLN:HE22 | 5        | 3.88          |
| (1,1318) | 1:4:A:LEU:HD13 | 1:84:A:GLN:HE21 | 5        | 3.88          |
| (1,1318) | 1:4:A:LEU:HD13 | 1:84:A:GLN:HE22 | 5        | 3.88          |
| (1,1229) | 1:4:A:LEU:HD21 | 1:84:A:GLN:HE22 | 1        | 3.83          |
| (1,1229) | 1:4:A:LEU:HD22 | 1:84:A:GLN:HE22 | 1        | 3.83          |
| (1,1229) | 1:4:A:LEU:HD23 | 1:84:A:GLN:HE22 | 1        | 3.83          |
| (1,1234) | 1:4:A:LEU:HD21 | 1:84:A:GLN:HE21 | 7        | 3.79          |
| (1,1234) | 1:4:A:LEU:HD22 | 1:84:A:GLN:HE21 | 7        | 3.79          |
| (1,1234) | 1:4:A:LEU:HD23 | 1:84:A:GLN:HE21 | 7        | 3.79          |
| (1,1234) | 1:4:A:LEU:HD21 | 1:84:A:GLN:HE21 | 8        | 3.74          |
| (1,1234) | 1:4:A:LEU:HD22 | 1:84:A:GLN:HE21 | 8        | 3.74          |
| (1,1234) | 1:4:A:LEU:HD23 | 1:84:A:GLN:HE21 | 8        | 3.74          |
| (1,1319) | 1:4:A:LEU:HD21 | 1:84:A:GLN:HE21 | 2        | 3.7           |
| (1,1319) | 1:4:A:LEU:HD21 | 1:84:A:GLN:HE22 | 2        | 3.7           |
| (1,1319) | 1:4:A:LEU:HD22 | 1:84:A:GLN:HE21 | 2        | 3.7           |
| (1,1319) | 1:4:A:LEU:HD22 | 1:84:A:GLN:HE22 | 2        | 3.7           |
| (1,1319) | 1:4:A:LEU:HD23 | 1:84:A:GLN:HE21 | 2        | 3.7           |
| (1,1319) | 1:4:A:LEU:HD23 | 1:84:A:GLN:HE22 | 2        | 3.7           |
| (1,1327) | 1:7:A:MET:HE1  | 1:84:A:GLN:HE21 | 2        | 3.68          |
| (1,1327) | 1:7:A:MET:HE1  | 1:84:A:GLN:HE22 | 2        | 3.68          |
| (1,1327) | 1:7:A:MET:HE2  | 1:84:A:GLN:HE21 | 2        | 3.68          |
| (1,1327) | 1:7:A:MET:HE2  | 1:84:A:GLN:HE22 | 2        | 3.68          |
| (1,1327) | 1:7:A:MET:HE3  | 1:84:A:GLN:HE21 | 2        | 3.68          |
| (1,1327) | 1:7:A:MET:HE3  | 1:84:A:GLN:HE22 | 2        | 3.68          |
| (1,315)  | 1:7:A:MET:HE1  | 1:84:A:GLN:HE21 | 10       | 3.62          |
| (1,315)  | 1:7:A:MET:HE2  | 1:84:A:GLN:HE21 | 10       | 3.62          |
| (1,315)  | 1:7:A:MET:HE3  | 1:84:A:GLN:HE21 | 10       | 3.62          |
| (1,1327) | 1:7:A:MET:HE1  | 1:84:A:GLN:HE21 | 6        | 3.59          |
| (1,1327) | 1:7:A:MET:HE1  | 1:84:A:GLN:HE22 | 6        | 3.59          |
| (1,1327) | 1:7:A:MET:HE2  | 1:84:A:GLN:HE21 | 6        | 3.59          |
| (1,1327) | 1:7:A:MET:HE2  | 1:84:A:GLN:HE22 | 6        | 3.59          |
| (1,1327) | 1:7:A:MET:HE3  | 1:84:A:GLN:HE21 | 6        | 3.59          |
| (1,1327) | 1:7:A:MET:HE3  | 1:84:A:GLN:HE22 | 6        | 3.59          |
| (1,1318) | 1:4:A:LEU:HD11 | 1:84:A:GLN:HE21 | 4        | 3.59          |
| (1,1318) | 1:4:A:LEU:HD11 | 1:84:A:GLN:HE22 | 4        | 3.59          |
| (1,1318) | 1:4:A:LEU:HD12 | 1:84:A:GLN:HE21 | 4        | 3.59          |
| (1,1318) | 1:4:A:LEU:HD12 | 1:84:A:GLN:HE22 | 4        | 3.59          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,1318) | 1:4:A:LEU:HD13 | 1:84:A:GLN:HE21 | 4        | 3.59          |
| (1,1318) | 1:4:A:LEU:HD13 | 1:84:A:GLN:HE22 | 4        | 3.59          |
| (1,309)  | 1:7:A:MET:HE1  | 1:84:A:GLN:HE22 | 8        | 3.59          |
| (1,309)  | 1:7:A:MET:HE2  | 1:84:A:GLN:HE22 | 8        | 3.59          |
| (1,309)  | 1:7:A:MET:HE3  | 1:84:A:GLN:HE22 | 8        | 3.59          |
| (1,1234) | 1:4:A:LEU:HD21 | 1:84:A:GLN:HE21 | 2        | 3.54          |
| (1,1234) | 1:4:A:LEU:HD22 | 1:84:A:GLN:HE21 | 2        | 3.54          |
| (1,1234) | 1:4:A:LEU:HD23 | 1:84:A:GLN:HE21 | 2        | 3.54          |
| (1,1319) | 1:4:A:LEU:HD21 | 1:84:A:GLN:HE21 | 4        | 3.52          |
| (1,1319) | 1:4:A:LEU:HD21 | 1:84:A:GLN:HE22 | 4        | 3.52          |
| (1,1319) | 1:4:A:LEU:HD22 | 1:84:A:GLN:HE21 | 4        | 3.52          |
| (1,1319) | 1:4:A:LEU:HD22 | 1:84:A:GLN:HE22 | 4        | 3.52          |
| (1,1319) | 1:4:A:LEU:HD23 | 1:84:A:GLN:HE21 | 4        | 3.52          |
| (1,1319) | 1:4:A:LEU:HD23 | 1:84:A:GLN:HE22 | 4        | 3.52          |
| (1,315)  | 1:7:A:MET:HE1  | 1:84:A:GLN:HE21 | 8        | 3.51          |
| (1,315)  | 1:7:A:MET:HE2  | 1:84:A:GLN:HE21 | 8        | 3.51          |
| (1,315)  | 1:7:A:MET:HE3  | 1:84:A:GLN:HE21 | 8        | 3.51          |
| (1,285)  | 1:72:A:PHE:HB2 | 1:87:A:LEU:HB3  | 10       | 3.5           |
| (1,309)  | 1:7:A:MET:HE1  | 1:84:A:GLN:HE22 | 10       | 3.49          |
| (1,309)  | 1:7:A:MET:HE2  | 1:84:A:GLN:HE22 | 10       | 3.49          |
| (1,309)  | 1:7:A:MET:HE3  | 1:84:A:GLN:HE22 | 10       | 3.49          |
| (1,1319) | 1:4:A:LEU:HD21 | 1:84:A:GLN:HE21 | 1        | 3.47          |
| (1,1319) | 1:4:A:LEU:HD21 | 1:84:A:GLN:HE22 | 1        | 3.47          |
| (1,1319) | 1:4:A:LEU:HD22 | 1:84:A:GLN:HE21 | 1        | 3.47          |
| (1,1319) | 1:4:A:LEU:HD22 | 1:84:A:GLN:HE22 | 1        | 3.47          |
| (1,1319) | 1:4:A:LEU:HD23 | 1:84:A:GLN:HE21 | 1        | 3.47          |
| (1,1319) | 1:4:A:LEU:HD23 | 1:84:A:GLN:HE22 | 1        | 3.47          |
| (1,1229) | 1:4:A:LEU:HD21 | 1:84:A:GLN:HE22 | 10       | 3.47          |
| (1,1229) | 1:4:A:LEU:HD22 | 1:84:A:GLN:HE22 | 10       | 3.47          |
| (1,1229) | 1:4:A:LEU:HD23 | 1:84:A:GLN:HE22 | 10       | 3.47          |
| (1,284)  | 1:72:A:PHE:HB2 | 1:87:A:LEU:HB2  | 6        | 3.38          |
| (1,1319) | 1:4:A:LEU:HD21 | 1:84:A:GLN:HE21 | 7        | 3.34          |
| (1,1319) | 1:4:A:LEU:HD21 | 1:84:A:GLN:HE22 | 7        | 3.34          |
| (1,1319) | 1:4:A:LEU:HD22 | 1:84:A:GLN:HE21 | 7        | 3.34          |
| (1,1319) | 1:4:A:LEU:HD22 | 1:84:A:GLN:HE22 | 7        | 3.34          |
| (1,1319) | 1:4:A:LEU:HD23 | 1:84:A:GLN:HE21 | 7        | 3.34          |
| (1,1319) | 1:4:A:LEU:HD23 | 1:84:A:GLN:HE22 | 7        | 3.34          |
| (1,1085) | 1:6:A:ASN:HA   | 1:32:A:LYS:H    | 9        | 3.34          |
| (1,1318) | 1:4:A:LEU:HD11 | 1:84:A:GLN:HE21 | 1        | 3.32          |
| (1,1318) | 1:4:A:LEU:HD11 | 1:84:A:GLN:HE22 | 1        | 3.32          |
| (1,1318) | 1:4:A:LEU:HD12 | 1:84:A:GLN:HE21 | 1        | 3.32          |
| (1,1318) | 1:4:A:LEU:HD12 | 1:84:A:GLN:HE22 | 1        | 3.32          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,1318) | 1:4:A:LEU:HD13 | 1:84:A:GLN:HE21 | 1        | 3.32          |
| (1,1318) | 1:4:A:LEU:HD13 | 1:84:A:GLN:HE22 | 1        | 3.32          |
| (1,1319) | 1:4:A:LEU:HD21 | 1:84:A:GLN:HE21 | 10       | 3.3           |
| (1,1319) | 1:4:A:LEU:HD21 | 1:84:A:GLN:HE22 | 10       | 3.3           |
| (1,1319) | 1:4:A:LEU:HD22 | 1:84:A:GLN:HE21 | 10       | 3.3           |
| (1,1319) | 1:4:A:LEU:HD22 | 1:84:A:GLN:HE22 | 10       | 3.3           |
| (1,1319) | 1:4:A:LEU:HD23 | 1:84:A:GLN:HE21 | 10       | 3.3           |
| (1,1319) | 1:4:A:LEU:HD23 | 1:84:A:GLN:HE22 | 10       | 3.3           |
| (1,315)  | 1:7:A:MET:HE1  | 1:84:A:GLN:HE21 | 7        | 3.26          |
| (1,315)  | 1:7:A:MET:HE2  | 1:84:A:GLN:HE21 | 7        | 3.26          |
| (1,315)  | 1:7:A:MET:HE3  | 1:84:A:GLN:HE21 | 7        | 3.26          |
| (1,1234) | 1:4:A:LEU:HD21 | 1:84:A:GLN:HE21 | 1        | 3.25          |
| (1,1234) | 1:4:A:LEU:HD22 | 1:84:A:GLN:HE21 | 1        | 3.25          |
| (1,1234) | 1:4:A:LEU:HD23 | 1:84:A:GLN:HE21 | 1        | 3.25          |
| (1,1085) | 1:6:A:ASN:HA   | 1:32:A:LYS:H    | 1        | 3.22          |
| (1,1234) | 1:4:A:LEU:HD21 | 1:84:A:GLN:HE21 | 4        | 3.21          |
| (1,1234) | 1:4:A:LEU:HD22 | 1:84:A:GLN:HE21 | 4        | 3.21          |
| (1,1234) | 1:4:A:LEU:HD23 | 1:84:A:GLN:HE21 | 4        | 3.21          |
| (1,1234) | 1:4:A:LEU:HD21 | 1:84:A:GLN:HE21 | 10       | 3.18          |
| (1,1234) | 1:4:A:LEU:HD22 | 1:84:A:GLN:HE21 | 10       | 3.18          |
| (1,1234) | 1:4:A:LEU:HD23 | 1:84:A:GLN:HE21 | 10       | 3.18          |
| (1,309)  | 1:7:A:MET:HE1  | 1:84:A:GLN:HE22 | 3        | 3.17          |
| (1,309)  | 1:7:A:MET:HE2  | 1:84:A:GLN:HE22 | 3        | 3.17          |
| (1,309)  | 1:7:A:MET:HE3  | 1:84:A:GLN:HE22 | 3        | 3.17          |
| (1,1085) | 1:6:A:ASN:HA   | 1:32:A:LYS:H    | 8        | 3.16          |
| (1,902)  | 1:72:A:PHE:HB3 | 1:87:A:LEU:H    | 10       | 3.14          |
| (1,902)  | 1:72:A:PHE:HB3 | 1:87:A:LEU:H    | 2        | 3.1           |
| (1,1413) | 1:23:A:LYS:HE2 | 1:27:A:GLU:H    | 5        | 3.08          |
| (1,1413) | 1:23:A:LYS:HE3 | 1:27:A:GLU:H    | 5        | 3.08          |
| (1,1085) | 1:6:A:ASN:HA   | 1:32:A:LYS:H    | 5        | 3.08          |
| (1,1085) | 1:6:A:ASN:HA   | 1:32:A:LYS:H    | 7        | 3.08          |
| (1,170)  | 1:89:A:ALA:H   | 1:92:A:LEU:HB2  | 9        | 3.08          |
| (1,309)  | 1:7:A:MET:HE1  | 1:84:A:GLN:HE22 | 4        | 3.06          |
| (1,309)  | 1:7:A:MET:HE2  | 1:84:A:GLN:HE22 | 4        | 3.06          |
| (1,309)  | 1:7:A:MET:HE3  | 1:84:A:GLN:HE22 | 4        | 3.06          |
| (1,1229) | 1:4:A:LEU:HD21 | 1:84:A:GLN:HE22 | 7        | 3.04          |
| (1,1229) | 1:4:A:LEU:HD22 | 1:84:A:GLN:HE22 | 7        | 3.04          |
| (1,1229) | 1:4:A:LEU:HD23 | 1:84:A:GLN:HE22 | 7        | 3.04          |
| (1,284)  | 1:72:A:PHE:HB2 | 1:87:A:LEU:HB2  | 8        | 3.04          |
| (1,1413) | 1:23:A:LYS:HE2 | 1:27:A:GLU:H    | 1        | 3.03          |
| (1,1413) | 1:23:A:LYS:HE3 | 1:27:A:GLU:H    | 1        | 3.03          |
| (1,902)  | 1:72:A:PHE:HB3 | 1:87:A:LEU:H    | 8        | 3.02          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,315)  | 1:7:A:MET:HE1  | 1:84:A:GLN:HE21 | 3        | 3.02          |
| (1,315)  | 1:7:A:MET:HE2  | 1:84:A:GLN:HE21 | 3        | 3.02          |
| (1,315)  | 1:7:A:MET:HE3  | 1:84:A:GLN:HE21 | 3        | 3.02          |
| (1,1413) | 1:23:A:LYS:HE2 | 1:27:A:GLU:H    | 8        | 3.01          |
| (1,1413) | 1:23:A:LYS:HE3 | 1:27:A:GLU:H    | 8        | 3.01          |
| (1,1413) | 1:23:A:LYS:HE2 | 1:27:A:GLU:H    | 4        | 2.99          |
| (1,1413) | 1:23:A:LYS:HE3 | 1:27:A:GLU:H    | 4        | 2.99          |
| (1,1234) | 1:4:A:LEU:HD21 | 1:84:A:GLN:HE21 | 3        | 2.97          |
| (1,1234) | 1:4:A:LEU:HD22 | 1:84:A:GLN:HE21 | 3        | 2.97          |
| (1,1234) | 1:4:A:LEU:HD23 | 1:84:A:GLN:HE21 | 3        | 2.97          |
| (1,902)  | 1:72:A:PHE:HB3 | 1:87:A:LEU:H    | 6        | 2.97          |
| (1,902)  | 1:72:A:PHE:HB3 | 1:87:A:LEU:H    | 9        | 2.97          |
| (1,331)  | 1:72:A:PHE:HB3 | 1:87:A:LEU:HA   | 10       | 2.97          |
| (1,1327) | 1:7:A:MET:HE1  | 1:84:A:GLN:HE21 | 5        | 2.96          |
| (1,1327) | 1:7:A:MET:HE1  | 1:84:A:GLN:HE22 | 5        | 2.96          |
| (1,1327) | 1:7:A:MET:HE2  | 1:84:A:GLN:HE21 | 5        | 2.96          |
| (1,1327) | 1:7:A:MET:HE2  | 1:84:A:GLN:HE22 | 5        | 2.96          |
| (1,1327) | 1:7:A:MET:HE3  | 1:84:A:GLN:HE21 | 5        | 2.96          |
| (1,1327) | 1:7:A:MET:HE3  | 1:84:A:GLN:HE22 | 5        | 2.96          |
| (1,1085) | 1:6:A:ASN:HA   | 1:32:A:LYS:H    | 3        | 2.96          |
| (1,1085) | 1:6:A:ASN:HA   | 1:32:A:LYS:H    | 10       | 2.96          |
| (1,902)  | 1:72:A:PHE:HB3 | 1:87:A:LEU:H    | 7        | 2.95          |
| (1,1543) | 1:72:A:PHE:HB2 | 1:87:A:LEU:HB2  | 10       | 2.94          |
| (1,1543) | 1:72:A:PHE:HB2 | 1:87:A:LEU:HB3  | 10       | 2.94          |
| (1,285)  | 1:72:A:PHE:HB2 | 1:87:A:LEU:HB3  | 9        | 2.92          |
| (1,315)  | 1:7:A:MET:HE1  | 1:84:A:GLN:HE21 | 9        | 2.91          |
| (1,315)  | 1:7:A:MET:HE2  | 1:84:A:GLN:HE21 | 9        | 2.91          |
| (1,315)  | 1:7:A:MET:HE3  | 1:84:A:GLN:HE21 | 9        | 2.91          |
| (1,1319) | 1:4:A:LEU:HD21 | 1:84:A:GLN:HE21 | 3        | 2.88          |
| (1,1319) | 1:4:A:LEU:HD21 | 1:84:A:GLN:HE22 | 3        | 2.88          |
| (1,1319) | 1:4:A:LEU:HD22 | 1:84:A:GLN:HE21 | 3        | 2.88          |
| (1,1319) | 1:4:A:LEU:HD22 | 1:84:A:GLN:HE22 | 3        | 2.88          |
| (1,1319) | 1:4:A:LEU:HD23 | 1:84:A:GLN:HE21 | 3        | 2.88          |
| (1,1319) | 1:4:A:LEU:HD23 | 1:84:A:GLN:HE22 | 3        | 2.88          |
| (1,315)  | 1:7:A:MET:HE1  | 1:84:A:GLN:HE21 | 4        | 2.86          |
| (1,315)  | 1:7:A:MET:HE2  | 1:84:A:GLN:HE21 | 4        | 2.86          |
| (1,315)  | 1:7:A:MET:HE3  | 1:84:A:GLN:HE21 | 4        | 2.86          |
| (1,1413) | 1:23:A:LYS:HE2 | 1:27:A:GLU:H    | 3        | 2.85          |
| (1,1413) | 1:23:A:LYS:HE3 | 1:27:A:GLU:H    | 3        | 2.85          |
| (1,902)  | 1:72:A:PHE:HB3 | 1:87:A:LEU:H    | 3        | 2.85          |
| (1,331)  | 1:72:A:PHE:HB3 | 1:87:A:LEU:HA   | 6        | 2.85          |
| (1,1229) | 1:4:A:LEU:HD21 | 1:84:A:GLN:HE22 | 9        | 2.84          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,1229) | 1:4:A:LEU:HD22 | 1:84:A:GLN:HE22 | 9        | 2.84          |
| (1,1229) | 1:4:A:LEU:HD23 | 1:84:A:GLN:HE22 | 9        | 2.84          |
| (1,284)  | 1:72:A:PHE:HB2 | 1:87:A:LEU:HB2  | 2        | 2.84          |
| (1,739)  | 1:16:A:SER:H   | 1:45:A:SER:H    | 5        | 2.79          |
| (1,309)  | 1:7:A:MET:HE1  | 1:84:A:GLN:HE22 | 7        | 2.78          |
| (1,309)  | 1:7:A:MET:HE2  | 1:84:A:GLN:HE22 | 7        | 2.78          |
| (1,309)  | 1:7:A:MET:HE3  | 1:84:A:GLN:HE22 | 7        | 2.78          |
| (1,309)  | 1:7:A:MET:HE1  | 1:84:A:GLN:HE22 | 9        | 2.77          |
| (1,309)  | 1:7:A:MET:HE2  | 1:84:A:GLN:HE22 | 9        | 2.77          |
| (1,309)  | 1:7:A:MET:HE3  | 1:84:A:GLN:HE22 | 9        | 2.77          |
| (1,170)  | 1:89:A:ALA:H   | 1:92:A:LEU:HB2  | 5        | 2.76          |
| (1,1229) | 1:4:A:LEU:HD21 | 1:84:A:GLN:HE22 | 3        | 2.74          |
| (1,1229) | 1:4:A:LEU:HD22 | 1:84:A:GLN:HE22 | 3        | 2.74          |
| (1,1229) | 1:4:A:LEU:HD23 | 1:84:A:GLN:HE22 | 3        | 2.74          |
| (1,1085) | 1:6:A:ASN:HA   | 1:32:A:LYS:H    | 2        | 2.74          |
| (1,773)  | 1:15:A:LEU:HA  | 1:45:A:SER:H    | 5        | 2.74          |
| (1,1413) | 1:23:A:LYS:HE2 | 1:27:A:GLU:H    | 10       | 2.73          |
| (1,1413) | 1:23:A:LYS:HE3 | 1:27:A:GLU:H    | 10       | 2.73          |
| (1,1085) | 1:6:A:ASN:HA   | 1:32:A:LYS:H    | 6        | 2.72          |
| (1,1319) | 1:4:A:LEU:HD21 | 1:84:A:GLN:HE21 | 9        | 2.71          |
| (1,1319) | 1:4:A:LEU:HD21 | 1:84:A:GLN:HE22 | 9        | 2.71          |
| (1,1319) | 1:4:A:LEU:HD22 | 1:84:A:GLN:HE21 | 9        | 2.71          |
| (1,1319) | 1:4:A:LEU:HD22 | 1:84:A:GLN:HE22 | 9        | 2.71          |
| (1,1319) | 1:4:A:LEU:HD23 | 1:84:A:GLN:HE21 | 9        | 2.71          |
| (1,1319) | 1:4:A:LEU:HD23 | 1:84:A:GLN:HE22 | 9        | 2.71          |
| (1,170)  | 1:89:A:ALA:H   | 1:92:A:LEU:HB2  | 6        | 2.71          |
| (1,1085) | 1:6:A:ASN:HA   | 1:32:A:LYS:H    | 4        | 2.7           |
| (1,1413) | 1:23:A:LYS:HE2 | 1:27:A:GLU:H    | 7        | 2.66          |
| (1,1413) | 1:23:A:LYS:HE3 | 1:27:A:GLU:H    | 7        | 2.66          |
| (1,902)  | 1:72:A:PHE:HB3 | 1:87:A:LEU:H    | 1        | 2.66          |
| (1,1413) | 1:23:A:LYS:HE2 | 1:27:A:GLU:H    | 6        | 2.64          |
| (1,1413) | 1:23:A:LYS:HE3 | 1:27:A:GLU:H    | 6        | 2.64          |
| (1,331)  | 1:72:A:PHE:HB3 | 1:87:A:LEU:HA   | 2        | 2.63          |
| (1,1327) | 1:7:A:MET:HE1  | 1:84:A:GLN:HE21 | 8        | 2.62          |
| (1,1327) | 1:7:A:MET:HE1  | 1:84:A:GLN:HE22 | 8        | 2.62          |
| (1,1327) | 1:7:A:MET:HE2  | 1:84:A:GLN:HE21 | 8        | 2.62          |
| (1,1327) | 1:7:A:MET:HE2  | 1:84:A:GLN:HE22 | 8        | 2.62          |
| (1,1327) | 1:7:A:MET:HE3  | 1:84:A:GLN:HE21 | 8        | 2.62          |
| (1,1327) | 1:7:A:MET:HE3  | 1:84:A:GLN:HE22 | 8        | 2.62          |
| (1,1327) | 1:7:A:MET:HE1  | 1:84:A:GLN:HE21 | 10       | 2.62          |
| (1,1327) | 1:7:A:MET:HE1  | 1:84:A:GLN:HE22 | 10       | 2.62          |
| (1,1327) | 1:7:A:MET:HE2  | 1:84:A:GLN:HE21 | 10       | 2.62          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,1327) | 1:7:A:MET:HE2  | 1:84:A:GLN:HE22 | 10       | 2.62          |
| (1,1327) | 1:7:A:MET:HE3  | 1:84:A:GLN:HE21 | 10       | 2.62          |
| (1,1327) | 1:7:A:MET:HE3  | 1:84:A:GLN:HE22 | 10       | 2.62          |
| (1,331)  | 1:72:A:PHE:HB3 | 1:87:A:LEU:HA   | 8        | 2.61          |
| (1,285)  | 1:72:A:PHE:HB2 | 1:87:A:LEU:HB3  | 6        | 2.6           |
| (1,739)  | 1:16:A:SER:H   | 1:45:A:SER:H    | 9        | 2.56          |
| (1,331)  | 1:72:A:PHE:HB3 | 1:87:A:LEU:HA   | 9        | 2.53          |
| (1,315)  | 1:7:A:MET:HE1  | 1:84:A:GLN:HE21 | 1        | 2.53          |
| (1,315)  | 1:7:A:MET:HE2  | 1:84:A:GLN:HE21 | 1        | 2.53          |
| (1,315)  | 1:7:A:MET:HE3  | 1:84:A:GLN:HE21 | 1        | 2.53          |
| (1,902)  | 1:72:A:PHE:HB3 | 1:87:A:LEU:H    | 5        | 2.52          |
| (1,1234) | 1:4:A:LEU:HD21 | 1:84:A:GLN:HE21 | 9        | 2.5           |
| (1,1234) | 1:4:A:LEU:HD22 | 1:84:A:GLN:HE21 | 9        | 2.5           |
| (1,1234) | 1:4:A:LEU:HD23 | 1:84:A:GLN:HE21 | 9        | 2.5           |
| (1,284)  | 1:72:A:PHE:HB2 | 1:87:A:LEU:HB2  | 7        | 2.48          |
| (1,1543) | 1:72:A:PHE:HB2 | 1:87:A:LEU:HB2  | 9        | 2.43          |
| (1,1543) | 1:72:A:PHE:HB2 | 1:87:A:LEU:HB3  | 9        | 2.43          |
| (1,309)  | 1:7:A:MET:HE1  | 1:84:A:GLN:HE22 | 1        | 2.41          |
| (1,309)  | 1:7:A:MET:HE2  | 1:84:A:GLN:HE22 | 1        | 2.41          |
| (1,309)  | 1:7:A:MET:HE3  | 1:84:A:GLN:HE22 | 1        | 2.41          |
| (1,1414) | 1:23:A:LYS:HE2 | 1:27:A:GLU:HG3  | 4        | 2.4           |
| (1,1414) | 1:23:A:LYS:HE3 | 1:27:A:GLU:HG3  | 4        | 2.4           |
| (1,331)  | 1:72:A:PHE:HB3 | 1:87:A:LEU:HA   | 7        | 2.38          |
| (1,284)  | 1:72:A:PHE:HB2 | 1:87:A:LEU:HB2  | 1        | 2.37          |
| (1,902)  | 1:72:A:PHE:HB3 | 1:87:A:LEU:H    | 4        | 2.36          |
| (1,1413) | 1:23:A:LYS:HE2 | 1:27:A:GLU:H    | 2        | 2.35          |
| (1,1413) | 1:23:A:LYS:HE3 | 1:27:A:GLU:H    | 2        | 2.35          |
| (1,739)  | 1:16:A:SER:H   | 1:45:A:SER:H    | 3        | 2.35          |
| (1,284)  | 1:72:A:PHE:HB2 | 1:87:A:LEU:HB2  | 3        | 2.33          |
| (1,1623) | 1:99:A:VAL:H   | 1:100:A:LYS:HD2 | 3        | 2.31          |
| (1,1623) | 1:99:A:VAL:H   | 1:100:A:LYS:HD3 | 3        | 2.31          |
| (1,1623) | 1:99:A:VAL:H   | 1:100:A:LYS:HD2 | 5        | 2.28          |
| (1,1623) | 1:99:A:VAL:H   | 1:100:A:LYS:HD3 | 5        | 2.28          |
| (1,331)  | 1:72:A:PHE:HB3 | 1:87:A:LEU:HA   | 1        | 2.25          |
| (1,331)  | 1:72:A:PHE:HB3 | 1:87:A:LEU:HA   | 3        | 2.25          |
| (1,282)  | 1:72:A:PHE:HB2 | 1:86:A:LEU:HB2  | 8        | 2.25          |
| (1,1327) | 1:7:A:MET:HE1  | 1:84:A:GLN:HE21 | 3        | 2.21          |
| (1,1327) | 1:7:A:MET:HE1  | 1:84:A:GLN:HE22 | 3        | 2.21          |
| (1,1327) | 1:7:A:MET:HE2  | 1:84:A:GLN:HE21 | 3        | 2.21          |
| (1,1327) | 1:7:A:MET:HE2  | 1:84:A:GLN:HE22 | 3        | 2.21          |
| (1,1327) | 1:7:A:MET:HE3  | 1:84:A:GLN:HE21 | 3        | 2.21          |
| (1,1327) | 1:7:A:MET:HE3  | 1:84:A:GLN:HE22 | 3        | 2.21          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,285)  | 1:72:A:PHE:HB2 | 1:87:A:LEU:HB3  | 8        | 2.19          |
| (1,284)  | 1:72:A:PHE:HB2 | 1:87:A:LEU:HB2  | 5        | 2.19          |
| (1,1414) | 1:23:A:LYS:HE2 | 1:27:A:GLU:HG3  | 5        | 2.18          |
| (1,1414) | 1:23:A:LYS:HE3 | 1:27:A:GLU:HG3  | 5        | 2.18          |
| (1,282)  | 1:72:A:PHE:HB2 | 1:86:A:LEU:HB2  | 3        | 2.16          |
| (1,1414) | 1:23:A:LYS:HE2 | 1:27:A:GLU:HG3  | 1        | 2.15          |
| (1,1414) | 1:23:A:LYS:HE3 | 1:27:A:GLU:HG3  | 1        | 2.15          |
| (1,369)  | 1:76:A:VAL:HA  | 1:83:A:LEU:HA   | 6        | 2.15          |
| (1,284)  | 1:72:A:PHE:HB2 | 1:87:A:LEU:HB2  | 4        | 2.13          |
| (1,1327) | 1:7:A:MET:HE1  | 1:84:A:GLN:HE21 | 7        | 2.12          |
| (1,1327) | 1:7:A:MET:HE1  | 1:84:A:GLN:HE22 | 7        | 2.12          |
| (1,1327) | 1:7:A:MET:HE2  | 1:84:A:GLN:HE21 | 7        | 2.12          |
| (1,1327) | 1:7:A:MET:HE2  | 1:84:A:GLN:HE22 | 7        | 2.12          |
| (1,1327) | 1:7:A:MET:HE3  | 1:84:A:GLN:HE21 | 7        | 2.12          |
| (1,1327) | 1:7:A:MET:HE3  | 1:84:A:GLN:HE22 | 7        | 2.12          |
| (1,1177) | 1:52:A:LYS:HE2 | 1:54:A:SER:H    | 9        | 2.12          |
| (1,1327) | 1:7:A:MET:HE1  | 1:84:A:GLN:HE21 | 4        | 2.09          |
| (1,1327) | 1:7:A:MET:HE1  | 1:84:A:GLN:HE22 | 4        | 2.09          |
| (1,1327) | 1:7:A:MET:HE2  | 1:84:A:GLN:HE21 | 4        | 2.09          |
| (1,1327) | 1:7:A:MET:HE2  | 1:84:A:GLN:HE22 | 4        | 2.09          |
| (1,1327) | 1:7:A:MET:HE3  | 1:84:A:GLN:HE21 | 4        | 2.09          |
| (1,1327) | 1:7:A:MET:HE3  | 1:84:A:GLN:HE22 | 4        | 2.09          |
| (1,282)  | 1:72:A:PHE:HB2 | 1:86:A:LEU:HB2  | 2        | 2.09          |
| (1,155)  | 1:68:A:VAL:H   | 1:92:A:LEU:HD21 | 6        | 2.08          |
| (1,155)  | 1:68:A:VAL:H   | 1:92:A:LEU:HD22 | 6        | 2.08          |
| (1,155)  | 1:68:A:VAL:H   | 1:92:A:LEU:HD23 | 6        | 2.08          |
| (1,1543) | 1:72:A:PHE:HB2 | 1:87:A:LEU:HB2  | 6        | 2.06          |
| (1,1543) | 1:72:A:PHE:HB2 | 1:87:A:LEU:HB3  | 6        | 2.06          |
| (1,369)  | 1:76:A:VAL:HA  | 1:83:A:LEU:HA   | 8        | 2.06          |
| (1,1414) | 1:23:A:LYS:HE2 | 1:27:A:GLU:HG3  | 10       | 2.04          |
| (1,1414) | 1:23:A:LYS:HE3 | 1:27:A:GLU:HG3  | 10       | 2.04          |
| (1,331)  | 1:72:A:PHE:HB3 | 1:87:A:LEU:HA   | 5        | 2.04          |
| (1,901)  | 1:72:A:PHE:HB2 | 1:87:A:LEU:H    | 10       | 2.01          |
| (1,331)  | 1:72:A:PHE:HB3 | 1:87:A:LEU:HA   | 4        | 2.01          |
| (1,901)  | 1:72:A:PHE:HB2 | 1:87:A:LEU:H    | 6        | 2.0           |
| (1,1327) | 1:7:A:MET:HE1  | 1:84:A:GLN:HE21 | 9        | 1.99          |
| (1,1327) | 1:7:A:MET:HE1  | 1:84:A:GLN:HE22 | 9        | 1.99          |
| (1,1327) | 1:7:A:MET:HE2  | 1:84:A:GLN:HE21 | 9        | 1.99          |
| (1,1327) | 1:7:A:MET:HE2  | 1:84:A:GLN:HE22 | 9        | 1.99          |
| (1,1327) | 1:7:A:MET:HE3  | 1:84:A:GLN:HE21 | 9        | 1.99          |
| (1,1327) | 1:7:A:MET:HE3  | 1:84:A:GLN:HE22 | 9        | 1.99          |
| (1,155)  | 1:68:A:VAL:H   | 1:92:A:LEU:HD21 | 5        | 1.99          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,155)  | 1:68:A:VAL:H    | 1:92:A:LEU:HD22 | 5        | 1.99          |
| (1,155)  | 1:68:A:VAL:H    | 1:92:A:LEU:HD23 | 5        | 1.99          |
| (1,765)  | 1:38:A:ASN:HD22 | 1:98:A:GLU:H    | 1        | 1.98          |
| (1,739)  | 1:16:A:SER:H    | 1:45:A:SER:H    | 7        | 1.97          |
| (1,285)  | 1:72:A:PHE:HB2  | 1:87:A:LEU:HB3  | 2        | 1.94          |
| (1,285)  | 1:72:A:PHE:HB2  | 1:87:A:LEU:HB3  | 7        | 1.94          |
| (1,282)  | 1:72:A:PHE:HB2  | 1:86:A:LEU:HB2  | 6        | 1.94          |
| (1,1222) | 1:5:A:SER:H     | 1:7:A:MET:HB3   | 5        | 1.93          |
| (1,739)  | 1:16:A:SER:H    | 1:45:A:SER:H    | 1        | 1.93          |
| (1,901)  | 1:72:A:PHE:HB2  | 1:87:A:LEU:H    | 8        | 1.92          |
| (1,282)  | 1:72:A:PHE:HB2  | 1:86:A:LEU:HB2  | 9        | 1.92          |
| (1,1414) | 1:23:A:LYS:HE2  | 1:27:A:GLU:HG3  | 8        | 1.91          |
| (1,1414) | 1:23:A:LYS:HE3  | 1:27:A:GLU:HG3  | 8        | 1.91          |
| (1,1414) | 1:23:A:LYS:HE2  | 1:27:A:GLU:HG3  | 3        | 1.9           |
| (1,1414) | 1:23:A:LYS:HE3  | 1:27:A:GLU:HG3  | 3        | 1.9           |
| (1,369)  | 1:76:A:VAL:HA   | 1:83:A:LEU:HA   | 1        | 1.9           |
| (1,282)  | 1:72:A:PHE:HB2  | 1:86:A:LEU:HB2  | 1        | 1.9           |
| (1,1222) | 1:5:A:SER:H     | 1:7:A:MET:HB3   | 2        | 1.89          |
| (1,901)  | 1:72:A:PHE:HB2  | 1:87:A:LEU:H    | 2        | 1.89          |
| (1,155)  | 1:68:A:VAL:H    | 1:92:A:LEU:HD21 | 9        | 1.89          |
| (1,155)  | 1:68:A:VAL:H    | 1:92:A:LEU:HD22 | 9        | 1.89          |
| (1,155)  | 1:68:A:VAL:H    | 1:92:A:LEU:HD23 | 9        | 1.89          |
| (1,282)  | 1:72:A:PHE:HB2  | 1:86:A:LEU:HB2  | 7        | 1.88          |
| (1,1178) | 1:52:A:LYS:HE3  | 1:54:A:SER:H    | 6        | 1.87          |
| (1,1108) | 1:49:A:GLU:HB3  | 1:54:A:SER:H    | 2        | 1.87          |
| (1,765)  | 1:38:A:ASN:HD22 | 1:98:A:GLU:H    | 5        | 1.86          |
| (1,739)  | 1:16:A:SER:H    | 1:45:A:SER:H    | 10       | 1.86          |
| (1,282)  | 1:72:A:PHE:HB2  | 1:86:A:LEU:HB2  | 10       | 1.86          |
| (1,765)  | 1:38:A:ASN:HD22 | 1:98:A:GLU:H    | 10       | 1.85          |
| (1,285)  | 1:72:A:PHE:HB2  | 1:87:A:LEU:HB3  | 3        | 1.83          |
| (1,1222) | 1:5:A:SER:H     | 1:7:A:MET:HB3   | 9        | 1.81          |
| (1,765)  | 1:38:A:ASN:HD22 | 1:98:A:GLU:H    | 6        | 1.81          |
| (1,119)  | 1:57:A:MET:HE1  | 1:92:A:LEU:HD11 | 10       | 1.81          |
| (1,119)  | 1:57:A:MET:HE1  | 1:92:A:LEU:HD12 | 10       | 1.81          |
| (1,119)  | 1:57:A:MET:HE1  | 1:92:A:LEU:HD13 | 10       | 1.81          |
| (1,119)  | 1:57:A:MET:HE2  | 1:92:A:LEU:HD11 | 10       | 1.81          |
| (1,119)  | 1:57:A:MET:HE2  | 1:92:A:LEU:HD12 | 10       | 1.81          |
| (1,119)  | 1:57:A:MET:HE2  | 1:92:A:LEU:HD13 | 10       | 1.81          |
| (1,119)  | 1:57:A:MET:HE3  | 1:92:A:LEU:HD11 | 10       | 1.81          |
| (1,119)  | 1:57:A:MET:HE3  | 1:92:A:LEU:HD12 | 10       | 1.81          |
| (1,119)  | 1:57:A:MET:HE3  | 1:92:A:LEU:HD13 | 10       | 1.81          |
| (1,118)  | 1:57:A:MET:HE1  | 1:92:A:LEU:HD11 | 10       | 1.81          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,118)  | 1:57:A:MET:HE1 | 1:92:A:LEU:HD12 | 10       | 1.81          |
| (1,118)  | 1:57:A:MET:HE1 | 1:92:A:LEU:HD13 | 10       | 1.81          |
| (1,118)  | 1:57:A:MET:HE2 | 1:92:A:LEU:HD11 | 10       | 1.81          |
| (1,118)  | 1:57:A:MET:HE2 | 1:92:A:LEU:HD12 | 10       | 1.81          |
| (1,118)  | 1:57:A:MET:HE2 | 1:92:A:LEU:HD13 | 10       | 1.81          |
| (1,118)  | 1:57:A:MET:HE3 | 1:92:A:LEU:HD11 | 10       | 1.81          |
| (1,118)  | 1:57:A:MET:HE3 | 1:92:A:LEU:HD12 | 10       | 1.81          |
| (1,118)  | 1:57:A:MET:HE3 | 1:92:A:LEU:HD13 | 10       | 1.81          |
| (1,1222) | 1:5:A:SER:H    | 1:7:A:MET:HB3   | 1        | 1.8           |
| (1,1177) | 1:52:A:LYS:HE2 | 1:54:A:SER:H    | 3        | 1.8           |
| (1,155)  | 1:68:A:VAL:H   | 1:92:A:LEU:HD21 | 4        | 1.78          |
| (1,155)  | 1:68:A:VAL:H   | 1:92:A:LEU:HD22 | 4        | 1.78          |
| (1,155)  | 1:68:A:VAL:H   | 1:92:A:LEU:HD23 | 4        | 1.78          |
| (1,285)  | 1:72:A:PHE:HB2 | 1:87:A:LEU:HB3  | 5        | 1.77          |
| (1,773)  | 1:15:A:LEU:HA  | 1:45:A:SER:H    | 9        | 1.75          |
| (1,1134) | 1:91:A:SER:H   | 1:92:A:LEU:HB2  | 3        | 1.73          |
| (1,901)  | 1:72:A:PHE:HB2 | 1:87:A:LEU:H    | 3        | 1.72          |
| (1,1543) | 1:72:A:PHE:HB2 | 1:87:A:LEU:HB2  | 8        | 1.71          |
| (1,1543) | 1:72:A:PHE:HB2 | 1:87:A:LEU:HB3  | 8        | 1.71          |
| (1,1109) | 1:7:A:MET:HG2  | 1:32:A:LYS:H    | 5        | 1.71          |
| (1,155)  | 1:68:A:VAL:H   | 1:92:A:LEU:HD21 | 8        | 1.71          |
| (1,155)  | 1:68:A:VAL:H   | 1:92:A:LEU:HD22 | 8        | 1.71          |
| (1,155)  | 1:68:A:VAL:H   | 1:92:A:LEU:HD23 | 8        | 1.71          |
| (1,1111) | 1:7:A:MET:HB3  | 1:32:A:LYS:H    | 7        | 1.69          |
| (1,369)  | 1:76:A:VAL:HA  | 1:83:A:LEU:HA   | 10       | 1.69          |
| (1,1134) | 1:91:A:SER:H   | 1:92:A:LEU:HB2  | 1        | 1.68          |
| (1,369)  | 1:76:A:VAL:HA  | 1:83:A:LEU:HA   | 7        | 1.68          |
| (1,285)  | 1:72:A:PHE:HB2 | 1:87:A:LEU:HB3  | 1        | 1.68          |
| (1,1222) | 1:5:A:SER:H    | 1:7:A:MET:HB3   | 4        | 1.67          |
| (1,901)  | 1:72:A:PHE:HB2 | 1:87:A:LEU:H    | 9        | 1.67          |
| (1,86)   | 1:9:A:ILE:HD11 | 1:42:A:LEU:HD21 | 6        | 1.67          |
| (1,86)   | 1:9:A:ILE:HD11 | 1:42:A:LEU:HD22 | 6        | 1.67          |
| (1,86)   | 1:9:A:ILE:HD11 | 1:42:A:LEU:HD23 | 6        | 1.67          |
| (1,86)   | 1:9:A:ILE:HD12 | 1:42:A:LEU:HD21 | 6        | 1.67          |
| (1,86)   | 1:9:A:ILE:HD12 | 1:42:A:LEU:HD22 | 6        | 1.67          |
| (1,86)   | 1:9:A:ILE:HD12 | 1:42:A:LEU:HD23 | 6        | 1.67          |
| (1,86)   | 1:9:A:ILE:HD13 | 1:42:A:LEU:HD21 | 6        | 1.67          |
| (1,86)   | 1:9:A:ILE:HD13 | 1:42:A:LEU:HD22 | 6        | 1.67          |
| (1,86)   | 1:9:A:ILE:HD13 | 1:42:A:LEU:HD23 | 6        | 1.67          |
| (1,85)   | 1:9:A:ILE:HD11 | 1:42:A:LEU:HD21 | 6        | 1.67          |
| (1,85)   | 1:9:A:ILE:HD11 | 1:42:A:LEU:HD22 | 6        | 1.67          |
| (1,85)   | 1:9:A:ILE:HD11 | 1:42:A:LEU:HD23 | 6        | 1.67          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,85)   | 1:9:A:ILE:HD12 | 1:42:A:LEU:HD21 | 6        | 1.67          |
| (1,85)   | 1:9:A:ILE:HD12 | 1:42:A:LEU:HD22 | 6        | 1.67          |
| (1,85)   | 1:9:A:ILE:HD12 | 1:42:A:LEU:HD23 | 6        | 1.67          |
| (1,85)   | 1:9:A:ILE:HD13 | 1:42:A:LEU:HD21 | 6        | 1.67          |
| (1,85)   | 1:9:A:ILE:HD13 | 1:42:A:LEU:HD22 | 6        | 1.67          |
| (1,85)   | 1:9:A:ILE:HD13 | 1:42:A:LEU:HD23 | 6        | 1.67          |
| (1,1327) | 1:7:A:MET:HE1  | 1:84:A:GLN:HE21 | 1        | 1.66          |
| (1,1327) | 1:7:A:MET:HE1  | 1:84:A:GLN:HE22 | 1        | 1.66          |
| (1,1327) | 1:7:A:MET:HE2  | 1:84:A:GLN:HE21 | 1        | 1.66          |
| (1,1327) | 1:7:A:MET:HE2  | 1:84:A:GLN:HE22 | 1        | 1.66          |
| (1,1327) | 1:7:A:MET:HE3  | 1:84:A:GLN:HE21 | 1        | 1.66          |
| (1,1327) | 1:7:A:MET:HE3  | 1:84:A:GLN:HE22 | 1        | 1.66          |
| (1,1178) | 1:52:A:LYS:HE3 | 1:54:A:SER:H    | 1        | 1.66          |
| (1,1108) | 1:49:A:GLU:HB3 | 1:54:A:SER:H    | 9        | 1.66          |
| (1,369)  | 1:76:A:VAL:HA  | 1:83:A:LEU:HA   | 5        | 1.66          |
| (1,155)  | 1:68:A:VAL:H   | 1:92:A:LEU:HD21 | 1        | 1.66          |
| (1,155)  | 1:68:A:VAL:H   | 1:92:A:LEU:HD22 | 1        | 1.66          |
| (1,155)  | 1:68:A:VAL:H   | 1:92:A:LEU:HD23 | 1        | 1.66          |
| (1,1111) | 1:7:A:MET:HB3  | 1:32:A:LYS:H    | 8        | 1.65          |
| (1,1177) | 1:52:A:LYS:HE2 | 1:54:A:SER:H    | 7        | 1.64          |
| (1,1111) | 1:7:A:MET:HB3  | 1:32:A:LYS:H    | 1        | 1.64          |
| (1,227)  | 1:4:A:LEU:HB3  | 1:30:A:GLY:HA2  | 2        | 1.64          |
| (1,1109) | 1:7:A:MET:HG2  | 1:32:A:LYS:H    | 9        | 1.63          |
| (1,773)  | 1:15:A:LEU:HA  | 1:45:A:SER:H    | 3        | 1.63          |
| (1,1623) | 1:99:A:VAL:H   | 1:100:A:LYS:HD2 | 2        | 1.62          |
| (1,1623) | 1:99:A:VAL:H   | 1:100:A:LYS:HD3 | 2        | 1.62          |
| (1,901)  | 1:72:A:PHE:HB2 | 1:87:A:LEU:H    | 7        | 1.62          |
| (1,1111) | 1:7:A:MET:HB3  | 1:32:A:LYS:H    | 5        | 1.61          |
| (1,282)  | 1:72:A:PHE:HB2 | 1:86:A:LEU:HB2  | 5        | 1.61          |
| (1,1414) | 1:23:A:LYS:HE2 | 1:27:A:GLU:HG3  | 6        | 1.6           |
| (1,1414) | 1:23:A:LYS:HE3 | 1:27:A:GLU:HG3  | 6        | 1.6           |
| (1,1134) | 1:91:A:SER:H   | 1:92:A:LEU:HB2  | 2        | 1.6           |
| (1,773)  | 1:15:A:LEU:HA  | 1:45:A:SER:H    | 7        | 1.6           |
| (1,739)  | 1:16:A:SER:H   | 1:45:A:SER:H    | 6        | 1.6           |
| (1,1223) | 1:5:A:SER:H    | 1:7:A:MET:HE1   | 1        | 1.59          |
| (1,1223) | 1:5:A:SER:H    | 1:7:A:MET:HE2   | 1        | 1.59          |
| (1,1223) | 1:5:A:SER:H    | 1:7:A:MET:HE3   | 1        | 1.59          |
| (1,1222) | 1:5:A:SER:H    | 1:7:A:MET:HB3   | 3        | 1.59          |
| (1,1177) | 1:52:A:LYS:HE2 | 1:54:A:SER:H    | 6        | 1.59          |
| (1,369)  | 1:76:A:VAL:HA  | 1:83:A:LEU:HA   | 2        | 1.58          |
| (1,1177) | 1:52:A:LYS:HE2 | 1:54:A:SER:H    | 2        | 1.57          |
| (1,1134) | 1:91:A:SER:H   | 1:92:A:LEU:HB2  | 4        | 1.57          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,1222) | 1:5:A:SER:H    | 1:7:A:MET:HB3   | 7        | 1.56          |
| (1,1222) | 1:5:A:SER:H    | 1:7:A:MET:HB3   | 8        | 1.56          |
| (1,1134) | 1:91:A:SER:H   | 1:92:A:LEU:HB2  | 8        | 1.56          |
| (1,901)  | 1:72:A:PHE:HB2 | 1:87:A:LEU:H    | 1        | 1.56          |
| (1,282)  | 1:72:A:PHE:HB2 | 1:86:A:LEU:HB2  | 4        | 1.56          |
| (1,1125) | 1:83:A:LEU:HG  | 1:84:A:GLN:H    | 8        | 1.55          |
| (1,1414) | 1:23:A:LYS:HE2 | 1:27:A:GLU:HG3  | 7        | 1.54          |
| (1,1414) | 1:23:A:LYS:HE3 | 1:27:A:GLU:HG3  | 7        | 1.54          |
| (1,1111) | 1:7:A:MET:HB3  | 1:32:A:LYS:H    | 9        | 1.54          |
| (1,285)  | 1:72:A:PHE:HB2 | 1:87:A:LEU:HB3  | 4        | 1.54          |
| (1,119)  | 1:57:A:MET:HE1 | 1:92:A:LEU:HD11 | 4        | 1.54          |
| (1,119)  | 1:57:A:MET:HE1 | 1:92:A:LEU:HD12 | 4        | 1.54          |
| (1,119)  | 1:57:A:MET:HE1 | 1:92:A:LEU:HD13 | 4        | 1.54          |
| (1,119)  | 1:57:A:MET:HE2 | 1:92:A:LEU:HD11 | 4        | 1.54          |
| (1,119)  | 1:57:A:MET:HE2 | 1:92:A:LEU:HD12 | 4        | 1.54          |
| (1,119)  | 1:57:A:MET:HE2 | 1:92:A:LEU:HD13 | 4        | 1.54          |
| (1,119)  | 1:57:A:MET:HE3 | 1:92:A:LEU:HD11 | 4        | 1.54          |
| (1,119)  | 1:57:A:MET:HE3 | 1:92:A:LEU:HD12 | 4        | 1.54          |
| (1,119)  | 1:57:A:MET:HE3 | 1:92:A:LEU:HD13 | 4        | 1.54          |
| (1,118)  | 1:57:A:MET:HE1 | 1:92:A:LEU:HD11 | 4        | 1.54          |
| (1,118)  | 1:57:A:MET:HE1 | 1:92:A:LEU:HD12 | 4        | 1.54          |
| (1,118)  | 1:57:A:MET:HE1 | 1:92:A:LEU:HD13 | 4        | 1.54          |
| (1,118)  | 1:57:A:MET:HE2 | 1:92:A:LEU:HD11 | 4        | 1.54          |
| (1,118)  | 1:57:A:MET:HE2 | 1:92:A:LEU:HD12 | 4        | 1.54          |
| (1,118)  | 1:57:A:MET:HE2 | 1:92:A:LEU:HD13 | 4        | 1.54          |
| (1,118)  | 1:57:A:MET:HE3 | 1:92:A:LEU:HD11 | 4        | 1.54          |
| (1,118)  | 1:57:A:MET:HE3 | 1:92:A:LEU:HD12 | 4        | 1.54          |
| (1,118)  | 1:57:A:MET:HE3 | 1:92:A:LEU:HD13 | 4        | 1.54          |
| (1,119)  | 1:57:A:MET:HE1 | 1:92:A:LEU:HD11 | 8        | 1.52          |
| (1,119)  | 1:57:A:MET:HE1 | 1:92:A:LEU:HD12 | 8        | 1.52          |
| (1,119)  | 1:57:A:MET:HE1 | 1:92:A:LEU:HD13 | 8        | 1.52          |
| (1,119)  | 1:57:A:MET:HE2 | 1:92:A:LEU:HD11 | 8        | 1.52          |
| (1,119)  | 1:57:A:MET:HE2 | 1:92:A:LEU:HD12 | 8        | 1.52          |
| (1,119)  | 1:57:A:MET:HE2 | 1:92:A:LEU:HD13 | 8        | 1.52          |
| (1,119)  | 1:57:A:MET:HE3 | 1:92:A:LEU:HD11 | 8        | 1.52          |
| (1,119)  | 1:57:A:MET:HE3 | 1:92:A:LEU:HD12 | 8        | 1.52          |
| (1,119)  | 1:57:A:MET:HE3 | 1:92:A:LEU:HD13 | 8        | 1.52          |
| (1,118)  | 1:57:A:MET:HE1 | 1:92:A:LEU:HD11 | 8        | 1.52          |
| (1,118)  | 1:57:A:MET:HE1 | 1:92:A:LEU:HD12 | 8        | 1.52          |
| (1,118)  | 1:57:A:MET:HE1 | 1:92:A:LEU:HD13 | 8        | 1.52          |
| (1,118)  | 1:57:A:MET:HE2 | 1:92:A:LEU:HD11 | 8        | 1.52          |
| (1,118)  | 1:57:A:MET:HE2 | 1:92:A:LEU:HD12 | 8        | 1.52          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,118)  | 1:57:A:MET:HE2 | 1:92:A:LEU:HD13 | 8        | 1.52          |
| (1,118)  | 1:57:A:MET:HE3 | 1:92:A:LEU:HD11 | 8        | 1.52          |
| (1,118)  | 1:57:A:MET:HE3 | 1:92:A:LEU:HD12 | 8        | 1.52          |
| (1,118)  | 1:57:A:MET:HE3 | 1:92:A:LEU:HD13 | 8        | 1.52          |
| (1,1414) | 1:23:A:LYS:HE2 | 1:27:A:GLU:HG3  | 2        | 1.51          |
| (1,1414) | 1:23:A:LYS:HE3 | 1:27:A:GLU:HG3  | 2        | 1.51          |
| (1,1223) | 1:5:A:SER:H    | 1:7:A:MET:HE1   | 4        | 1.51          |
| (1,1223) | 1:5:A:SER:H    | 1:7:A:MET:HE2   | 4        | 1.51          |
| (1,1223) | 1:5:A:SER:H    | 1:7:A:MET:HE3   | 4        | 1.51          |
| (1,119)  | 1:57:A:MET:HE1 | 1:92:A:LEU:HD11 | 6        | 1.51          |
| (1,119)  | 1:57:A:MET:HE1 | 1:92:A:LEU:HD12 | 6        | 1.51          |
| (1,119)  | 1:57:A:MET:HE1 | 1:92:A:LEU:HD13 | 6        | 1.51          |
| (1,119)  | 1:57:A:MET:HE2 | 1:92:A:LEU:HD11 | 6        | 1.51          |
| (1,119)  | 1:57:A:MET:HE2 | 1:92:A:LEU:HD12 | 6        | 1.51          |
| (1,119)  | 1:57:A:MET:HE2 | 1:92:A:LEU:HD13 | 6        | 1.51          |
| (1,119)  | 1:57:A:MET:HE3 | 1:92:A:LEU:HD11 | 6        | 1.51          |
| (1,119)  | 1:57:A:MET:HE3 | 1:92:A:LEU:HD12 | 6        | 1.51          |
| (1,119)  | 1:57:A:MET:HE3 | 1:92:A:LEU:HD13 | 6        | 1.51          |
| (1,118)  | 1:57:A:MET:HE1 | 1:92:A:LEU:HD11 | 6        | 1.51          |
| (1,118)  | 1:57:A:MET:HE1 | 1:92:A:LEU:HD12 | 6        | 1.51          |
| (1,118)  | 1:57:A:MET:HE1 | 1:92:A:LEU:HD13 | 6        | 1.51          |
| (1,118)  | 1:57:A:MET:HE2 | 1:92:A:LEU:HD11 | 6        | 1.51          |
| (1,118)  | 1:57:A:MET:HE2 | 1:92:A:LEU:HD12 | 6        | 1.51          |
| (1,118)  | 1:57:A:MET:HE2 | 1:92:A:LEU:HD13 | 6        | 1.51          |
| (1,118)  | 1:57:A:MET:HE3 | 1:92:A:LEU:HD11 | 6        | 1.51          |
| (1,118)  | 1:57:A:MET:HE3 | 1:92:A:LEU:HD12 | 6        | 1.51          |
| (1,118)  | 1:57:A:MET:HE3 | 1:92:A:LEU:HD13 | 6        | 1.51          |
| (1,1543) | 1:72:A:PHE:HB2 | 1:87:A:LEU:HB2  | 2        | 1.5           |
| (1,1543) | 1:72:A:PHE:HB2 | 1:87:A:LEU:HB3  | 2        | 1.5           |
| (1,1222) | 1:5:A:SER:H    | 1:7:A:MET:HB3   | 10       | 1.5           |
| (1,1125) | 1:83:A:LEU:HG  | 1:84:A:GLN:H    | 10       | 1.5           |
| (1,1111) | 1:7:A:MET:HB3  | 1:32:A:LYS:H    | 3        | 1.5           |
| (1,1178) | 1:52:A:LYS:HE3 | 1:54:A:SER:H    | 9        | 1.49          |
| (1,1134) | 1:91:A:SER:H   | 1:92:A:LEU:HB2  | 7        | 1.49          |
| (1,369)  | 1:76:A:VAL:HA  | 1:83:A:LEU:HA   | 4        | 1.49          |
| (1,1177) | 1:52:A:LYS:HE2 | 1:54:A:SER:H    | 4        | 1.48          |
| (1,1134) | 1:91:A:SER:H   | 1:92:A:LEU:HB2  | 10       | 1.48          |
| (1,739)  | 1:16:A:SER:H   | 1:45:A:SER:H    | 2        | 1.47          |
| (1,155)  | 1:68:A:VAL:H   | 1:92:A:LEU:HD21 | 2        | 1.47          |
| (1,155)  | 1:68:A:VAL:H   | 1:92:A:LEU:HD22 | 2        | 1.47          |
| (1,155)  | 1:68:A:VAL:H   | 1:92:A:LEU:HD23 | 2        | 1.47          |
| (1,155)  | 1:68:A:VAL:H   | 1:92:A:LEU:HD21 | 3        | 1.47          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,155)  | 1:68:A:VAL:H    | 1:92:A:LEU:HD22 | 3        | 1.47          |
| (1,155)  | 1:68:A:VAL:H    | 1:92:A:LEU:HD23 | 3        | 1.47          |
| (1,1413) | 1:23:A:LYS:HE2  | 1:27:A:GLU:H    | 9        | 1.45          |
| (1,1413) | 1:23:A:LYS:HE3  | 1:27:A:GLU:H    | 9        | 1.45          |
| (1,1109) | 1:7:A:MET:HG2   | 1:32:A:LYS:H    | 7        | 1.45          |
| (1,1060) | 1:6:A:ASN:H     | 1:32:A:LYS:H    | 7        | 1.44          |
| (1,1125) | 1:83:A:LEU:HG   | 1:84:A:GLN:H    | 6        | 1.43          |
| (1,739)  | 1:16:A:SER:H    | 1:45:A:SER:H    | 8        | 1.43          |
| (1,1259) | 1:38:A:ASN:HD22 | 1:96:A:GLY:H    | 1        | 1.42          |
| (1,769)  | 1:15:A:LEU:HA   | 1:70:A:GLU:H    | 5        | 1.42          |
| (1,1144) | 1:4:A:LEU:HD11  | 1:32:A:LYS:H    | 5        | 1.4           |
| (1,1144) | 1:4:A:LEU:HD12  | 1:32:A:LYS:H    | 5        | 1.4           |
| (1,1144) | 1:4:A:LEU:HD13  | 1:32:A:LYS:H    | 5        | 1.4           |
| (1,1543) | 1:72:A:PHE:HB2  | 1:87:A:LEU:HB2  | 7        | 1.39          |
| (1,1543) | 1:72:A:PHE:HB2  | 1:87:A:LEU:HB3  | 7        | 1.39          |
| (1,1109) | 1:7:A:MET:HG2   | 1:32:A:LYS:H    | 2        | 1.39          |
| (1,1069) | 1:5:A:SER:H     | 1:32:A:LYS:H    | 10       | 1.39          |
| (1,614)  | 1:67:A:VAL:H    | 1:96:A:GLY:H    | 6        | 1.39          |
| (1,1111) | 1:7:A:MET:HB3   | 1:32:A:LYS:H    | 10       | 1.38          |
| (1,773)  | 1:15:A:LEU:HA   | 1:45:A:SER:H    | 10       | 1.38          |
| (1,287)  | 1:53:A:MET:HE1  | 1:61:A:LYS:HE2  | 8        | 1.38          |
| (1,287)  | 1:53:A:MET:HE2  | 1:61:A:LYS:HE2  | 8        | 1.38          |
| (1,287)  | 1:53:A:MET:HE3  | 1:61:A:LYS:HE2  | 8        | 1.38          |
| (1,1223) | 1:5:A:SER:H     | 1:7:A:MET:HE1   | 10       | 1.37          |
| (1,1223) | 1:5:A:SER:H     | 1:7:A:MET:HE2   | 10       | 1.37          |
| (1,1223) | 1:5:A:SER:H     | 1:7:A:MET:HE3   | 10       | 1.37          |
| (1,369)  | 1:76:A:VAL:HA   | 1:83:A:LEU:HA   | 3        | 1.37          |
| (1,227)  | 1:4:A:LEU:HB3   | 1:30:A:GLY:HA2  | 3        | 1.37          |
| (1,119)  | 1:57:A:MET:HE1  | 1:92:A:LEU:HD11 | 1        | 1.37          |
| (1,119)  | 1:57:A:MET:HE1  | 1:92:A:LEU:HD12 | 1        | 1.37          |
| (1,119)  | 1:57:A:MET:HE1  | 1:92:A:LEU:HD13 | 1        | 1.37          |
| (1,119)  | 1:57:A:MET:HE2  | 1:92:A:LEU:HD11 | 1        | 1.37          |
| (1,119)  | 1:57:A:MET:HE2  | 1:92:A:LEU:HD12 | 1        | 1.37          |
| (1,119)  | 1:57:A:MET:HE2  | 1:92:A:LEU:HD13 | 1        | 1.37          |
| (1,119)  | 1:57:A:MET:HE3  | 1:92:A:LEU:HD11 | 1        | 1.37          |
| (1,119)  | 1:57:A:MET:HE3  | 1:92:A:LEU:HD12 | 1        | 1.37          |
| (1,119)  | 1:57:A:MET:HE3  | 1:92:A:LEU:HD13 | 1        | 1.37          |
| (1,118)  | 1:57:A:MET:HE1  | 1:92:A:LEU:HD11 | 1        | 1.37          |
| (1,118)  | 1:57:A:MET:HE1  | 1:92:A:LEU:HD12 | 1        | 1.37          |
| (1,118)  | 1:57:A:MET:HE1  | 1:92:A:LEU:HD13 | 1        | 1.37          |
| (1,118)  | 1:57:A:MET:HE2  | 1:92:A:LEU:HD11 | 1        | 1.37          |
| (1,118)  | 1:57:A:MET:HE2  | 1:92:A:LEU:HD12 | 1        | 1.37          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,118)  | 1:57:A:MET:HE2  | 1:92:A:LEU:HD13 | 1        | 1.37          |
| (1,118)  | 1:57:A:MET:HE3  | 1:92:A:LEU:HD11 | 1        | 1.37          |
| (1,118)  | 1:57:A:MET:HE3  | 1:92:A:LEU:HD12 | 1        | 1.37          |
| (1,118)  | 1:57:A:MET:HE3  | 1:92:A:LEU:HD13 | 1        | 1.37          |
| (1,1223) | 1:5:A:SER:H     | 1:7:A:MET:HE1   | 3        | 1.36          |
| (1,1223) | 1:5:A:SER:H     | 1:7:A:MET:HE2   | 3        | 1.36          |
| (1,1223) | 1:5:A:SER:H     | 1:7:A:MET:HE3   | 3        | 1.36          |
| (1,1069) | 1:5:A:SER:H     | 1:32:A:LYS:H    | 6        | 1.36          |
| (1,901)  | 1:72:A:PHE:HB2  | 1:87:A:LEU:H    | 5        | 1.36          |
| (1,82)   | 1:28:A:LYS:HG3  | 1:29:A:LEU:HG   | 8        | 1.36          |
| (1,1060) | 1:6:A:ASN:H     | 1:32:A:LYS:H    | 9        | 1.35          |
| (1,634)  | 1:69:A:CYS:HB2  | 1:92:A:LEU:H    | 9        | 1.35          |
| (1,614)  | 1:67:A:VAL:H    | 1:96:A:GLY:H    | 8        | 1.35          |
| (1,227)  | 1:4:A:LEU:HB3   | 1:30:A:GLY:HA2  | 7        | 1.35          |
| (1,1178) | 1:52:A:LYS:HE3  | 1:54:A:SER:H    | 8        | 1.34          |
| (1,1108) | 1:49:A:GLU:HB3  | 1:54:A:SER:H    | 8        | 1.34          |
| (1,227)  | 1:4:A:LEU:HB3   | 1:30:A:GLY:HA2  | 10       | 1.34          |
| (1,1623) | 1:99:A:VAL:H    | 1:100:A:LYS:HD2 | 1        | 1.33          |
| (1,1623) | 1:99:A:VAL:H    | 1:100:A:LYS:HD3 | 1        | 1.33          |
| (1,1300) | 1:28:A:LYS:HG3  | 1:30:A:GLY:H    | 10       | 1.33          |
| (1,1178) | 1:52:A:LYS:HE3  | 1:54:A:SER:H    | 2        | 1.33          |
| (1,1178) | 1:52:A:LYS:HE3  | 1:54:A:SER:H    | 10       | 1.33          |
| (1,227)  | 1:4:A:LEU:HB3   | 1:30:A:GLY:HA2  | 9        | 1.33          |
| (1,1223) | 1:5:A:SER:H     | 1:7:A:MET:HE1   | 7        | 1.32          |
| (1,1223) | 1:5:A:SER:H     | 1:7:A:MET:HE2   | 7        | 1.32          |
| (1,1223) | 1:5:A:SER:H     | 1:7:A:MET:HE3   | 7        | 1.32          |
| (1,1048) | 1:4:A:LEU:HD11  | 1:7:A:MET:H     | 10       | 1.32          |
| (1,1048) | 1:4:A:LEU:HD12  | 1:7:A:MET:H     | 10       | 1.32          |
| (1,1048) | 1:4:A:LEU:HD13  | 1:7:A:MET:H     | 10       | 1.32          |
| (1,1259) | 1:38:A:ASN:HD22 | 1:96:A:GLY:H    | 3        | 1.31          |
| (1,773)  | 1:15:A:LEU:HA   | 1:45:A:SER:H    | 6        | 1.31          |
| (1,408)  | 1:72:A:PHE:HA   | 1:87:A:LEU:HA   | 10       | 1.31          |
| (1,1300) | 1:28:A:LYS:HG3  | 1:30:A:GLY:H    | 9        | 1.3           |
| (1,1109) | 1:7:A:MET:HG2   | 1:32:A:LYS:H    | 3        | 1.3           |
| (1,1300) | 1:28:A:LYS:HG3  | 1:30:A:GLY:H    | 4        | 1.29          |
| (1,1223) | 1:5:A:SER:H     | 1:7:A:MET:HE1   | 9        | 1.29          |
| (1,1223) | 1:5:A:SER:H     | 1:7:A:MET:HE2   | 9        | 1.29          |
| (1,1223) | 1:5:A:SER:H     | 1:7:A:MET:HE3   | 9        | 1.29          |
| (1,1222) | 1:5:A:SER:H     | 1:7:A:MET:HB3   | 6        | 1.29          |
| (1,1543) | 1:72:A:PHE:HB2  | 1:87:A:LEU:HB2  | 3        | 1.28          |
| (1,1543) | 1:72:A:PHE:HB2  | 1:87:A:LEU:HB3  | 3        | 1.28          |
| (1,1300) | 1:28:A:LYS:HG3  | 1:30:A:GLY:H    | 6        | 1.28          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1300) | 1:28:A:LYS:HG3  | 1:30:A:GLY:H    | 8        | 1.28          |
| (1,1259) | 1:38:A:ASN:HD22 | 1:96:A:GLY:H    | 6        | 1.28          |
| (1,1069) | 1:5:A:SER:H     | 1:32:A:LYS:H    | 9        | 1.28          |
| (1,1060) | 1:6:A:ASN:H     | 1:32:A:LYS:H    | 1        | 1.28          |
| (1,1060) | 1:6:A:ASN:H     | 1:32:A:LYS:H    | 3        | 1.28          |
| (1,1048) | 1:4:A:LEU:HD11  | 1:7:A:MET:H     | 2        | 1.28          |
| (1,1048) | 1:4:A:LEU:HD12  | 1:7:A:MET:H     | 2        | 1.28          |
| (1,1048) | 1:4:A:LEU:HD13  | 1:7:A:MET:H     | 2        | 1.28          |
| (1,901)  | 1:72:A:PHE:HB2  | 1:87:A:LEU:H    | 4        | 1.28          |
| (1,1550) | 1:74:A:GLN:HA   | 1:74:A:GLN:HE21 | 5        | 1.27          |
| (1,1550) | 1:74:A:GLN:HA   | 1:74:A:GLN:HE22 | 5        | 1.27          |
| (1,1300) | 1:28:A:LYS:HG3  | 1:30:A:GLY:H    | 3        | 1.27          |
| (1,1259) | 1:38:A:ASN:HD22 | 1:96:A:GLY:H    | 2        | 1.27          |
| (1,1223) | 1:5:A:SER:H     | 1:7:A:MET:HE1   | 8        | 1.27          |
| (1,1223) | 1:5:A:SER:H     | 1:7:A:MET:HE2   | 8        | 1.27          |
| (1,1223) | 1:5:A:SER:H     | 1:7:A:MET:HE3   | 8        | 1.27          |
| (1,1177) | 1:52:A:LYS:HE2  | 1:54:A:SER:H    | 5        | 1.27          |
| (1,614)  | 1:67:A:VAL:H    | 1:96:A:GLY:H    | 4        | 1.27          |
| (1,1623) | 1:99:A:VAL:H    | 1:100:A:LYS:HD2 | 9        | 1.26          |
| (1,1623) | 1:99:A:VAL:H    | 1:100:A:LYS:HD3 | 9        | 1.26          |
| (1,1300) | 1:28:A:LYS:HG3  | 1:30:A:GLY:H    | 1        | 1.26          |
| (1,1111) | 1:7:A:MET:HB3   | 1:32:A:LYS:H    | 2        | 1.26          |
| (1,1109) | 1:7:A:MET:HG2   | 1:32:A:LYS:H    | 1        | 1.26          |
| (1,802)  | 1:53:A:MET:HE1  | 1:58:A:GLU:H    | 4        | 1.26          |
| (1,802)  | 1:53:A:MET:HE2  | 1:58:A:GLU:H    | 4        | 1.26          |
| (1,802)  | 1:53:A:MET:HE3  | 1:58:A:GLU:H    | 4        | 1.26          |
| (1,1178) | 1:52:A:LYS:HE3  | 1:54:A:SER:H    | 3        | 1.25          |
| (1,1109) | 1:7:A:MET:HG2   | 1:32:A:LYS:H    | 8        | 1.25          |
| (1,1108) | 1:49:A:GLU:HB3  | 1:54:A:SER:H    | 6        | 1.24          |
| (1,1048) | 1:4:A:LEU:HD11  | 1:7:A:MET:H     | 7        | 1.24          |
| (1,1048) | 1:4:A:LEU:HD12  | 1:7:A:MET:H     | 7        | 1.24          |
| (1,1048) | 1:4:A:LEU:HD13  | 1:7:A:MET:H     | 7        | 1.24          |
| (1,369)  | 1:76:A:VAL:HA   | 1:83:A:LEU:HA   | 9        | 1.24          |
| (1,119)  | 1:57:A:MET:HE1  | 1:92:A:LEU:HD11 | 9        | 1.24          |
| (1,119)  | 1:57:A:MET:HE1  | 1:92:A:LEU:HD12 | 9        | 1.24          |
| (1,119)  | 1:57:A:MET:HE1  | 1:92:A:LEU:HD13 | 9        | 1.24          |
| (1,119)  | 1:57:A:MET:HE2  | 1:92:A:LEU:HD11 | 9        | 1.24          |
| (1,119)  | 1:57:A:MET:HE2  | 1:92:A:LEU:HD12 | 9        | 1.24          |
| (1,119)  | 1:57:A:MET:HE2  | 1:92:A:LEU:HD13 | 9        | 1.24          |
| (1,119)  | 1:57:A:MET:HE3  | 1:92:A:LEU:HD11 | 9        | 1.24          |
| (1,119)  | 1:57:A:MET:HE3  | 1:92:A:LEU:HD12 | 9        | 1.24          |
| (1,119)  | 1:57:A:MET:HE3  | 1:92:A:LEU:HD13 | 9        | 1.24          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,118)  | 1:57:A:MET:HE1  | 1:92:A:LEU:HD11 | 9        | 1.24          |
| (1,118)  | 1:57:A:MET:HE1  | 1:92:A:LEU:HD12 | 9        | 1.24          |
| (1,118)  | 1:57:A:MET:HE1  | 1:92:A:LEU:HD13 | 9        | 1.24          |
| (1,118)  | 1:57:A:MET:HE2  | 1:92:A:LEU:HD11 | 9        | 1.24          |
| (1,118)  | 1:57:A:MET:HE2  | 1:92:A:LEU:HD12 | 9        | 1.24          |
| (1,118)  | 1:57:A:MET:HE2  | 1:92:A:LEU:HD13 | 9        | 1.24          |
| (1,118)  | 1:57:A:MET:HE3  | 1:92:A:LEU:HD11 | 9        | 1.24          |
| (1,118)  | 1:57:A:MET:HE3  | 1:92:A:LEU:HD12 | 9        | 1.24          |
| (1,118)  | 1:57:A:MET:HE3  | 1:92:A:LEU:HD13 | 9        | 1.24          |
| (1,1116) | 1:73:A:LEU:H    | 1:74:A:GLN:HG2  | 6        | 1.23          |
| (1,1116) | 1:73:A:LEU:H    | 1:74:A:GLN:HG2  | 9        | 1.23          |
| (1,1111) | 1:7:A:MET:HB3   | 1:32:A:LYS:H    | 6        | 1.23          |
| (1,614)  | 1:67:A:VAL:H    | 1:96:A:GLY:H    | 9        | 1.23          |
| (1,119)  | 1:57:A:MET:HE1  | 1:92:A:LEU:HD11 | 2        | 1.23          |
| (1,119)  | 1:57:A:MET:HE1  | 1:92:A:LEU:HD12 | 2        | 1.23          |
| (1,119)  | 1:57:A:MET:HE1  | 1:92:A:LEU:HD13 | 2        | 1.23          |
| (1,119)  | 1:57:A:MET:HE2  | 1:92:A:LEU:HD11 | 2        | 1.23          |
| (1,119)  | 1:57:A:MET:HE2  | 1:92:A:LEU:HD12 | 2        | 1.23          |
| (1,119)  | 1:57:A:MET:HE2  | 1:92:A:LEU:HD13 | 2        | 1.23          |
| (1,119)  | 1:57:A:MET:HE3  | 1:92:A:LEU:HD11 | 2        | 1.23          |
| (1,119)  | 1:57:A:MET:HE3  | 1:92:A:LEU:HD12 | 2        | 1.23          |
| (1,119)  | 1:57:A:MET:HE3  | 1:92:A:LEU:HD13 | 2        | 1.23          |
| (1,118)  | 1:57:A:MET:HE1  | 1:92:A:LEU:HD11 | 2        | 1.23          |
| (1,118)  | 1:57:A:MET:HE1  | 1:92:A:LEU:HD12 | 2        | 1.23          |
| (1,118)  | 1:57:A:MET:HE1  | 1:92:A:LEU:HD13 | 2        | 1.23          |
| (1,118)  | 1:57:A:MET:HE2  | 1:92:A:LEU:HD11 | 2        | 1.23          |
| (1,118)  | 1:57:A:MET:HE2  | 1:92:A:LEU:HD12 | 2        | 1.23          |
| (1,118)  | 1:57:A:MET:HE2  | 1:92:A:LEU:HD13 | 2        | 1.23          |
| (1,118)  | 1:57:A:MET:HE3  | 1:92:A:LEU:HD11 | 2        | 1.23          |
| (1,118)  | 1:57:A:MET:HE3  | 1:92:A:LEU:HD12 | 2        | 1.23          |
| (1,118)  | 1:57:A:MET:HE3  | 1:92:A:LEU:HD13 | 2        | 1.23          |
| (1,773)  | 1:15:A:LEU:HA   | 1:45:A:SER:H    | 2        | 1.22          |
| (1,155)  | 1:68:A:VAL:H    | 1:92:A:LEU:HD21 | 10       | 1.22          |
| (1,155)  | 1:68:A:VAL:H    | 1:92:A:LEU:HD22 | 10       | 1.22          |
| (1,155)  | 1:68:A:VAL:H    | 1:92:A:LEU:HD23 | 10       | 1.22          |
| (1,1543) | 1:72:A:PHE:HB2  | 1:87:A:LEU:HB2  | 1        | 1.21          |
| (1,1543) | 1:72:A:PHE:HB2  | 1:87:A:LEU:HB3  | 1        | 1.21          |
| (1,1259) | 1:38:A:ASN:HD22 | 1:96:A:GLY:H    | 5        | 1.21          |
| (1,1048) | 1:4:A:LEU:HD11  | 1:7:A:MET:H     | 3        | 1.21          |
| (1,1048) | 1:4:A:LEU:HD12  | 1:7:A:MET:H     | 3        | 1.21          |
| (1,1048) | 1:4:A:LEU:HD13  | 1:7:A:MET:H     | 3        | 1.21          |
| (1,408)  | 1:72:A:PPHE:HA  | 1:87:A:LEU:HA   | 6        | 1.21          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1543) | 1:72:A:PHE:HB2  | 1:87:A:LEU:HB2  | 5        | 1.2           |
| (1,1543) | 1:72:A:PHE:HB2  | 1:87:A:LEU:HB3  | 5        | 1.2           |
| (1,1111) | 1:7:A:MET:HB3   | 1:32:A:LYS:H    | 4        | 1.2           |
| (1,1108) | 1:49:A:GLU:HB3  | 1:54:A:SER:H    | 4        | 1.2           |
| (1,773)  | 1:15:A:LEU:HA   | 1:45:A:SER:H    | 1        | 1.2           |
| (1,1300) | 1:28:A:LYS:HG3  | 1:30:A:GLY:H    | 2        | 1.19          |
| (1,1116) | 1:73:A:LEU:H    | 1:74:A:GLN:HG2  | 5        | 1.18          |
| (1,1108) | 1:49:A:GLU:HB3  | 1:54:A:SER:H    | 3        | 1.18          |
| (1,765)  | 1:38:A:ASN:HD22 | 1:98:A:GLU:H    | 8        | 1.18          |
| (1,82)   | 1:28:A:LYS:HG3  | 1:29:A:LEU:HG   | 5        | 1.18          |
| (1,1259) | 1:38:A:ASN:HD22 | 1:96:A:GLY:H    | 8        | 1.16          |
| (1,82)   | 1:28:A:LYS:HG3  | 1:29:A:LEU:HG   | 3        | 1.16          |
| (1,82)   | 1:28:A:LYS:HG3  | 1:29:A:LEU:HG   | 4        | 1.16          |
| (1,1607) | 1:91:A:SER:HB2  | 1:92:A:LEU:HD11 | 10       | 1.15          |
| (1,1607) | 1:91:A:SER:HB2  | 1:92:A:LEU:HD12 | 10       | 1.15          |
| (1,1607) | 1:91:A:SER:HB2  | 1:92:A:LEU:HD13 | 10       | 1.15          |
| (1,1607) | 1:91:A:SER:HB3  | 1:92:A:LEU:HD11 | 10       | 1.15          |
| (1,1607) | 1:91:A:SER:HB3  | 1:92:A:LEU:HD12 | 10       | 1.15          |
| (1,1607) | 1:91:A:SER:HB3  | 1:92:A:LEU:HD13 | 10       | 1.15          |
| (1,769)  | 1:15:A:LEU:HA   | 1:70:A:GLU:H    | 9        | 1.15          |
| (1,82)   | 1:28:A:LYS:HG3  | 1:29:A:LEU:HG   | 6        | 1.15          |
| (1,614)  | 1:67:A:VAL:H    | 1:96:A:GLY:H    | 2        | 1.14          |
| (1,1264) | 1:94:A:SER:HA   | 1:96:A:GLY:H    | 5        | 1.13          |
| (1,1069) | 1:5:A:SER:H     | 1:32:A:LYS:H    | 8        | 1.13          |
| (1,227)  | 1:4:A:LEU:HB3   | 1:30:A:GLY:HA2  | 1        | 1.13          |
| (1,1300) | 1:28:A:LYS:HG3  | 1:30:A:GLY:H    | 5        | 1.12          |
| (1,1108) | 1:49:A:GLU:HB3  | 1:54:A:SER:H    | 7        | 1.12          |
| (1,614)  | 1:67:A:VAL:H    | 1:96:A:GLY:H    | 3        | 1.12          |
| (1,408)  | 1:72:A:PHE:HA   | 1:87:A:LEU:HA   | 2        | 1.12          |
| (1,119)  | 1:57:A:MET:HE1  | 1:92:A:LEU:HD11 | 7        | 1.12          |
| (1,119)  | 1:57:A:MET:HE1  | 1:92:A:LEU:HD12 | 7        | 1.12          |
| (1,119)  | 1:57:A:MET:HE1  | 1:92:A:LEU:HD13 | 7        | 1.12          |
| (1,119)  | 1:57:A:MET:HE2  | 1:92:A:LEU:HD11 | 7        | 1.12          |
| (1,119)  | 1:57:A:MET:HE2  | 1:92:A:LEU:HD12 | 7        | 1.12          |
| (1,119)  | 1:57:A:MET:HE2  | 1:92:A:LEU:HD13 | 7        | 1.12          |
| (1,119)  | 1:57:A:MET:HE3  | 1:92:A:LEU:HD11 | 7        | 1.12          |
| (1,119)  | 1:57:A:MET:HE3  | 1:92:A:LEU:HD12 | 7        | 1.12          |
| (1,119)  | 1:57:A:MET:HE3  | 1:92:A:LEU:HD13 | 7        | 1.12          |
| (1,118)  | 1:57:A:MET:HE1  | 1:92:A:LEU:HD11 | 7        | 1.12          |
| (1,118)  | 1:57:A:MET:HE1  | 1:92:A:LEU:HD12 | 7        | 1.12          |
| (1,118)  | 1:57:A:MET:HE1  | 1:92:A:LEU:HD13 | 7        | 1.12          |
| (1,118)  | 1:57:A:MET:HE2  | 1:92:A:LEU:HD11 | 7        | 1.12          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,118)  | 1:57:A:MET:HE2  | 1:92:A:LEU:HD12 | 7        | 1.12          |
| (1,118)  | 1:57:A:MET:HE2  | 1:92:A:LEU:HD13 | 7        | 1.12          |
| (1,118)  | 1:57:A:MET:HE3  | 1:92:A:LEU:HD11 | 7        | 1.12          |
| (1,118)  | 1:57:A:MET:HE3  | 1:92:A:LEU:HD12 | 7        | 1.12          |
| (1,118)  | 1:57:A:MET:HE3  | 1:92:A:LEU:HD13 | 7        | 1.12          |
| (1,1259) | 1:38:A:ASN:HD22 | 1:96:A:GLY:H    | 9        | 1.11          |
| (1,1259) | 1:38:A:ASN:HD22 | 1:96:A:GLY:H    | 10       | 1.11          |
| (1,1069) | 1:5:A:SER:H     | 1:32:A:LYS:H    | 5        | 1.11          |
| (1,619)  | 1:38:A:ASN:HD21 | 1:97:A:ALA:H    | 7        | 1.11          |
| (1,480)  | 1:49:A:GLU:HB2  | 1:57:A:MET:HG3  | 4        | 1.11          |
| (1,476)  | 1:69:A:CYS:HB3  | 1:71:A:ASP:HA   | 8        | 1.11          |
| (1,1060) | 1:6:A:ASN:H     | 1:32:A:LYS:H    | 8        | 1.1           |
| (1,480)  | 1:49:A:GLU:HB2  | 1:57:A:MET:HG3  | 9        | 1.1           |
| (1,476)  | 1:69:A:CYS:HB3  | 1:71:A:ASP:HA   | 9        | 1.1           |
| (1,1223) | 1:5:A:SER:H     | 1:7:A:MET:HE1   | 5        | 1.09          |
| (1,1223) | 1:5:A:SER:H     | 1:7:A:MET:HE2   | 5        | 1.09          |
| (1,1223) | 1:5:A:SER:H     | 1:7:A:MET:HE3   | 5        | 1.09          |
| (1,1178) | 1:52:A:LYS:HE3  | 1:54:A:SER:H    | 4        | 1.09          |
| (1,1125) | 1:83:A:LEU:HG   | 1:84:A:GLN:H    | 9        | 1.09          |
| (1,582)  | 1:10:A:LEU:H    | 1:42:A:LEU:HD21 | 1        | 1.09          |
| (1,582)  | 1:10:A:LEU:H    | 1:42:A:LEU:HD22 | 1        | 1.09          |
| (1,582)  | 1:10:A:LEU:H    | 1:42:A:LEU:HD23 | 1        | 1.09          |
| (1,480)  | 1:49:A:GLU:HB2  | 1:57:A:MET:HG3  | 8        | 1.08          |
| (1,476)  | 1:69:A:CYS:HB3  | 1:71:A:ASP:HA   | 3        | 1.08          |
| (1,408)  | 1:72:A:PHE:HA   | 1:87:A:LEU:HA   | 9        | 1.08          |
| (1,157)  | 1:68:A:VAL:H    | 1:92:A:LEU:HD21 | 6        | 1.08          |
| (1,157)  | 1:68:A:VAL:H    | 1:92:A:LEU:HD22 | 6        | 1.08          |
| (1,157)  | 1:68:A:VAL:H    | 1:92:A:LEU:HD23 | 6        | 1.08          |
| (1,156)  | 1:68:A:VAL:H    | 1:92:A:LEU:HD21 | 6        | 1.08          |
| (1,156)  | 1:68:A:VAL:H    | 1:92:A:LEU:HD22 | 6        | 1.08          |
| (1,156)  | 1:68:A:VAL:H    | 1:92:A:LEU:HD23 | 6        | 1.08          |
| (1,802)  | 1:53:A:MET:HE1  | 1:58:A:GLU:H    | 7        | 1.07          |
| (1,802)  | 1:53:A:MET:HE2  | 1:58:A:GLU:H    | 7        | 1.07          |
| (1,802)  | 1:53:A:MET:HE3  | 1:58:A:GLU:H    | 7        | 1.07          |
| (1,634)  | 1:69:A:CYS:HB2  | 1:92:A:LEU:H    | 10       | 1.07          |
| (1,1607) | 1:91:A:SER:HB2  | 1:92:A:LEU:HD11 | 7        | 1.06          |
| (1,1607) | 1:91:A:SER:HB2  | 1:92:A:LEU:HD12 | 7        | 1.06          |
| (1,1607) | 1:91:A:SER:HB2  | 1:92:A:LEU:HD13 | 7        | 1.06          |
| (1,1607) | 1:91:A:SER:HB3  | 1:92:A:LEU:HD11 | 7        | 1.06          |
| (1,1607) | 1:91:A:SER:HB3  | 1:92:A:LEU:HD12 | 7        | 1.06          |
| (1,1607) | 1:91:A:SER:HB3  | 1:92:A:LEU:HD13 | 7        | 1.06          |
| (1,1093) | 1:90:A:HIS:HB3  | 1:91:A:SER:H    | 10       | 1.06          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,614)  | 1:67:A:VAL:H    | 1:96:A:GLY:H    | 7        | 1.06          |
| (1,480)  | 1:49:A:GLU:HB2  | 1:57:A:MET:HG3  | 2        | 1.06          |
| (1,1607) | 1:91:A:SER:HB2  | 1:92:A:LEU:HD11 | 4        | 1.05          |
| (1,1607) | 1:91:A:SER:HB2  | 1:92:A:LEU:HD12 | 4        | 1.05          |
| (1,1607) | 1:91:A:SER:HB2  | 1:92:A:LEU:HD13 | 4        | 1.05          |
| (1,1607) | 1:91:A:SER:HB3  | 1:92:A:LEU:HD11 | 4        | 1.05          |
| (1,1607) | 1:91:A:SER:HB3  | 1:92:A:LEU:HD12 | 4        | 1.05          |
| (1,1607) | 1:91:A:SER:HB3  | 1:92:A:LEU:HD13 | 4        | 1.05          |
| (1,1543) | 1:72:A:PHE:HB2  | 1:87:A:LEU:HB2  | 4        | 1.05          |
| (1,1543) | 1:72:A:PHE:HB2  | 1:87:A:LEU:HB3  | 4        | 1.05          |
| (1,1178) | 1:52:A:LYS:HE3  | 1:54:A:SER:H    | 5        | 1.05          |
| (1,865)  | 1:18:A:ASN:HD22 | 1:20:A:ASP:H    | 10       | 1.05          |
| (1,765)  | 1:38:A:ASN:HD22 | 1:98:A:GLU:H    | 2        | 1.05          |
| (1,614)  | 1:67:A:VAL:H    | 1:96:A:GLY:H    | 1        | 1.05          |
| (1,480)  | 1:49:A:GLU:HB2  | 1:57:A:MET:HG3  | 7        | 1.05          |
| (1,1607) | 1:91:A:SER:HB2  | 1:92:A:LEU:HD11 | 2        | 1.04          |
| (1,1607) | 1:91:A:SER:HB2  | 1:92:A:LEU:HD12 | 2        | 1.04          |
| (1,1607) | 1:91:A:SER:HB2  | 1:92:A:LEU:HD13 | 2        | 1.04          |
| (1,1607) | 1:91:A:SER:HB3  | 1:92:A:LEU:HD11 | 2        | 1.04          |
| (1,1607) | 1:91:A:SER:HB3  | 1:92:A:LEU:HD12 | 2        | 1.04          |
| (1,1607) | 1:91:A:SER:HB3  | 1:92:A:LEU:HD13 | 2        | 1.04          |
| (1,1300) | 1:28:A:LYS:HG3  | 1:30:A:GLY:H    | 7        | 1.04          |
| (1,1178) | 1:52:A:LYS:HE3  | 1:54:A:SER:H    | 7        | 1.04          |
| (1,1177) | 1:52:A:LYS:HE2  | 1:54:A:SER:H    | 8        | 1.04          |
| (1,1069) | 1:5:A:SER:H     | 1:32:A:LYS:H    | 1        | 1.04          |
| (1,802)  | 1:53:A:MET:HE1  | 1:58:A:GLU:H    | 5        | 1.04          |
| (1,802)  | 1:53:A:MET:HE2  | 1:58:A:GLU:H    | 5        | 1.04          |
| (1,802)  | 1:53:A:MET:HE3  | 1:58:A:GLU:H    | 5        | 1.04          |
| (1,614)  | 1:67:A:VAL:H    | 1:96:A:GLY:H    | 10       | 1.04          |
| (1,476)  | 1:69:A:CYS:HB3  | 1:71:A:ASP:HA   | 1        | 1.04          |
| (1,1607) | 1:91:A:SER:HB2  | 1:92:A:LEU:HD11 | 1        | 1.03          |
| (1,1607) | 1:91:A:SER:HB2  | 1:92:A:LEU:HD12 | 1        | 1.03          |
| (1,1607) | 1:91:A:SER:HB2  | 1:92:A:LEU:HD13 | 1        | 1.03          |
| (1,1607) | 1:91:A:SER:HB3  | 1:92:A:LEU:HD11 | 1        | 1.03          |
| (1,1607) | 1:91:A:SER:HB3  | 1:92:A:LEU:HD12 | 1        | 1.03          |
| (1,1607) | 1:91:A:SER:HB3  | 1:92:A:LEU:HD13 | 1        | 1.03          |
| (1,802)  | 1:53:A:MET:HE1  | 1:58:A:GLU:H    | 3        | 1.03          |
| (1,802)  | 1:53:A:MET:HE2  | 1:58:A:GLU:H    | 3        | 1.03          |
| (1,802)  | 1:53:A:MET:HE3  | 1:58:A:GLU:H    | 3        | 1.03          |
| (1,476)  | 1:69:A:CYS:HB3  | 1:71:A:ASP:HA   | 10       | 1.03          |
| (1,1177) | 1:52:A:LYS:HE2  | 1:54:A:SER:H    | 10       | 1.02          |
| (1,582)  | 1:10:A:LEU:H    | 1:42:A:LEU:HD21 | 8        | 1.01          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,582)  | 1:10:A:LEU:H   | 1:42:A:LEU:HD22 | 8        | 1.01          |
| (1,582)  | 1:10:A:LEU:H   | 1:42:A:LEU:HD23 | 8        | 1.01          |
| (1,408)  | 1:72:A:PHE:HA  | 1:87:A:LEU:HA   | 8        | 1.01          |
| (1,1623) | 1:99:A:VAL:H   | 1:100:A:LYS:HD2 | 7        | 1.0           |
| (1,1623) | 1:99:A:VAL:H   | 1:100:A:LYS:HD3 | 7        | 1.0           |
| (1,1108) | 1:49:A:GLU:HB3 | 1:54:A:SER:H    | 1        | 1.0           |
| (1,802)  | 1:53:A:MET:HE1 | 1:58:A:GLU:H    | 8        | 1.0           |
| (1,802)  | 1:53:A:MET:HE2 | 1:58:A:GLU:H    | 8        | 1.0           |
| (1,802)  | 1:53:A:MET:HE3 | 1:58:A:GLU:H    | 8        | 1.0           |
| (1,155)  | 1:68:A:VAL:H   | 1:92:A:LEU:HD21 | 7        | 1.0           |
| (1,155)  | 1:68:A:VAL:H   | 1:92:A:LEU:HD22 | 7        | 1.0           |
| (1,155)  | 1:68:A:VAL:H   | 1:92:A:LEU:HD23 | 7        | 1.0           |
| (1,119)  | 1:57:A:MET:HE1 | 1:92:A:LEU:HD11 | 3        | 1.0           |
| (1,119)  | 1:57:A:MET:HE1 | 1:92:A:LEU:HD12 | 3        | 1.0           |
| (1,119)  | 1:57:A:MET:HE1 | 1:92:A:LEU:HD13 | 3        | 1.0           |
| (1,119)  | 1:57:A:MET:HE2 | 1:92:A:LEU:HD11 | 3        | 1.0           |
| (1,119)  | 1:57:A:MET:HE2 | 1:92:A:LEU:HD12 | 3        | 1.0           |
| (1,119)  | 1:57:A:MET:HE2 | 1:92:A:LEU:HD13 | 3        | 1.0           |
| (1,119)  | 1:57:A:MET:HE3 | 1:92:A:LEU:HD11 | 3        | 1.0           |
| (1,119)  | 1:57:A:MET:HE3 | 1:92:A:LEU:HD12 | 3        | 1.0           |
| (1,119)  | 1:57:A:MET:HE3 | 1:92:A:LEU:HD13 | 3        | 1.0           |
| (1,118)  | 1:57:A:MET:HE1 | 1:92:A:LEU:HD11 | 3        | 1.0           |
| (1,118)  | 1:57:A:MET:HE1 | 1:92:A:LEU:HD12 | 3        | 1.0           |
| (1,118)  | 1:57:A:MET:HE1 | 1:92:A:LEU:HD13 | 3        | 1.0           |
| (1,118)  | 1:57:A:MET:HE2 | 1:92:A:LEU:HD11 | 3        | 1.0           |
| (1,118)  | 1:57:A:MET:HE2 | 1:92:A:LEU:HD12 | 3        | 1.0           |
| (1,118)  | 1:57:A:MET:HE2 | 1:92:A:LEU:HD13 | 3        | 1.0           |
| (1,118)  | 1:57:A:MET:HE3 | 1:92:A:LEU:HD11 | 3        | 1.0           |
| (1,118)  | 1:57:A:MET:HE3 | 1:92:A:LEU:HD12 | 3        | 1.0           |
| (1,118)  | 1:57:A:MET:HE3 | 1:92:A:LEU:HD13 | 3        | 1.0           |
| (1,1607) | 1:91:A:SER:HB2 | 1:92:A:LEU:HD11 | 8        | 0.99          |
| (1,1607) | 1:91:A:SER:HB2 | 1:92:A:LEU:HD12 | 8        | 0.99          |
| (1,1607) | 1:91:A:SER:HB2 | 1:92:A:LEU:HD13 | 8        | 0.99          |
| (1,1607) | 1:91:A:SER:HB3 | 1:92:A:LEU:HD11 | 8        | 0.99          |
| (1,1607) | 1:91:A:SER:HB3 | 1:92:A:LEU:HD12 | 8        | 0.99          |
| (1,1607) | 1:91:A:SER:HB3 | 1:92:A:LEU:HD13 | 8        | 0.99          |
| (1,157)  | 1:68:A:VAL:H   | 1:92:A:LEU:HD21 | 5        | 0.99          |
| (1,157)  | 1:68:A:VAL:H   | 1:92:A:LEU:HD22 | 5        | 0.99          |
| (1,157)  | 1:68:A:VAL:H   | 1:92:A:LEU:HD23 | 5        | 0.99          |
| (1,156)  | 1:68:A:VAL:H   | 1:92:A:LEU:HD21 | 5        | 0.99          |
| (1,156)  | 1:68:A:VAL:H   | 1:92:A:LEU:HD22 | 5        | 0.99          |
| (1,156)  | 1:68:A:VAL:H   | 1:92:A:LEU:HD23 | 5        | 0.99          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1048) | 1:4:A:LEU:HD11  | 1:7:A:MET:H     | 9        | 0.98          |
| (1,1048) | 1:4:A:LEU:HD12  | 1:7:A:MET:H     | 9        | 0.98          |
| (1,1048) | 1:4:A:LEU:HD13  | 1:7:A:MET:H     | 9        | 0.98          |
| (1,119)  | 1:57:A:MET:HE1  | 1:92:A:LEU:HD11 | 5        | 0.98          |
| (1,119)  | 1:57:A:MET:HE1  | 1:92:A:LEU:HD12 | 5        | 0.98          |
| (1,119)  | 1:57:A:MET:HE1  | 1:92:A:LEU:HD13 | 5        | 0.98          |
| (1,119)  | 1:57:A:MET:HE2  | 1:92:A:LEU:HD11 | 5        | 0.98          |
| (1,119)  | 1:57:A:MET:HE2  | 1:92:A:LEU:HD12 | 5        | 0.98          |
| (1,119)  | 1:57:A:MET:HE2  | 1:92:A:LEU:HD13 | 5        | 0.98          |
| (1,119)  | 1:57:A:MET:HE3  | 1:92:A:LEU:HD11 | 5        | 0.98          |
| (1,119)  | 1:57:A:MET:HE3  | 1:92:A:LEU:HD12 | 5        | 0.98          |
| (1,119)  | 1:57:A:MET:HE3  | 1:92:A:LEU:HD13 | 5        | 0.98          |
| (1,118)  | 1:57:A:MET:HE1  | 1:92:A:LEU:HD11 | 5        | 0.98          |
| (1,118)  | 1:57:A:MET:HE1  | 1:92:A:LEU:HD12 | 5        | 0.98          |
| (1,118)  | 1:57:A:MET:HE1  | 1:92:A:LEU:HD13 | 5        | 0.98          |
| (1,118)  | 1:57:A:MET:HE2  | 1:92:A:LEU:HD11 | 5        | 0.98          |
| (1,118)  | 1:57:A:MET:HE2  | 1:92:A:LEU:HD12 | 5        | 0.98          |
| (1,118)  | 1:57:A:MET:HE2  | 1:92:A:LEU:HD13 | 5        | 0.98          |
| (1,118)  | 1:57:A:MET:HE3  | 1:92:A:LEU:HD11 | 5        | 0.98          |
| (1,118)  | 1:57:A:MET:HE3  | 1:92:A:LEU:HD12 | 5        | 0.98          |
| (1,118)  | 1:57:A:MET:HE3  | 1:92:A:LEU:HD13 | 5        | 0.98          |
| (1,1125) | 1:83:A:LEU:HG   | 1:84:A:GLN:H    | 1        | 0.97          |
| (1,865)  | 1:18:A:ASN:HD22 | 1:20:A:ASP:H    | 6        | 0.97          |
| (1,865)  | 1:18:A:ASN:HD22 | 1:20:A:ASP:H    | 7        | 0.97          |
| (1,480)  | 1:49:A:GLU:HB2  | 1:57:A:MET:HG3  | 3        | 0.97          |
| (1,227)  | 1:4:A:LEU:HB3   | 1:30:A:GLY:HA2  | 4        | 0.97          |
| (1,1223) | 1:5:A:SER:H     | 1:7:A:MET:HE1   | 2        | 0.96          |
| (1,1223) | 1:5:A:SER:H     | 1:7:A:MET:HE2   | 2        | 0.96          |
| (1,1223) | 1:5:A:SER:H     | 1:7:A:MET:HE3   | 2        | 0.96          |
| (1,1223) | 1:5:A:SER:H     | 1:7:A:MET:HE1   | 6        | 0.96          |
| (1,1223) | 1:5:A:SER:H     | 1:7:A:MET:HE2   | 6        | 0.96          |
| (1,1223) | 1:5:A:SER:H     | 1:7:A:MET:HE3   | 6        | 0.96          |
| (1,1093) | 1:90:A:HIS:HB3  | 1:91:A:SER:H    | 6        | 0.96          |
| (1,408)  | 1:72:A:PHE:HA   | 1:87:A:LEU:HA   | 3        | 0.96          |
| (1,82)   | 1:28:A:LYS:HG3  | 1:29:A:LEU:HG   | 1        | 0.96          |
| (1,1125) | 1:83:A:LEU:HG   | 1:84:A:GLN:H    | 4        | 0.95          |
| (1,1108) | 1:49:A:GLU:HB3  | 1:54:A:SER:H    | 5        | 0.95          |
| (1,1060) | 1:6:A:ASN:H     | 1:32:A:LYS:H    | 5        | 0.95          |
| (1,408)  | 1:72:A:PHE:HA   | 1:87:A:LEU:HA   | 7        | 0.95          |
| (1,82)   | 1:28:A:LYS:HG3  | 1:29:A:LEU:HG   | 2        | 0.95          |
| (1,1093) | 1:90:A:HIS:HB3  | 1:91:A:SER:H    | 9        | 0.94          |
| (1,756)  | 1:34:A:THR:H    | 1:40:A:ALA:H    | 6        | 0.94          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,665)  | 1:65:A:VAL:HG11 | 1:97:A:ALA:H    | 7        | 0.93          |
| (1,665)  | 1:65:A:VAL:HG12 | 1:97:A:ALA:H    | 7        | 0.93          |
| (1,665)  | 1:65:A:VAL:HG13 | 1:97:A:ALA:H    | 7        | 0.93          |
| (1,347)  | 1:25:A:MET:HE1  | 1:29:A:LEU:HD21 | 7        | 0.93          |
| (1,347)  | 1:25:A:MET:HE1  | 1:29:A:LEU:HD22 | 7        | 0.93          |
| (1,347)  | 1:25:A:MET:HE1  | 1:29:A:LEU:HD23 | 7        | 0.93          |
| (1,347)  | 1:25:A:MET:HE2  | 1:29:A:LEU:HD21 | 7        | 0.93          |
| (1,347)  | 1:25:A:MET:HE2  | 1:29:A:LEU:HD22 | 7        | 0.93          |
| (1,347)  | 1:25:A:MET:HE2  | 1:29:A:LEU:HD23 | 7        | 0.93          |
| (1,347)  | 1:25:A:MET:HE3  | 1:29:A:LEU:HD21 | 7        | 0.93          |
| (1,347)  | 1:25:A:MET:HE3  | 1:29:A:LEU:HD22 | 7        | 0.93          |
| (1,347)  | 1:25:A:MET:HE3  | 1:29:A:LEU:HD23 | 7        | 0.93          |
| (1,227)  | 1:4:A:LEU:HB3   | 1:30:A:GLY:HA2  | 8        | 0.93          |
| (1,1069) | 1:5:A:SER:H     | 1:32:A:LYS:H    | 3        | 0.92          |
| (1,865)  | 1:18:A:ASN:HD22 | 1:20:A:ASP:H    | 3        | 0.92          |
| (1,739)  | 1:16:A:SER:H    | 1:45:A:SER:H    | 4        | 0.92          |
| (1,227)  | 1:4:A:LEU:HB3   | 1:30:A:GLY:HA2  | 6        | 0.92          |
| (1,86)   | 1:9:A:ILE:HD11  | 1:42:A:LEU:HD21 | 8        | 0.92          |
| (1,86)   | 1:9:A:ILE:HD11  | 1:42:A:LEU:HD22 | 8        | 0.92          |
| (1,86)   | 1:9:A:ILE:HD11  | 1:42:A:LEU:HD23 | 8        | 0.92          |
| (1,86)   | 1:9:A:ILE:HD12  | 1:42:A:LEU:HD21 | 8        | 0.92          |
| (1,86)   | 1:9:A:ILE:HD12  | 1:42:A:LEU:HD22 | 8        | 0.92          |
| (1,86)   | 1:9:A:ILE:HD12  | 1:42:A:LEU:HD23 | 8        | 0.92          |
| (1,86)   | 1:9:A:ILE:HD13  | 1:42:A:LEU:HD21 | 8        | 0.92          |
| (1,86)   | 1:9:A:ILE:HD13  | 1:42:A:LEU:HD22 | 8        | 0.92          |
| (1,86)   | 1:9:A:ILE:HD13  | 1:42:A:LEU:HD23 | 8        | 0.92          |
| (1,85)   | 1:9:A:ILE:HD11  | 1:42:A:LEU:HD21 | 8        | 0.92          |
| (1,85)   | 1:9:A:ILE:HD11  | 1:42:A:LEU:HD22 | 8        | 0.92          |
| (1,85)   | 1:9:A:ILE:HD11  | 1:42:A:LEU:HD23 | 8        | 0.92          |
| (1,85)   | 1:9:A:ILE:HD12  | 1:42:A:LEU:HD21 | 8        | 0.92          |
| (1,85)   | 1:9:A:ILE:HD12  | 1:42:A:LEU:HD22 | 8        | 0.92          |
| (1,85)   | 1:9:A:ILE:HD12  | 1:42:A:LEU:HD23 | 8        | 0.92          |
| (1,85)   | 1:9:A:ILE:HD13  | 1:42:A:LEU:HD21 | 8        | 0.92          |
| (1,85)   | 1:9:A:ILE:HD13  | 1:42:A:LEU:HD22 | 8        | 0.92          |
| (1,85)   | 1:9:A:ILE:HD13  | 1:42:A:LEU:HD23 | 8        | 0.92          |
| (1,1125) | 1:83:A:LEU:HG   | 1:84:A:GLN:H    | 3        | 0.91          |
| (1,1069) | 1:5:A:SER:H     | 1:32:A:LYS:H    | 7        | 0.91          |
| (1,865)  | 1:18:A:ASN:HD22 | 1:20:A:ASP:H    | 2        | 0.91          |
| (1,773)  | 1:15:A:LEU:HA   | 1:45:A:SER:H    | 8        | 0.91          |
| (1,1507) | 1:58:A:GLU:HG2  | 1:59:A:GLU:H    | 4        | 0.9           |
| (1,1507) | 1:58:A:GLU:HG3  | 1:59:A:GLU:H    | 4        | 0.9           |
| (1,1259) | 1:38:A:ASN:HD22 | 1:96:A:GLY:H    | 4        | 0.89          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,1060) | 1:6:A:ASN:H    | 1:32:A:LYS:H    | 4        | 0.89          |
| (1,769)  | 1:15:A:LEU:HA  | 1:70:A:GLU:H    | 2        | 0.89          |
| (1,756)  | 1:34:A:THR:H   | 1:40:A:ALA:H    | 2        | 0.89          |
| (1,157)  | 1:68:A:VAL:H   | 1:92:A:LEU:HD21 | 9        | 0.89          |
| (1,157)  | 1:68:A:VAL:H   | 1:92:A:LEU:HD22 | 9        | 0.89          |
| (1,157)  | 1:68:A:VAL:H   | 1:92:A:LEU:HD23 | 9        | 0.89          |
| (1,156)  | 1:68:A:VAL:H   | 1:92:A:LEU:HD21 | 9        | 0.89          |
| (1,156)  | 1:68:A:VAL:H   | 1:92:A:LEU:HD22 | 9        | 0.89          |
| (1,156)  | 1:68:A:VAL:H   | 1:92:A:LEU:HD23 | 9        | 0.89          |
| (1,1507) | 1:58:A:GLU:HG2 | 1:59:A:GLU:H    | 2        | 0.88          |
| (1,1507) | 1:58:A:GLU:HG3 | 1:59:A:GLU:H    | 2        | 0.88          |
| (1,802)  | 1:53:A:MET:HE1 | 1:58:A:GLU:H    | 10       | 0.88          |
| (1,802)  | 1:53:A:MET:HE2 | 1:58:A:GLU:H    | 10       | 0.88          |
| (1,802)  | 1:53:A:MET:HE3 | 1:58:A:GLU:H    | 10       | 0.88          |
| (1,227)  | 1:4:A:LEU:HB3  | 1:30:A:GLY:HA2  | 5        | 0.88          |
| (1,1109) | 1:7:A:MET:HG2  | 1:32:A:LYS:H    | 4        | 0.87          |
| (1,1109) | 1:7:A:MET:HG2  | 1:32:A:LYS:H    | 6        | 0.87          |
| (1,802)  | 1:53:A:MET:HE1 | 1:58:A:GLU:H    | 6        | 0.87          |
| (1,802)  | 1:53:A:MET:HE2 | 1:58:A:GLU:H    | 6        | 0.87          |
| (1,802)  | 1:53:A:MET:HE3 | 1:58:A:GLU:H    | 6        | 0.87          |
| (1,1125) | 1:83:A:LEU:HG  | 1:84:A:GLN:H    | 2        | 0.86          |
| (1,1069) | 1:5:A:SER:H    | 1:32:A:LYS:H    | 4        | 0.86          |
| (1,408)  | 1:72:A:PHE:HA  | 1:87:A:LEU:HA   | 1        | 0.86          |
| (1,1507) | 1:58:A:GLU:HG2 | 1:59:A:GLU:H    | 5        | 0.85          |
| (1,1507) | 1:58:A:GLU:HG3 | 1:59:A:GLU:H    | 5        | 0.85          |
| (1,1507) | 1:58:A:GLU:HG2 | 1:59:A:GLU:H    | 8        | 0.85          |
| (1,1507) | 1:58:A:GLU:HG3 | 1:59:A:GLU:H    | 8        | 0.85          |
| (1,802)  | 1:53:A:MET:HE1 | 1:58:A:GLU:H    | 1        | 0.85          |
| (1,802)  | 1:53:A:MET:HE2 | 1:58:A:GLU:H    | 1        | 0.85          |
| (1,802)  | 1:53:A:MET:HE3 | 1:58:A:GLU:H    | 1        | 0.85          |
| (1,480)  | 1:49:A:GLU:HB2 | 1:57:A:MET:HG3  | 6        | 0.85          |
| (1,108)  | 1:9:A:ILE:HA   | 1:10:A:LEU:HD11 | 2        | 0.85          |
| (1,108)  | 1:9:A:ILE:HA   | 1:10:A:LEU:HD12 | 2        | 0.85          |
| (1,108)  | 1:9:A:ILE:HA   | 1:10:A:LEU:HD13 | 2        | 0.85          |
| (1,108)  | 1:9:A:ILE:HA   | 1:10:A:LEU:HD11 | 7        | 0.85          |
| (1,108)  | 1:9:A:ILE:HA   | 1:10:A:LEU:HD12 | 7        | 0.85          |
| (1,108)  | 1:9:A:ILE:HA   | 1:10:A:LEU:HD13 | 7        | 0.85          |
| (1,1607) | 1:91:A:SER:HB2 | 1:92:A:LEU:HD11 | 3        | 0.84          |
| (1,1607) | 1:91:A:SER:HB2 | 1:92:A:LEU:HD12 | 3        | 0.84          |
| (1,1607) | 1:91:A:SER:HB2 | 1:92:A:LEU:HD13 | 3        | 0.84          |
| (1,1607) | 1:91:A:SER:HB3 | 1:92:A:LEU:HD11 | 3        | 0.84          |
| (1,1607) | 1:91:A:SER:HB3 | 1:92:A:LEU:HD12 | 3        | 0.84          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1607) | 1:91:A:SER:HB3  | 1:92:A:LEU:HD13 | 3        | 0.84          |
| (1,1540) | 1:70:A:GLU:HG2  | 1:71:A:ASP:HA   | 6        | 0.84          |
| (1,1540) | 1:70:A:GLU:HG3  | 1:71:A:ASP:HA   | 6        | 0.84          |
| (1,1507) | 1:58:A:GLU:HG2  | 1:59:A:GLU:H    | 3        | 0.84          |
| (1,1507) | 1:58:A:GLU:HG3  | 1:59:A:GLU:H    | 3        | 0.84          |
| (1,1093) | 1:90:A:HIS:HB3  | 1:91:A:SER:H    | 7        | 0.84          |
| (1,865)  | 1:18:A:ASN:HD22 | 1:20:A:ASP:H    | 1        | 0.84          |
| (1,769)  | 1:15:A:LEU:HA   | 1:70:A:GLU:H    | 10       | 0.84          |
| (1,756)  | 1:34:A:THR:H    | 1:40:A:ALA:H    | 8        | 0.84          |
| (1,634)  | 1:69:A:CYS:HB2  | 1:92:A:LEU:H    | 6        | 0.84          |
| (1,619)  | 1:38:A:ASN:HD21 | 1:97:A:ALA:H    | 1        | 0.84          |
| (1,1540) | 1:70:A:GLU:HG2  | 1:71:A:ASP:HA   | 4        | 0.83          |
| (1,1540) | 1:70:A:GLU:HG3  | 1:71:A:ASP:HA   | 4        | 0.83          |
| (1,1540) | 1:70:A:GLU:HG2  | 1:71:A:ASP:HA   | 8        | 0.83          |
| (1,1540) | 1:70:A:GLU:HG3  | 1:71:A:ASP:HA   | 8        | 0.83          |
| (1,1507) | 1:58:A:GLU:HG2  | 1:59:A:GLU:H    | 1        | 0.83          |
| (1,1507) | 1:58:A:GLU:HG3  | 1:59:A:GLU:H    | 1        | 0.83          |
| (1,634)  | 1:69:A:CYS:HB2  | 1:92:A:LEU:H    | 1        | 0.83          |
| (1,1507) | 1:58:A:GLU:HG2  | 1:59:A:GLU:H    | 10       | 0.82          |
| (1,1507) | 1:58:A:GLU:HG3  | 1:59:A:GLU:H    | 10       | 0.82          |
| (1,1396) | 1:19:A:LYS:HD2  | 1:21:A:GLU:H    | 8        | 0.82          |
| (1,1396) | 1:19:A:LYS:HD3  | 1:21:A:GLU:H    | 8        | 0.82          |
| (1,1177) | 1:52:A:LYS:HE2  | 1:54:A:SER:H    | 1        | 0.82          |
| (1,1134) | 1:91:A:SER:H    | 1:92:A:LEU:HB2  | 5        | 0.82          |
| (1,865)  | 1:18:A:ASN:HD22 | 1:20:A:ASP:H    | 5        | 0.82          |
| (1,802)  | 1:53:A:MET:HE1  | 1:58:A:GLU:H    | 2        | 0.82          |
| (1,802)  | 1:53:A:MET:HE2  | 1:58:A:GLU:H    | 2        | 0.82          |
| (1,802)  | 1:53:A:MET:HE3  | 1:58:A:GLU:H    | 2        | 0.82          |
| (1,480)  | 1:49:A:GLU:HB2  | 1:57:A:MET:HG3  | 1        | 0.82          |
| (1,224)  | 1:4:A:LEU:HB2   | 1:30:A:GLY:HA2  | 5        | 0.82          |
| (1,1109) | 1:7:A:MET:HG2   | 1:32:A:LYS:H    | 10       | 0.81          |
| (1,802)  | 1:53:A:MET:HE1  | 1:58:A:GLU:H    | 9        | 0.81          |
| (1,802)  | 1:53:A:MET:HE2  | 1:58:A:GLU:H    | 9        | 0.81          |
| (1,802)  | 1:53:A:MET:HE3  | 1:58:A:GLU:H    | 9        | 0.81          |
| (1,108)  | 1:9:A:ILE:HA    | 1:10:A:LEU:HD11 | 5        | 0.81          |
| (1,108)  | 1:9:A:ILE:HA    | 1:10:A:LEU:HD12 | 5        | 0.81          |
| (1,108)  | 1:9:A:ILE:HA    | 1:10:A:LEU:HD13 | 5        | 0.81          |
| (1,108)  | 1:9:A:ILE:HA    | 1:10:A:LEU:HD11 | 8        | 0.81          |
| (1,108)  | 1:9:A:ILE:HA    | 1:10:A:LEU:HD12 | 8        | 0.81          |
| (1,108)  | 1:9:A:ILE:HA    | 1:10:A:LEU:HD13 | 8        | 0.81          |
| (1,1550) | 1:74:A:GLN:HA   | 1:74:A:GLN:HE21 | 6        | 0.8           |
| (1,1550) | 1:74:A:GLN:HA   | 1:74:A:GLN:HE22 | 6        | 0.8           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,773)  | 1:15:A:LEU:HA   | 1:45:A:SER:H    | 4        | 0.8           |
| (1,765)  | 1:38:A:ASN:HD22 | 1:98:A:GLU:H    | 9        | 0.8           |
| (1,756)  | 1:34:A:THR:H    | 1:40:A:ALA:H    | 5        | 0.8           |
| (1,108)  | 1:9:A:ILE:HA    | 1:10:A:LEU:HD11 | 10       | 0.8           |
| (1,108)  | 1:9:A:ILE:HA    | 1:10:A:LEU:HD12 | 10       | 0.8           |
| (1,108)  | 1:9:A:ILE:HA    | 1:10:A:LEU:HD13 | 10       | 0.8           |
| (1,634)  | 1:69:A:CYS:HB2  | 1:92:A:LEU:H    | 8        | 0.79          |
| (1,600)  | 1:65:A:VAL:HG21 | 1:66:A:ARG:H    | 3        | 0.79          |
| (1,600)  | 1:65:A:VAL:HG22 | 1:66:A:ARG:H    | 3        | 0.79          |
| (1,600)  | 1:65:A:VAL:HG23 | 1:66:A:ARG:H    | 3        | 0.79          |
| (1,44)   | 1:63:A:ALA:HA   | 1:65:A:VAL:HG11 | 10       | 0.79          |
| (1,44)   | 1:63:A:ALA:HA   | 1:65:A:VAL:HG12 | 10       | 0.79          |
| (1,44)   | 1:63:A:ALA:HA   | 1:65:A:VAL:HG13 | 10       | 0.79          |
| (1,43)   | 1:63:A:ALA:HA   | 1:65:A:VAL:HG11 | 10       | 0.79          |
| (1,43)   | 1:63:A:ALA:HA   | 1:65:A:VAL:HG12 | 10       | 0.79          |
| (1,43)   | 1:63:A:ALA:HA   | 1:65:A:VAL:HG13 | 10       | 0.79          |
| (1,157)  | 1:68:A:VAL:H    | 1:92:A:LEU:HD21 | 4        | 0.78          |
| (1,157)  | 1:68:A:VAL:H    | 1:92:A:LEU:HD22 | 4        | 0.78          |
| (1,157)  | 1:68:A:VAL:H    | 1:92:A:LEU:HD23 | 4        | 0.78          |
| (1,156)  | 1:68:A:VAL:H    | 1:92:A:LEU:HD21 | 4        | 0.78          |
| (1,156)  | 1:68:A:VAL:H    | 1:92:A:LEU:HD22 | 4        | 0.78          |
| (1,156)  | 1:68:A:VAL:H    | 1:92:A:LEU:HD23 | 4        | 0.78          |
| (1,108)  | 1:9:A:ILE:HA    | 1:10:A:LEU:HD11 | 4        | 0.78          |
| (1,108)  | 1:9:A:ILE:HA    | 1:10:A:LEU:HD12 | 4        | 0.78          |
| (1,108)  | 1:9:A:ILE:HA    | 1:10:A:LEU:HD13 | 4        | 0.78          |
| (1,82)   | 1:28:A:LYS:HG3  | 1:29:A:LEU:HG   | 9        | 0.78          |
| (1,1550) | 1:74:A:GLN:HA   | 1:74:A:GLN:HE21 | 9        | 0.77          |
| (1,1550) | 1:74:A:GLN:HA   | 1:74:A:GLN:HE22 | 9        | 0.77          |
| (1,1060) | 1:6:A:ASN:H     | 1:32:A:LYS:H    | 2        | 0.77          |
| (1,1540) | 1:70:A:GLU:HG2  | 1:71:A:ASP:HA   | 10       | 0.76          |
| (1,1540) | 1:70:A:GLU:HG3  | 1:71:A:ASP:HA   | 10       | 0.76          |
| (1,408)  | 1:72:A:PHE:HA   | 1:87:A:LEU:HA   | 5        | 0.76          |
| (1,649)  | 1:9:A:ILE:H     | 1:33:A:LEU:HG   | 8        | 0.75          |
| (1,600)  | 1:65:A:VAL:HG21 | 1:66:A:ARG:H    | 6        | 0.75          |
| (1,600)  | 1:65:A:VAL:HG22 | 1:66:A:ARG:H    | 6        | 0.75          |
| (1,600)  | 1:65:A:VAL:HG23 | 1:66:A:ARG:H    | 6        | 0.75          |
| (1,108)  | 1:9:A:ILE:HA    | 1:10:A:LEU:HD11 | 3        | 0.75          |
| (1,108)  | 1:9:A:ILE:HA    | 1:10:A:LEU:HD12 | 3        | 0.75          |
| (1,108)  | 1:9:A:ILE:HA    | 1:10:A:LEU:HD13 | 3        | 0.75          |
| (1,44)   | 1:63:A:ALA:HA   | 1:65:A:VAL:HG11 | 7        | 0.75          |
| (1,44)   | 1:63:A:ALA:HA   | 1:65:A:VAL:HG12 | 7        | 0.75          |
| (1,44)   | 1:63:A:ALA:HA   | 1:65:A:VAL:HG13 | 7        | 0.75          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,43)   | 1:63:A:ALA:HA   | 1:65:A:VAL:HG11 | 7        | 0.75          |
| (1,43)   | 1:63:A:ALA:HA   | 1:65:A:VAL:HG12 | 7        | 0.75          |
| (1,43)   | 1:63:A:ALA:HA   | 1:65:A:VAL:HG13 | 7        | 0.75          |
| (1,865)  | 1:18:A:ASN:HD22 | 1:20:A:ASP:H    | 9        | 0.74          |
| (1,649)  | 1:9:A:ILE:H     | 1:33:A:LEU:HG   | 7        | 0.74          |
| (1,600)  | 1:65:A:VAL:HG21 | 1:66:A:ARG:H    | 8        | 0.74          |
| (1,600)  | 1:65:A:VAL:HG22 | 1:66:A:ARG:H    | 8        | 0.74          |
| (1,600)  | 1:65:A:VAL:HG23 | 1:66:A:ARG:H    | 8        | 0.74          |
| (1,1607) | 1:91:A:SER:HB2  | 1:92:A:LEU:HD11 | 6        | 0.73          |
| (1,1607) | 1:91:A:SER:HB2  | 1:92:A:LEU:HD12 | 6        | 0.73          |
| (1,1607) | 1:91:A:SER:HB2  | 1:92:A:LEU:HD13 | 6        | 0.73          |
| (1,1607) | 1:91:A:SER:HB3  | 1:92:A:LEU:HD11 | 6        | 0.73          |
| (1,1607) | 1:91:A:SER:HB3  | 1:92:A:LEU:HD12 | 6        | 0.73          |
| (1,1607) | 1:91:A:SER:HB3  | 1:92:A:LEU:HD13 | 6        | 0.73          |
| (1,769)  | 1:15:A:LEU:HA   | 1:70:A:GLU:H    | 4        | 0.73          |
| (1,600)  | 1:65:A:VAL:HG21 | 1:66:A:ARG:H    | 10       | 0.73          |
| (1,600)  | 1:65:A:VAL:HG22 | 1:66:A:ARG:H    | 10       | 0.73          |
| (1,600)  | 1:65:A:VAL:HG23 | 1:66:A:ARG:H    | 10       | 0.73          |
| (1,44)   | 1:63:A:ALA:HA   | 1:65:A:VAL:HG11 | 8        | 0.73          |
| (1,44)   | 1:63:A:ALA:HA   | 1:65:A:VAL:HG12 | 8        | 0.73          |
| (1,44)   | 1:63:A:ALA:HA   | 1:65:A:VAL:HG13 | 8        | 0.73          |
| (1,43)   | 1:63:A:ALA:HA   | 1:65:A:VAL:HG11 | 8        | 0.73          |
| (1,43)   | 1:63:A:ALA:HA   | 1:65:A:VAL:HG12 | 8        | 0.73          |
| (1,43)   | 1:63:A:ALA:HA   | 1:65:A:VAL:HG13 | 8        | 0.73          |
| (1,600)  | 1:65:A:VAL:HG21 | 1:66:A:ARG:H    | 9        | 0.72          |
| (1,600)  | 1:65:A:VAL:HG22 | 1:66:A:ARG:H    | 9        | 0.72          |
| (1,600)  | 1:65:A:VAL:HG23 | 1:66:A:ARG:H    | 9        | 0.72          |
| (1,480)  | 1:49:A:GLU:HB2  | 1:57:A:MET:HG3  | 5        | 0.72          |
| (1,281)  | 1:72:A:PHE:HB2  | 1:86:A:LEU:HB3  | 3        | 0.72          |
| (1,224)  | 1:4:A:LEU:HB2   | 1:30:A:GLY:HA2  | 1        | 0.72          |
| (1,224)  | 1:4:A:LEU:HB2   | 1:30:A:GLY:HA2  | 4        | 0.72          |
| (1,1623) | 1:99:A:VAL:H    | 1:100:A:LYS:HD2 | 10       | 0.71          |
| (1,1623) | 1:99:A:VAL:H    | 1:100:A:LYS:HD3 | 10       | 0.71          |
| (1,1395) | 1:19:A:LYS:HD2  | 1:20:A:ASP:HA   | 4        | 0.71          |
| (1,1395) | 1:19:A:LYS:HD3  | 1:20:A:ASP:HA   | 4        | 0.71          |
| (1,614)  | 1:67:A:VAL:H    | 1:96:A:GLY:H    | 5        | 0.71          |
| (1,224)  | 1:4:A:LEU:HB2   | 1:30:A:GLY:HA2  | 8        | 0.71          |
| (1,157)  | 1:68:A:VAL:H    | 1:92:A:LEU:HD21 | 8        | 0.71          |
| (1,157)  | 1:68:A:VAL:H    | 1:92:A:LEU:HD22 | 8        | 0.71          |
| (1,157)  | 1:68:A:VAL:H    | 1:92:A:LEU:HD23 | 8        | 0.71          |
| (1,156)  | 1:68:A:VAL:H    | 1:92:A:LEU:HD21 | 8        | 0.71          |
| (1,156)  | 1:68:A:VAL:H    | 1:92:A:LEU:HD22 | 8        | 0.71          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,156)  | 1:68:A:VAL:H    | 1:92:A:LEU:HD23 | 8        | 0.71          |
| (1,82)   | 1:28:A:LYS:HG3  | 1:29:A:LEU:HG   | 7        | 0.71          |
| (1,44)   | 1:63:A:ALA:HA   | 1:65:A:VAL:HG11 | 9        | 0.71          |
| (1,44)   | 1:63:A:ALA:HA   | 1:65:A:VAL:HG12 | 9        | 0.71          |
| (1,44)   | 1:63:A:ALA:HA   | 1:65:A:VAL:HG13 | 9        | 0.71          |
| (1,43)   | 1:63:A:ALA:HA   | 1:65:A:VAL:HG11 | 9        | 0.71          |
| (1,43)   | 1:63:A:ALA:HA   | 1:65:A:VAL:HG12 | 9        | 0.71          |
| (1,43)   | 1:63:A:ALA:HA   | 1:65:A:VAL:HG13 | 9        | 0.71          |
| (1,1093) | 1:90:A:HIS:HB3  | 1:91:A:SER:H    | 8        | 0.7           |
| (1,649)  | 1:9:A:ILE:H     | 1:33:A:LEU:HG   | 1        | 0.7           |
| (1,287)  | 1:53:A:MET:HE1  | 1:61:A:LYS:HE2  | 2        | 0.7           |
| (1,287)  | 1:53:A:MET:HE2  | 1:61:A:LYS:HE2  | 2        | 0.7           |
| (1,287)  | 1:53:A:MET:HE3  | 1:61:A:LYS:HE2  | 2        | 0.7           |
| (1,44)   | 1:63:A:ALA:HA   | 1:65:A:VAL:HG11 | 3        | 0.7           |
| (1,44)   | 1:63:A:ALA:HA   | 1:65:A:VAL:HG12 | 3        | 0.7           |
| (1,44)   | 1:63:A:ALA:HA   | 1:65:A:VAL:HG13 | 3        | 0.7           |
| (1,43)   | 1:63:A:ALA:HA   | 1:65:A:VAL:HG11 | 3        | 0.7           |
| (1,43)   | 1:63:A:ALA:HA   | 1:65:A:VAL:HG12 | 3        | 0.7           |
| (1,43)   | 1:63:A:ALA:HA   | 1:65:A:VAL:HG13 | 3        | 0.7           |
| (1,665)  | 1:65:A:VAL:HG11 | 1:97:A:ALA:H    | 8        | 0.69          |
| (1,665)  | 1:65:A:VAL:HG12 | 1:97:A:ALA:H    | 8        | 0.69          |
| (1,665)  | 1:65:A:VAL:HG13 | 1:97:A:ALA:H    | 8        | 0.69          |
| (1,108)  | 1:9:A:ILE:HA    | 1:10:A:LEU:HD11 | 6        | 0.69          |
| (1,108)  | 1:9:A:ILE:HA    | 1:10:A:LEU:HD12 | 6        | 0.69          |
| (1,108)  | 1:9:A:ILE:HA    | 1:10:A:LEU:HD13 | 6        | 0.69          |
| (1,1125) | 1:83:A:LEU:HG   | 1:84:A:GLN:H    | 7        | 0.68          |
| (1,769)  | 1:15:A:LEU:HA   | 1:70:A:GLU:H    | 7        | 0.68          |
| (1,665)  | 1:65:A:VAL:HG11 | 1:97:A:ALA:H    | 6        | 0.68          |
| (1,665)  | 1:65:A:VAL:HG12 | 1:97:A:ALA:H    | 6        | 0.68          |
| (1,665)  | 1:65:A:VAL:HG13 | 1:97:A:ALA:H    | 6        | 0.68          |
| (1,446)  | 1:4:A:LEU:HD11  | 1:7:A:MET:HB2   | 10       | 0.68          |
| (1,446)  | 1:4:A:LEU:HD12  | 1:7:A:MET:HB2   | 10       | 0.68          |
| (1,446)  | 1:4:A:LEU:HD13  | 1:7:A:MET:HB2   | 10       | 0.68          |
| (1,304)  | 1:50:A:VAL:H    | 1:53:A:MET:HE1  | 10       | 0.68          |
| (1,304)  | 1:50:A:VAL:H    | 1:53:A:MET:HE2  | 10       | 0.68          |
| (1,304)  | 1:50:A:VAL:H    | 1:53:A:MET:HE3  | 10       | 0.68          |
| (1,224)  | 1:4:A:LEU:HB2   | 1:30:A:GLY:HA2  | 10       | 0.68          |
| (1,44)   | 1:63:A:ALA:HA   | 1:65:A:VAL:HG11 | 5        | 0.68          |
| (1,44)   | 1:63:A:ALA:HA   | 1:65:A:VAL:HG12 | 5        | 0.68          |
| (1,44)   | 1:63:A:ALA:HA   | 1:65:A:VAL:HG13 | 5        | 0.68          |
| (1,43)   | 1:63:A:ALA:HA   | 1:65:A:VAL:HG11 | 5        | 0.68          |
| (1,43)   | 1:63:A:ALA:HA   | 1:65:A:VAL:HG12 | 5        | 0.68          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,43)   | 1:63:A:ALA:HA   | 1:65:A:VAL:HG13 | 5        | 0.68          |
| (1,1446) | 1:45:A:SER:H    | 1:70:A:GLU:HG2  | 5        | 0.67          |
| (1,1446) | 1:45:A:SER:H    | 1:70:A:GLU:HG3  | 5        | 0.67          |
| (1,1108) | 1:49:A:GLU:HB3  | 1:54:A:SER:H    | 10       | 0.67          |
| (1,582)  | 1:10:A:LEU:H    | 1:42:A:LEU:HD21 | 2        | 0.67          |
| (1,582)  | 1:10:A:LEU:H    | 1:42:A:LEU:HD22 | 2        | 0.67          |
| (1,582)  | 1:10:A:LEU:H    | 1:42:A:LEU:HD23 | 2        | 0.67          |
| (1,281)  | 1:72:A:PHE:HB2  | 1:86:A:LEU:HB3  | 2        | 0.67          |
| (1,1264) | 1:94:A:SER:HA   | 1:96:A:GLY:H    | 9        | 0.66          |
| (1,621)  | 1:38:A:ASN:HD22 | 1:97:A:ALA:H    | 7        | 0.66          |
| (1,481)  | 1:49:A:GLU:HB3  | 1:57:A:MET:HG3  | 9        | 0.66          |
| (1,224)  | 1:4:A:LEU:HB2   | 1:30:A:GLY:HA2  | 6        | 0.66          |
| (1,157)  | 1:68:A:VAL:H    | 1:92:A:LEU:HD21 | 1        | 0.66          |
| (1,157)  | 1:68:A:VAL:H    | 1:92:A:LEU:HD22 | 1        | 0.66          |
| (1,157)  | 1:68:A:VAL:H    | 1:92:A:LEU:HD23 | 1        | 0.66          |
| (1,156)  | 1:68:A:VAL:H    | 1:92:A:LEU:HD21 | 1        | 0.66          |
| (1,156)  | 1:68:A:VAL:H    | 1:92:A:LEU:HD22 | 1        | 0.66          |
| (1,156)  | 1:68:A:VAL:H    | 1:92:A:LEU:HD23 | 1        | 0.66          |
| (1,108)  | 1:9:A:ILE:HA    | 1:10:A:LEU:HD11 | 1        | 0.66          |
| (1,108)  | 1:9:A:ILE:HA    | 1:10:A:LEU:HD12 | 1        | 0.66          |
| (1,108)  | 1:9:A:ILE:HA    | 1:10:A:LEU:HD13 | 1        | 0.66          |
| (1,1607) | 1:91:A:SER:HB2  | 1:92:A:LEU:HD11 | 9        | 0.65          |
| (1,1607) | 1:91:A:SER:HB2  | 1:92:A:LEU:HD12 | 9        | 0.65          |
| (1,1607) | 1:91:A:SER:HB2  | 1:92:A:LEU:HD13 | 9        | 0.65          |
| (1,1607) | 1:91:A:SER:HB3  | 1:92:A:LEU:HD11 | 9        | 0.65          |
| (1,1607) | 1:91:A:SER:HB3  | 1:92:A:LEU:HD12 | 9        | 0.65          |
| (1,1607) | 1:91:A:SER:HB3  | 1:92:A:LEU:HD13 | 9        | 0.65          |
| (1,769)  | 1:15:A:LEU:HA   | 1:70:A:GLU:H    | 8        | 0.65          |
| (1,649)  | 1:9:A:ILE:H     | 1:33:A:LEU:HG   | 3        | 0.65          |
| (1,600)  | 1:65:A:VAL:HG21 | 1:66:A:ARG:H    | 2        | 0.65          |
| (1,600)  | 1:65:A:VAL:HG22 | 1:66:A:ARG:H    | 2        | 0.65          |
| (1,600)  | 1:65:A:VAL:HG23 | 1:66:A:ARG:H    | 2        | 0.65          |
| (1,600)  | 1:65:A:VAL:HG21 | 1:66:A:ARG:H    | 5        | 0.65          |
| (1,600)  | 1:65:A:VAL:HG22 | 1:66:A:ARG:H    | 5        | 0.65          |
| (1,600)  | 1:65:A:VAL:HG23 | 1:66:A:ARG:H    | 5        | 0.65          |
| (1,281)  | 1:72:A:PHE:HB2  | 1:86:A:LEU:HB3  | 8        | 0.65          |
| (1,44)   | 1:63:A:ALA:HA   | 1:65:A:VAL:HG11 | 1        | 0.65          |
| (1,44)   | 1:63:A:ALA:HA   | 1:65:A:VAL:HG12 | 1        | 0.65          |
| (1,44)   | 1:63:A:ALA:HA   | 1:65:A:VAL:HG13 | 1        | 0.65          |
| (1,44)   | 1:63:A:ALA:HA   | 1:65:A:VAL:HG11 | 2        | 0.65          |
| (1,44)   | 1:63:A:ALA:HA   | 1:65:A:VAL:HG12 | 2        | 0.65          |
| (1,44)   | 1:63:A:ALA:HA   | 1:65:A:VAL:HG13 | 2        | 0.65          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,43)   | 1:63:A:ALA:HA   | 1:65:A:VAL:HG11 | 1        | 0.65          |
| (1,43)   | 1:63:A:ALA:HA   | 1:65:A:VAL:HG12 | 1        | 0.65          |
| (1,43)   | 1:63:A:ALA:HA   | 1:65:A:VAL:HG13 | 1        | 0.65          |
| (1,43)   | 1:63:A:ALA:HA   | 1:65:A:VAL:HG11 | 2        | 0.65          |
| (1,43)   | 1:63:A:ALA:HA   | 1:65:A:VAL:HG12 | 2        | 0.65          |
| (1,43)   | 1:63:A:ALA:HA   | 1:65:A:VAL:HG13 | 2        | 0.65          |
| (1,1048) | 1:4:A:LEU:HD11  | 1:7:A:MET:H     | 5        | 0.64          |
| (1,1048) | 1:4:A:LEU:HD12  | 1:7:A:MET:H     | 5        | 0.64          |
| (1,1048) | 1:4:A:LEU:HD13  | 1:7:A:MET:H     | 5        | 0.64          |
| (1,224)  | 1:4:A:LEU:HB2   | 1:30:A:GLY:HA2  | 2        | 0.64          |
| (1,108)  | 1:9:A:ILE:HA    | 1:10:A:LEU:HD11 | 9        | 0.64          |
| (1,108)  | 1:9:A:ILE:HA    | 1:10:A:LEU:HD12 | 9        | 0.64          |
| (1,108)  | 1:9:A:ILE:HA    | 1:10:A:LEU:HD13 | 9        | 0.64          |
| (1,1264) | 1:94:A:SER:HA   | 1:96:A:GLY:H    | 7        | 0.63          |
| (1,1062) | 1:7:A:MET:H     | 1:32:A:LYS:H    | 9        | 0.63          |
| (1,600)  | 1:65:A:VAL:HG21 | 1:66:A:ARG:H    | 1        | 0.63          |
| (1,600)  | 1:65:A:VAL:HG22 | 1:66:A:ARG:H    | 1        | 0.63          |
| (1,600)  | 1:65:A:VAL:HG23 | 1:66:A:ARG:H    | 1        | 0.63          |
| (1,600)  | 1:65:A:VAL:HG21 | 1:66:A:ARG:H    | 4        | 0.63          |
| (1,600)  | 1:65:A:VAL:HG22 | 1:66:A:ARG:H    | 4        | 0.63          |
| (1,600)  | 1:65:A:VAL:HG23 | 1:66:A:ARG:H    | 4        | 0.63          |
| (1,582)  | 1:10:A:LEU:H    | 1:42:A:LEU:HD21 | 6        | 0.63          |
| (1,582)  | 1:10:A:LEU:H    | 1:42:A:LEU:HD22 | 6        | 0.63          |
| (1,582)  | 1:10:A:LEU:H    | 1:42:A:LEU:HD23 | 6        | 0.63          |
| (1,347)  | 1:25:A:MET:HE1  | 1:29:A:LEU:HD21 | 10       | 0.63          |
| (1,347)  | 1:25:A:MET:HE1  | 1:29:A:LEU:HD22 | 10       | 0.63          |
| (1,347)  | 1:25:A:MET:HE1  | 1:29:A:LEU:HD23 | 10       | 0.63          |
| (1,347)  | 1:25:A:MET:HE2  | 1:29:A:LEU:HD21 | 10       | 0.63          |
| (1,347)  | 1:25:A:MET:HE2  | 1:29:A:LEU:HD22 | 10       | 0.63          |
| (1,347)  | 1:25:A:MET:HE2  | 1:29:A:LEU:HD23 | 10       | 0.63          |
| (1,347)  | 1:25:A:MET:HE3  | 1:29:A:LEU:HD21 | 10       | 0.63          |
| (1,347)  | 1:25:A:MET:HE3  | 1:29:A:LEU:HD22 | 10       | 0.63          |
| (1,347)  | 1:25:A:MET:HE3  | 1:29:A:LEU:HD23 | 10       | 0.63          |
| (1,82)   | 1:28:A:LYS:HG3  | 1:29:A:LEU:HG   | 10       | 0.63          |
| (1,683)  | 1:12:A:LEU:H    | 1:43:A:CYS:HA   | 7        | 0.62          |
| (1,582)  | 1:10:A:LEU:H    | 1:42:A:LEU:HD21 | 5        | 0.62          |
| (1,582)  | 1:10:A:LEU:H    | 1:42:A:LEU:HD22 | 5        | 0.62          |
| (1,582)  | 1:10:A:LEU:H    | 1:42:A:LEU:HD23 | 5        | 0.62          |
| (1,619)  | 1:38:A:ASN:HD21 | 1:97:A:ALA:H    | 6        | 0.61          |
| (1,600)  | 1:65:A:VAL:HG21 | 1:66:A:ARG:H    | 7        | 0.61          |
| (1,600)  | 1:65:A:VAL:HG22 | 1:66:A:ARG:H    | 7        | 0.61          |
| (1,600)  | 1:65:A:VAL:HG23 | 1:66:A:ARG:H    | 7        | 0.61          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1264) | 1:94:A:SER:HA   | 1:96:A:GLY:H    | 10       | 0.59          |
| (1,930)  | 1:68:A:VAL:H    | 1:92:A:LEU:HG   | 6        | 0.59          |
| (1,756)  | 1:34:A:THR:H    | 1:40:A:ALA:H    | 7        | 0.59          |
| (1,481)  | 1:49:A:GLU:HB3  | 1:57:A:MET:HG3  | 2        | 0.59          |
| (1,446)  | 1:4:A:LEU:HD11  | 1:7:A:MET:HB2   | 7        | 0.59          |
| (1,446)  | 1:4:A:LEU:HD12  | 1:7:A:MET:HB2   | 7        | 0.59          |
| (1,446)  | 1:4:A:LEU:HD13  | 1:7:A:MET:HB2   | 7        | 0.59          |
| (1,44)   | 1:63:A:ALA:HA   | 1:65:A:VAL:HG11 | 4        | 0.59          |
| (1,44)   | 1:63:A:ALA:HA   | 1:65:A:VAL:HG12 | 4        | 0.59          |
| (1,44)   | 1:63:A:ALA:HA   | 1:65:A:VAL:HG13 | 4        | 0.59          |
| (1,43)   | 1:63:A:ALA:HA   | 1:65:A:VAL:HG11 | 4        | 0.59          |
| (1,43)   | 1:63:A:ALA:HA   | 1:65:A:VAL:HG12 | 4        | 0.59          |
| (1,43)   | 1:63:A:ALA:HA   | 1:65:A:VAL:HG13 | 4        | 0.59          |
| (1,756)  | 1:34:A:THR:H    | 1:40:A:ALA:H    | 9        | 0.58          |
| (1,665)  | 1:65:A:VAL:HG11 | 1:97:A:ALA:H    | 1        | 0.58          |
| (1,665)  | 1:65:A:VAL:HG12 | 1:97:A:ALA:H    | 1        | 0.58          |
| (1,665)  | 1:65:A:VAL:HG13 | 1:97:A:ALA:H    | 1        | 0.58          |
| (1,582)  | 1:10:A:LEU:H    | 1:42:A:LEU:HD21 | 4        | 0.58          |
| (1,582)  | 1:10:A:LEU:H    | 1:42:A:LEU:HD22 | 4        | 0.58          |
| (1,582)  | 1:10:A:LEU:H    | 1:42:A:LEU:HD23 | 4        | 0.58          |
| (1,480)  | 1:49:A:GLU:HB2  | 1:57:A:MET:HG3  | 10       | 0.58          |
| (1,1062) | 1:7:A:MET:H     | 1:32:A:LYS:H    | 1        | 0.57          |
| (1,648)  | 1:65:A:VAL:HB   | 1:67:A:VAL:H    | 4        | 0.57          |
| (1,648)  | 1:65:A:VAL:HB   | 1:67:A:VAL:H    | 8        | 0.57          |
| (1,582)  | 1:10:A:LEU:H    | 1:42:A:LEU:HD21 | 9        | 0.57          |
| (1,582)  | 1:10:A:LEU:H    | 1:42:A:LEU:HD22 | 9        | 0.57          |
| (1,582)  | 1:10:A:LEU:H    | 1:42:A:LEU:HD23 | 9        | 0.57          |
| (1,481)  | 1:49:A:GLU:HB3  | 1:57:A:MET:HG3  | 7        | 0.57          |
| (1,224)  | 1:4:A:LEU:HB2   | 1:30:A:GLY:HA2  | 7        | 0.57          |
| (1,109)  | 1:28:A:LYS:HG3  | 1:29:A:LEU:HA   | 4        | 0.57          |
| (1,44)   | 1:63:A:ALA:HA   | 1:65:A:VAL:HG11 | 6        | 0.57          |
| (1,44)   | 1:63:A:ALA:HA   | 1:65:A:VAL:HG12 | 6        | 0.57          |
| (1,44)   | 1:63:A:ALA:HA   | 1:65:A:VAL:HG13 | 6        | 0.57          |
| (1,43)   | 1:63:A:ALA:HA   | 1:65:A:VAL:HG11 | 6        | 0.57          |
| (1,43)   | 1:63:A:ALA:HA   | 1:65:A:VAL:HG12 | 6        | 0.57          |
| (1,43)   | 1:63:A:ALA:HA   | 1:65:A:VAL:HG13 | 6        | 0.57          |
| (1,1264) | 1:94:A:SER:HA   | 1:96:A:GLY:H    | 1        | 0.56          |
| (1,1264) | 1:94:A:SER:HA   | 1:96:A:GLY:H    | 4        | 0.56          |
| (1,1062) | 1:7:A:MET:H     | 1:32:A:LYS:H    | 8        | 0.56          |
| (1,619)  | 1:38:A:ASN:HD21 | 1:97:A:ALA:H    | 10       | 0.56          |
| (1,607)  | 1:66:A:ARG:H    | 1:97:A:ALA:H    | 7        | 0.56          |
| (1,481)  | 1:49:A:GLU:HB3  | 1:57:A:MET:HG3  | 4        | 0.56          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,347)  | 1:25:A:MET:HE1  | 1:29:A:LEU:HD21 | 9        | 0.56          |
| (1,347)  | 1:25:A:MET:HE1  | 1:29:A:LEU:HD22 | 9        | 0.56          |
| (1,347)  | 1:25:A:MET:HE1  | 1:29:A:LEU:HD23 | 9        | 0.56          |
| (1,347)  | 1:25:A:MET:HE2  | 1:29:A:LEU:HD21 | 9        | 0.56          |
| (1,347)  | 1:25:A:MET:HE2  | 1:29:A:LEU:HD22 | 9        | 0.56          |
| (1,347)  | 1:25:A:MET:HE2  | 1:29:A:LEU:HD23 | 9        | 0.56          |
| (1,347)  | 1:25:A:MET:HE3  | 1:29:A:LEU:HD21 | 9        | 0.56          |
| (1,347)  | 1:25:A:MET:HE3  | 1:29:A:LEU:HD22 | 9        | 0.56          |
| (1,347)  | 1:25:A:MET:HE3  | 1:29:A:LEU:HD23 | 9        | 0.56          |
| (1,109)  | 1:28:A:LYS:HG3  | 1:29:A:LEU:HA   | 2        | 0.56          |
| (1,109)  | 1:28:A:LYS:HG3  | 1:29:A:LEU:HA   | 3        | 0.56          |
| (1,1119) | 1:74:A:GLN:H    | 1:74:A:GLN:HG2  | 6        | 0.55          |
| (1,1062) | 1:7:A:MET:H     | 1:32:A:LYS:H    | 7        | 0.55          |
| (1,408)  | 1:72:A:PHE:HA   | 1:87:A:LEU:HA   | 4        | 0.55          |
| (1,224)  | 1:4:A:LEU:HB2   | 1:30:A:GLY:HA2  | 9        | 0.55          |
| (1,1264) | 1:94:A:SER:HA   | 1:96:A:GLY:H    | 6        | 0.54          |
| (1,769)  | 1:15:A:LEU:HA   | 1:70:A:GLU:H    | 6        | 0.54          |
| (1,648)  | 1:65:A:VAL:HB   | 1:67:A:VAL:H    | 5        | 0.54          |
| (1,296)  | 1:53:A:MET:HE1  | 1:54:A:SER:H    | 10       | 0.54          |
| (1,296)  | 1:53:A:MET:HE2  | 1:54:A:SER:H    | 10       | 0.54          |
| (1,296)  | 1:53:A:MET:HE3  | 1:54:A:SER:H    | 10       | 0.54          |
| (1,1119) | 1:74:A:GLN:H    | 1:74:A:GLN:HG2  | 9        | 0.53          |
| (1,224)  | 1:4:A:LEU:HB2   | 1:30:A:GLY:HA2  | 3        | 0.53          |
| (1,1607) | 1:91:A:SER:HB2  | 1:92:A:LEU:HD11 | 5        | 0.52          |
| (1,1607) | 1:91:A:SER:HB2  | 1:92:A:LEU:HD12 | 5        | 0.52          |
| (1,1607) | 1:91:A:SER:HB2  | 1:92:A:LEU:HD13 | 5        | 0.52          |
| (1,1607) | 1:91:A:SER:HB3  | 1:92:A:LEU:HD11 | 5        | 0.52          |
| (1,1607) | 1:91:A:SER:HB3  | 1:92:A:LEU:HD12 | 5        | 0.52          |
| (1,1607) | 1:91:A:SER:HB3  | 1:92:A:LEU:HD13 | 5        | 0.52          |
| (1,1166) | 1:4:A:LEU:H     | 1:30:A:GLY:HA3  | 10       | 0.52          |
| (1,765)  | 1:38:A:ASN:HD22 | 1:98:A:GLU:H    | 4        | 0.52          |
| (1,648)  | 1:65:A:VAL:HB   | 1:67:A:VAL:H    | 6        | 0.52          |
| (1,281)  | 1:72:A:PHE:HB2  | 1:86:A:LEU:HB3  | 9        | 0.52          |
| (1,1264) | 1:94:A:SER:HA   | 1:96:A:GLY:H    | 2        | 0.51          |
| (1,1134) | 1:91:A:SER:H    | 1:92:A:LEU:HB2  | 9        | 0.51          |
| (1,865)  | 1:18:A:ASN:HD22 | 1:20:A:ASP:H    | 4        | 0.51          |
| (1,281)  | 1:72:A:PHE:HB2  | 1:86:A:LEU:HB3  | 1        | 0.51          |
| (1,132)  | 1:12:A:LEU:HD11 | 1:57:A:MET:H    | 7        | 0.51          |
| (1,132)  | 1:12:A:LEU:HD12 | 1:57:A:MET:H    | 7        | 0.51          |
| (1,132)  | 1:12:A:LEU:HD13 | 1:57:A:MET:H    | 7        | 0.51          |
| (1,109)  | 1:28:A:LYS:HG3  | 1:29:A:LEU:HA   | 6        | 0.51          |
| (1,1446) | 1:45:A:SER:H    | 1:70:A:GLU:HG2  | 3        | 0.5           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1446) | 1:45:A:SER:H    | 1:70:A:GLU:HG3  | 3        | 0.5           |
| (1,1412) | 1:23:A:LYS:HD2  | 1:33:A:LEU:HD11 | 9        | 0.5           |
| (1,1412) | 1:23:A:LYS:HD2  | 1:33:A:LEU:HD12 | 9        | 0.5           |
| (1,1412) | 1:23:A:LYS:HD2  | 1:33:A:LEU:HD13 | 9        | 0.5           |
| (1,1412) | 1:23:A:LYS:HD3  | 1:33:A:LEU:HD11 | 9        | 0.5           |
| (1,1412) | 1:23:A:LYS:HD3  | 1:33:A:LEU:HD12 | 9        | 0.5           |
| (1,1412) | 1:23:A:LYS:HD3  | 1:33:A:LEU:HD13 | 9        | 0.5           |
| (1,1264) | 1:94:A:SER:HA   | 1:96:A:GLY:H    | 3        | 0.5           |
| (1,769)  | 1:15:A:LEU:HA   | 1:70:A:GLU:H    | 3        | 0.5           |
| (1,737)  | 1:15:A:LEU:HD11 | 1:22:A:ALA:H    | 10       | 0.5           |
| (1,737)  | 1:15:A:LEU:HD12 | 1:22:A:ALA:H    | 10       | 0.5           |
| (1,737)  | 1:15:A:LEU:HD13 | 1:22:A:ALA:H    | 10       | 0.5           |
| (1,736)  | 1:15:A:LEU:HD11 | 1:22:A:ALA:H    | 10       | 0.5           |
| (1,736)  | 1:15:A:LEU:HD12 | 1:22:A:ALA:H    | 10       | 0.5           |
| (1,736)  | 1:15:A:LEU:HD13 | 1:22:A:ALA:H    | 10       | 0.5           |
| (1,737)  | 1:15:A:LEU:HD11 | 1:22:A:ALA:H    | 7        | 0.49          |
| (1,737)  | 1:15:A:LEU:HD12 | 1:22:A:ALA:H    | 7        | 0.49          |
| (1,737)  | 1:15:A:LEU:HD13 | 1:22:A:ALA:H    | 7        | 0.49          |
| (1,736)  | 1:15:A:LEU:HD11 | 1:22:A:ALA:H    | 7        | 0.49          |
| (1,736)  | 1:15:A:LEU:HD12 | 1:22:A:ALA:H    | 7        | 0.49          |
| (1,736)  | 1:15:A:LEU:HD13 | 1:22:A:ALA:H    | 7        | 0.49          |
| (1,665)  | 1:65:A:VAL:HG11 | 1:97:A:ALA:H    | 10       | 0.49          |
| (1,665)  | 1:65:A:VAL:HG12 | 1:97:A:ALA:H    | 10       | 0.49          |
| (1,665)  | 1:65:A:VAL:HG13 | 1:97:A:ALA:H    | 10       | 0.49          |
| (1,621)  | 1:38:A:ASN:HD22 | 1:97:A:ALA:H    | 5        | 0.49          |
| (1,619)  | 1:38:A:ASN:HD21 | 1:97:A:ALA:H    | 5        | 0.49          |
| (1,281)  | 1:72:A:PHE:HB2  | 1:86:A:LEU:HB3  | 7        | 0.49          |
| (1,26)   | 1:100:A:LYS:HA  | 1:100:A:LYS:HD2 | 3        | 0.49          |
| (1,1396) | 1:19:A:LYS:HD2  | 1:21:A:GLU:H    | 2        | 0.48          |
| (1,1396) | 1:19:A:LYS:HD3  | 1:21:A:GLU:H    | 2        | 0.48          |
| (1,1384) | 1:18:A:ASN:HD21 | 1:20:A:ASP:H    | 2        | 0.48          |
| (1,1384) | 1:18:A:ASN:HD22 | 1:20:A:ASP:H    | 2        | 0.48          |
| (1,1093) | 1:90:A:HIS:HB3  | 1:91:A:SER:H    | 5        | 0.48          |
| (1,768)  | 1:11:A:THR:HA   | 1:45:A:SER:H    | 5        | 0.48          |
| (1,665)  | 1:65:A:VAL:HG11 | 1:97:A:ALA:H    | 2        | 0.48          |
| (1,665)  | 1:65:A:VAL:HG12 | 1:97:A:ALA:H    | 2        | 0.48          |
| (1,665)  | 1:65:A:VAL:HG13 | 1:97:A:ALA:H    | 2        | 0.48          |
| (1,481)  | 1:49:A:GLU:HB3  | 1:57:A:MET:HG3  | 6        | 0.48          |
| (1,446)  | 1:4:A:LEU:HD11  | 1:7:A:MET:HB2   | 2        | 0.48          |
| (1,446)  | 1:4:A:LEU:HD12  | 1:7:A:MET:HB2   | 2        | 0.48          |
| (1,446)  | 1:4:A:LEU:HD13  | 1:7:A:MET:HB2   | 2        | 0.48          |
| (1,1301) | 1:4:A:LEU:HB3   | 1:30:A:GLY:H    | 2        | 0.47          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,683)  | 1:12:A:LEU:H    | 1:43:A:CYS:HA   | 4        | 0.47          |
| (1,582)  | 1:10:A:LEU:H    | 1:42:A:LEU:HD21 | 3        | 0.47          |
| (1,582)  | 1:10:A:LEU:H    | 1:42:A:LEU:HD22 | 3        | 0.47          |
| (1,582)  | 1:10:A:LEU:H    | 1:42:A:LEU:HD23 | 3        | 0.47          |
| (1,446)  | 1:4:A:LEU:HD11  | 1:7:A:MET:HB2   | 3        | 0.47          |
| (1,446)  | 1:4:A:LEU:HD12  | 1:7:A:MET:HB2   | 3        | 0.47          |
| (1,446)  | 1:4:A:LEU:HD13  | 1:7:A:MET:HB2   | 3        | 0.47          |
| (1,157)  | 1:68:A:VAL:H    | 1:92:A:LEU:HD21 | 2        | 0.47          |
| (1,157)  | 1:68:A:VAL:H    | 1:92:A:LEU:HD22 | 2        | 0.47          |
| (1,157)  | 1:68:A:VAL:H    | 1:92:A:LEU:HD23 | 2        | 0.47          |
| (1,157)  | 1:68:A:VAL:H    | 1:92:A:LEU:HD21 | 3        | 0.47          |
| (1,157)  | 1:68:A:VAL:H    | 1:92:A:LEU:HD22 | 3        | 0.47          |
| (1,157)  | 1:68:A:VAL:H    | 1:92:A:LEU:HD23 | 3        | 0.47          |
| (1,156)  | 1:68:A:VAL:H    | 1:92:A:LEU:HD21 | 2        | 0.47          |
| (1,156)  | 1:68:A:VAL:H    | 1:92:A:LEU:HD22 | 2        | 0.47          |
| (1,156)  | 1:68:A:VAL:H    | 1:92:A:LEU:HD23 | 2        | 0.47          |
| (1,156)  | 1:68:A:VAL:H    | 1:92:A:LEU:HD21 | 3        | 0.47          |
| (1,156)  | 1:68:A:VAL:H    | 1:92:A:LEU:HD22 | 3        | 0.47          |
| (1,156)  | 1:68:A:VAL:H    | 1:92:A:LEU:HD23 | 3        | 0.47          |
| (1,1062) | 1:7:A:MET:H     | 1:32:A:LYS:H    | 10       | 0.46          |
| (1,943)  | 1:75:A:ASP:H    | 1:76:A:VAL:HB   | 7        | 0.46          |
| (1,837)  | 1:12:A:LEU:HD21 | 1:61:A:LYS:H    | 8        | 0.46          |
| (1,837)  | 1:12:A:LEU:HD22 | 1:61:A:LYS:H    | 8        | 0.46          |
| (1,837)  | 1:12:A:LEU:HD23 | 1:61:A:LYS:H    | 8        | 0.46          |
| (1,281)  | 1:72:A:PHE:HB2  | 1:86:A:LEU:HB3  | 10       | 0.46          |
| (1,1384) | 1:18:A:ASN:HD21 | 1:20:A:ASP:H    | 5        | 0.45          |
| (1,1384) | 1:18:A:ASN:HD22 | 1:20:A:ASP:H    | 5        | 0.45          |
| (1,1384) | 1:18:A:ASN:HD21 | 1:20:A:ASP:H    | 6        | 0.45          |
| (1,1384) | 1:18:A:ASN:HD22 | 1:20:A:ASP:H    | 6        | 0.45          |
| (1,943)  | 1:75:A:ASP:H    | 1:76:A:VAL:HB   | 3        | 0.45          |
| (1,943)  | 1:75:A:ASP:H    | 1:76:A:VAL:HB   | 10       | 0.45          |
| (1,683)  | 1:12:A:LEU:H    | 1:43:A:CYS:HA   | 1        | 0.45          |
| (1,683)  | 1:12:A:LEU:H    | 1:43:A:CYS:HA   | 5        | 0.45          |
| (1,607)  | 1:66:A:ARG:H    | 1:97:A:ALA:H    | 2        | 0.45          |
| (1,481)  | 1:49:A:GLU:HB3  | 1:57:A:MET:HG3  | 8        | 0.45          |
| (1,281)  | 1:72:A:PHE:HB2  | 1:86:A:LEU:HB3  | 6        | 0.45          |
| (1,1166) | 1:4:A:LEU:H     | 1:30:A:GLY:HA3  | 7        | 0.44          |
| (1,1033) | 1:4:A:LEU:HB2   | 1:6:A:ASN:H     | 6        | 0.44          |
| (1,943)  | 1:75:A:ASP:H    | 1:76:A:VAL:HB   | 1        | 0.44          |
| (1,320)  | 1:53:A:MET:HE1  | 1:57:A:MET:HA   | 8        | 0.44          |
| (1,320)  | 1:53:A:MET:HE2  | 1:57:A:MET:HA   | 8        | 0.44          |
| (1,320)  | 1:53:A:MET:HE3  | 1:57:A:MET:HA   | 8        | 0.44          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,320)  | 1:53:A:MET:HE1  | 1:57:A:MET:HA   | 10       | 0.44          |
| (1,320)  | 1:53:A:MET:HE2  | 1:57:A:MET:HA   | 10       | 0.44          |
| (1,320)  | 1:53:A:MET:HE3  | 1:57:A:MET:HA   | 10       | 0.44          |
| (1,109)  | 1:28:A:LYS:HG3  | 1:29:A:LEU:HA   | 9        | 0.44          |
| (1,1384) | 1:18:A:ASN:HD21 | 1:20:A:ASP:H    | 10       | 0.43          |
| (1,1384) | 1:18:A:ASN:HD22 | 1:20:A:ASP:H    | 10       | 0.43          |
| (1,1069) | 1:5:A:SER:H     | 1:32:A:LYS:H    | 2        | 0.43          |
| (1,943)  | 1:75:A:ASP:H    | 1:76:A:VAL:HB   | 2        | 0.43          |
| (1,648)  | 1:65:A:VAL:HB   | 1:67:A:VAL:H    | 7        | 0.43          |
| (1,634)  | 1:69:A:CYS:HB2  | 1:92:A:LEU:H    | 3        | 0.43          |
| (1,621)  | 1:38:A:ASN:HD22 | 1:97:A:ALA:H    | 1        | 0.43          |
| (1,582)  | 1:10:A:LEU:H    | 1:42:A:LEU:HD21 | 10       | 0.43          |
| (1,582)  | 1:10:A:LEU:H    | 1:42:A:LEU:HD22 | 10       | 0.43          |
| (1,582)  | 1:10:A:LEU:H    | 1:42:A:LEU:HD23 | 10       | 0.43          |
| (1,320)  | 1:53:A:MET:HE1  | 1:57:A:MET:HA   | 2        | 0.43          |
| (1,320)  | 1:53:A:MET:HE2  | 1:57:A:MET:HA   | 2        | 0.43          |
| (1,320)  | 1:53:A:MET:HE3  | 1:57:A:MET:HA   | 2        | 0.43          |
| (1,320)  | 1:53:A:MET:HE1  | 1:57:A:MET:HA   | 3        | 0.43          |
| (1,320)  | 1:53:A:MET:HE2  | 1:57:A:MET:HA   | 3        | 0.43          |
| (1,320)  | 1:53:A:MET:HE3  | 1:57:A:MET:HA   | 3        | 0.43          |
| (1,1264) | 1:94:A:SER:HA   | 1:96:A:GLY:H    | 8        | 0.42          |
| (1,1013) | 1:27:A:GLU:H    | 1:27:A:GLU:HG3  | 9        | 0.42          |
| (1,943)  | 1:75:A:ASP:H    | 1:76:A:VAL:HB   | 4        | 0.42          |
| (1,619)  | 1:38:A:ASN:HD21 | 1:97:A:ALA:H    | 8        | 0.42          |
| (1,607)  | 1:66:A:ARG:H    | 1:97:A:ALA:H    | 8        | 0.42          |
| (1,109)  | 1:28:A:LYS:HG3  | 1:29:A:LEU:HA   | 8        | 0.42          |
| (1,1485) | 1:52:A:LYS:HD2  | 1:54:A:SER:H    | 9        | 0.41          |
| (1,1485) | 1:52:A:LYS:HD3  | 1:54:A:SER:H    | 9        | 0.41          |
| (1,1395) | 1:19:A:LYS:HD2  | 1:20:A:ASP:HA   | 9        | 0.41          |
| (1,1395) | 1:19:A:LYS:HD3  | 1:20:A:ASP:HA   | 9        | 0.41          |
| (1,1344) | 1:9:A:ILE:HG12  | 1:32:A:LYS:HB3  | 10       | 0.41          |
| (1,1344) | 1:9:A:ILE:HG13  | 1:32:A:LYS:HB3  | 10       | 0.41          |
| (1,1137) | 1:41:A:SER:H    | 1:42:A:LEU:HD21 | 1        | 0.41          |
| (1,1137) | 1:41:A:SER:H    | 1:42:A:LEU:HD22 | 1        | 0.41          |
| (1,1137) | 1:41:A:SER:H    | 1:42:A:LEU:HD23 | 1        | 0.41          |
| (1,1136) | 1:41:A:SER:H    | 1:42:A:LEU:HD21 | 1        | 0.41          |
| (1,1136) | 1:41:A:SER:H    | 1:42:A:LEU:HD22 | 1        | 0.41          |
| (1,1136) | 1:41:A:SER:H    | 1:42:A:LEU:HD23 | 1        | 0.41          |
| (1,1119) | 1:74:A:GLN:H    | 1:74:A:GLN:HG2  | 5        | 0.41          |
| (1,943)  | 1:75:A:ASP:H    | 1:76:A:VAL:HB   | 5        | 0.41          |
| (1,648)  | 1:65:A:VAL:HB   | 1:67:A:VAL:H    | 9        | 0.41          |
| (1,310)  | 1:53:A:MET:HE1  | 1:61:A:LYS:H    | 6        | 0.41          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,310)  | 1:53:A:MET:HE2  | 1:61:A:LYS:H    | 6        | 0.41          |
| (1,310)  | 1:53:A:MET:HE3  | 1:61:A:LYS:H    | 6        | 0.41          |
| (1,292)  | 1:9:A:ILE:HG21  | 1:42:A:LEU:HD21 | 5        | 0.41          |
| (1,292)  | 1:9:A:ILE:HG21  | 1:42:A:LEU:HD22 | 5        | 0.41          |
| (1,292)  | 1:9:A:ILE:HG21  | 1:42:A:LEU:HD23 | 5        | 0.41          |
| (1,292)  | 1:9:A:ILE:HG22  | 1:42:A:LEU:HD21 | 5        | 0.41          |
| (1,292)  | 1:9:A:ILE:HG22  | 1:42:A:LEU:HD22 | 5        | 0.41          |
| (1,292)  | 1:9:A:ILE:HG22  | 1:42:A:LEU:HD23 | 5        | 0.41          |
| (1,292)  | 1:9:A:ILE:HG23  | 1:42:A:LEU:HD21 | 5        | 0.41          |
| (1,292)  | 1:9:A:ILE:HG23  | 1:42:A:LEU:HD22 | 5        | 0.41          |
| (1,292)  | 1:9:A:ILE:HG23  | 1:42:A:LEU:HD23 | 5        | 0.41          |
| (1,291)  | 1:9:A:ILE:HG21  | 1:42:A:LEU:HD21 | 5        | 0.41          |
| (1,291)  | 1:9:A:ILE:HG21  | 1:42:A:LEU:HD22 | 5        | 0.41          |
| (1,291)  | 1:9:A:ILE:HG21  | 1:42:A:LEU:HD23 | 5        | 0.41          |
| (1,291)  | 1:9:A:ILE:HG22  | 1:42:A:LEU:HD21 | 5        | 0.41          |
| (1,291)  | 1:9:A:ILE:HG22  | 1:42:A:LEU:HD22 | 5        | 0.41          |
| (1,291)  | 1:9:A:ILE:HG22  | 1:42:A:LEU:HD23 | 5        | 0.41          |
| (1,291)  | 1:9:A:ILE:HG23  | 1:42:A:LEU:HD21 | 5        | 0.41          |
| (1,291)  | 1:9:A:ILE:HG23  | 1:42:A:LEU:HD22 | 5        | 0.41          |
| (1,291)  | 1:9:A:ILE:HG23  | 1:42:A:LEU:HD23 | 5        | 0.41          |
| (1,288)  | 1:53:A:MET:HE1  | 1:61:A:LYS:HE3  | 6        | 0.41          |
| (1,288)  | 1:53:A:MET:HE2  | 1:61:A:LYS:HE3  | 6        | 0.41          |
| (1,288)  | 1:53:A:MET:HE3  | 1:61:A:LYS:HE3  | 6        | 0.41          |
| (1,1447) | 1:45:A:SER:HB2  | 1:46:A:THR:H    | 2        | 0.4           |
| (1,1447) | 1:45:A:SER:HB3  | 1:46:A:THR:H    | 2        | 0.4           |
| (1,1145) | 1:4:A:LEU:HD11  | 1:32:A:LYS:H    | 5        | 0.4           |
| (1,1145) | 1:4:A:LEU:HD12  | 1:32:A:LYS:H    | 5        | 0.4           |
| (1,1145) | 1:4:A:LEU:HD13  | 1:32:A:LYS:H    | 5        | 0.4           |
| (1,943)  | 1:75:A:ASP:H    | 1:76:A:VAL:HB   | 8        | 0.4           |
| (1,756)  | 1:34:A:THR:H    | 1:40:A:ALA:H    | 4        | 0.4           |
| (1,649)  | 1:9:A:ILE:H     | 1:33:A:LEU:HG   | 6        | 0.4           |
| (1,621)  | 1:38:A:ASN:HD22 | 1:97:A:ALA:H    | 6        | 0.4           |
| (1,607)  | 1:66:A:ARG:H    | 1:97:A:ALA:H    | 10       | 0.4           |
| (1,353)  | 1:7:A:MET:HE1   | 1:42:A:LEU:HD21 | 9        | 0.4           |
| (1,353)  | 1:7:A:MET:HE1   | 1:42:A:LEU:HD22 | 9        | 0.4           |
| (1,353)  | 1:7:A:MET:HE1   | 1:42:A:LEU:HD23 | 9        | 0.4           |
| (1,353)  | 1:7:A:MET:HE2   | 1:42:A:LEU:HD21 | 9        | 0.4           |
| (1,353)  | 1:7:A:MET:HE2   | 1:42:A:LEU:HD22 | 9        | 0.4           |
| (1,353)  | 1:7:A:MET:HE2   | 1:42:A:LEU:HD23 | 9        | 0.4           |
| (1,353)  | 1:7:A:MET:HE3   | 1:42:A:LEU:HD21 | 9        | 0.4           |
| (1,353)  | 1:7:A:MET:HE3   | 1:42:A:LEU:HD22 | 9        | 0.4           |
| (1,353)  | 1:7:A:MET:HE3   | 1:42:A:LEU:HD23 | 9        | 0.4           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,320)  | 1:53:A:MET:HE1  | 1:57:A:MET:HA   | 9        | 0.4           |
| (1,320)  | 1:53:A:MET:HE2  | 1:57:A:MET:HA   | 9        | 0.4           |
| (1,320)  | 1:53:A:MET:HE3  | 1:57:A:MET:HA   | 9        | 0.4           |
| (1,310)  | 1:53:A:MET:HE1  | 1:61:A:LYS:H    | 2        | 0.4           |
| (1,310)  | 1:53:A:MET:HE2  | 1:61:A:LYS:H    | 2        | 0.4           |
| (1,310)  | 1:53:A:MET:HE3  | 1:61:A:LYS:H    | 2        | 0.4           |
| (1,1446) | 1:45:A:SER:H    | 1:70:A:GLU:HG2  | 1        | 0.39          |
| (1,1446) | 1:45:A:SER:H    | 1:70:A:GLU:HG3  | 1        | 0.39          |
| (1,1166) | 1:4:A:LEU:H     | 1:30:A:GLY:HA3  | 5        | 0.39          |
| (1,1093) | 1:90:A:HIS:HB3  | 1:91:A:SER:H    | 1        | 0.39          |
| (1,983)  | 1:11:A:THR:H    | 1:43:A:CYS:HA   | 4        | 0.39          |
| (1,582)  | 1:10:A:LEU:H    | 1:42:A:LEU:HD21 | 7        | 0.39          |
| (1,582)  | 1:10:A:LEU:H    | 1:42:A:LEU:HD22 | 7        | 0.39          |
| (1,582)  | 1:10:A:LEU:H    | 1:42:A:LEU:HD23 | 7        | 0.39          |
| (1,353)  | 1:7:A:MET:HE1   | 1:42:A:LEU:HD21 | 5        | 0.39          |
| (1,353)  | 1:7:A:MET:HE1   | 1:42:A:LEU:HD22 | 5        | 0.39          |
| (1,353)  | 1:7:A:MET:HE1   | 1:42:A:LEU:HD23 | 5        | 0.39          |
| (1,353)  | 1:7:A:MET:HE2   | 1:42:A:LEU:HD21 | 5        | 0.39          |
| (1,353)  | 1:7:A:MET:HE2   | 1:42:A:LEU:HD22 | 5        | 0.39          |
| (1,353)  | 1:7:A:MET:HE2   | 1:42:A:LEU:HD23 | 5        | 0.39          |
| (1,353)  | 1:7:A:MET:HE3   | 1:42:A:LEU:HD21 | 5        | 0.39          |
| (1,353)  | 1:7:A:MET:HE3   | 1:42:A:LEU:HD22 | 5        | 0.39          |
| (1,353)  | 1:7:A:MET:HE3   | 1:42:A:LEU:HD23 | 5        | 0.39          |
| (1,1485) | 1:52:A:LYS:HD2  | 1:54:A:SER:H    | 3        | 0.38          |
| (1,1485) | 1:52:A:LYS:HD3  | 1:54:A:SER:H    | 3        | 0.38          |
| (1,1384) | 1:18:A:ASN:HD21 | 1:20:A:ASP:H    | 1        | 0.38          |
| (1,1384) | 1:18:A:ASN:HD22 | 1:20:A:ASP:H    | 1        | 0.38          |
| (1,1384) | 1:18:A:ASN:HD21 | 1:20:A:ASP:H    | 3        | 0.38          |
| (1,1384) | 1:18:A:ASN:HD22 | 1:20:A:ASP:H    | 3        | 0.38          |
| (1,1259) | 1:38:A:ASN:HD22 | 1:96:A:GLY:H    | 7        | 0.38          |
| (1,1166) | 1:4:A:LEU:H     | 1:30:A:GLY:HA3  | 9        | 0.38          |
| (1,1134) | 1:91:A:SER:H    | 1:92:A:LEU:HB2  | 6        | 0.38          |
| (1,1093) | 1:90:A:HIS:HB3  | 1:91:A:SER:H    | 3        | 0.38          |
| (1,1093) | 1:90:A:HIS:HB3  | 1:91:A:SER:H    | 4        | 0.38          |
| (1,943)  | 1:75:A:ASP:H    | 1:76:A:VAL:HB   | 9        | 0.38          |
| (1,619)  | 1:38:A:ASN:HD21 | 1:97:A:ALA:H    | 2        | 0.38          |
| (1,607)  | 1:66:A:ARG:H    | 1:97:A:ALA:H    | 1        | 0.38          |
| (1,1062) | 1:7:A:MET:H     | 1:32:A:LYS:H    | 3        | 0.37          |
| (1,1052) | 1:63:A:ALA:H    | 1:65:A:VAL:HG11 | 10       | 0.37          |
| (1,1052) | 1:63:A:ALA:H    | 1:65:A:VAL:HG12 | 10       | 0.37          |
| (1,1052) | 1:63:A:ALA:H    | 1:65:A:VAL:HG13 | 10       | 0.37          |
| (1,1051) | 1:63:A:ALA:H    | 1:65:A:VAL:HG11 | 10       | 0.37          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1051) | 1:63:A:ALA:H    | 1:65:A:VAL:HG12 | 10       | 0.37          |
| (1,1051) | 1:63:A:ALA:H    | 1:65:A:VAL:HG13 | 10       | 0.37          |
| (1,943)  | 1:75:A:ASP:H    | 1:76:A:VAL:HB   | 6        | 0.37          |
| (1,649)  | 1:9:A:ILE:H     | 1:33:A:LEU:HG   | 5        | 0.37          |
| (1,648)  | 1:65:A:VAL:HB   | 1:67:A:VAL:H    | 1        | 0.37          |
| (1,648)  | 1:65:A:VAL:HB   | 1:67:A:VAL:H    | 2        | 0.37          |
| (1,353)  | 1:7:A:MET:HE1   | 1:42:A:LEU:HD21 | 4        | 0.37          |
| (1,353)  | 1:7:A:MET:HE1   | 1:42:A:LEU:HD22 | 4        | 0.37          |
| (1,353)  | 1:7:A:MET:HE1   | 1:42:A:LEU:HD23 | 4        | 0.37          |
| (1,353)  | 1:7:A:MET:HE2   | 1:42:A:LEU:HD21 | 4        | 0.37          |
| (1,353)  | 1:7:A:MET:HE2   | 1:42:A:LEU:HD22 | 4        | 0.37          |
| (1,353)  | 1:7:A:MET:HE2   | 1:42:A:LEU:HD23 | 4        | 0.37          |
| (1,353)  | 1:7:A:MET:HE3   | 1:42:A:LEU:HD21 | 4        | 0.37          |
| (1,353)  | 1:7:A:MET:HE3   | 1:42:A:LEU:HD22 | 4        | 0.37          |
| (1,353)  | 1:7:A:MET:HE3   | 1:42:A:LEU:HD23 | 4        | 0.37          |
| (1,1396) | 1:19:A:LYS:HD2  | 1:21:A:GLU:H    | 9        | 0.36          |
| (1,1396) | 1:19:A:LYS:HD3  | 1:21:A:GLU:H    | 9        | 0.36          |
| (1,1276) | 1:4:A:LEU:HG    | 1:31:A:GLY:H    | 5        | 0.36          |
| (1,900)  | 1:45:A:SER:HB3  | 1:68:A:VAL:H    | 3        | 0.36          |
| (1,756)  | 1:34:A:THR:H    | 1:40:A:ALA:H    | 3        | 0.36          |
| (1,649)  | 1:9:A:ILE:H     | 1:33:A:LEU:HG   | 10       | 0.36          |
| (1,481)  | 1:49:A:GLU:HB3  | 1:57:A:MET:HG3  | 1        | 0.36          |
| (1,1606) | 1:91:A:SER:HB2  | 1:92:A:LEU:HG   | 7        | 0.35          |
| (1,1606) | 1:91:A:SER:HB3  | 1:92:A:LEU:HG   | 7        | 0.35          |
| (1,1344) | 1:9:A:ILE:HG12  | 1:32:A:LYS:HB3  | 1        | 0.35          |
| (1,1344) | 1:9:A:ILE:HG13  | 1:32:A:LYS:HB3  | 1        | 0.35          |
| (1,1344) | 1:9:A:ILE:HG12  | 1:32:A:LYS:HB3  | 8        | 0.35          |
| (1,1344) | 1:9:A:ILE:HG13  | 1:32:A:LYS:HB3  | 8        | 0.35          |
| (1,983)  | 1:11:A:THR:H    | 1:43:A:CYS:HA   | 5        | 0.35          |
| (1,768)  | 1:11:A:THR:HA   | 1:45:A:SER:H    | 4        | 0.35          |
| (1,665)  | 1:65:A:VAL:HG11 | 1:97:A:ALA:H    | 5        | 0.35          |
| (1,665)  | 1:65:A:VAL:HG12 | 1:97:A:ALA:H    | 5        | 0.35          |
| (1,665)  | 1:65:A:VAL:HG13 | 1:97:A:ALA:H    | 5        | 0.35          |
| (1,481)  | 1:49:A:GLU:HB3  | 1:57:A:MET:HG3  | 3        | 0.35          |
| (1,320)  | 1:53:A:MET:HE1  | 1:57:A:MET:HA   | 6        | 0.35          |
| (1,320)  | 1:53:A:MET:HE2  | 1:57:A:MET:HA   | 6        | 0.35          |
| (1,320)  | 1:53:A:MET:HE3  | 1:57:A:MET:HA   | 6        | 0.35          |
| (1,1447) | 1:45:A:SER:HB2  | 1:46:A:THR:H    | 5        | 0.34          |
| (1,1447) | 1:45:A:SER:HB3  | 1:46:A:THR:H    | 5        | 0.34          |
| (1,1384) | 1:18:A:ASN:HD21 | 1:20:A:ASP:H    | 7        | 0.34          |
| (1,1384) | 1:18:A:ASN:HD22 | 1:20:A:ASP:H    | 7        | 0.34          |
| (1,756)  | 1:34:A:THR:H    | 1:40:A:ALA:H    | 1        | 0.34          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,665)  | 1:65:A:VAL:HG11 | 1:97:A:ALA:H    | 9        | 0.34          |
| (1,665)  | 1:65:A:VAL:HG12 | 1:97:A:ALA:H    | 9        | 0.34          |
| (1,665)  | 1:65:A:VAL:HG13 | 1:97:A:ALA:H    | 9        | 0.34          |
| (1,607)  | 1:66:A:ARG:H    | 1:97:A:ALA:H    | 3        | 0.34          |
| (1,607)  | 1:66:A:ARG:H    | 1:97:A:ALA:H    | 6        | 0.34          |
| (1,353)  | 1:7:A:MET:HE1   | 1:42:A:LEU:HD21 | 6        | 0.34          |
| (1,353)  | 1:7:A:MET:HE1   | 1:42:A:LEU:HD22 | 6        | 0.34          |
| (1,353)  | 1:7:A:MET:HE1   | 1:42:A:LEU:HD23 | 6        | 0.34          |
| (1,353)  | 1:7:A:MET:HE2   | 1:42:A:LEU:HD21 | 6        | 0.34          |
| (1,353)  | 1:7:A:MET:HE2   | 1:42:A:LEU:HD22 | 6        | 0.34          |
| (1,353)  | 1:7:A:MET:HE2   | 1:42:A:LEU:HD23 | 6        | 0.34          |
| (1,353)  | 1:7:A:MET:HE3   | 1:42:A:LEU:HD21 | 6        | 0.34          |
| (1,353)  | 1:7:A:MET:HE3   | 1:42:A:LEU:HD22 | 6        | 0.34          |
| (1,353)  | 1:7:A:MET:HE3   | 1:42:A:LEU:HD23 | 6        | 0.34          |
| (1,353)  | 1:7:A:MET:HE1   | 1:42:A:LEU:HD21 | 7        | 0.34          |
| (1,353)  | 1:7:A:MET:HE1   | 1:42:A:LEU:HD22 | 7        | 0.34          |
| (1,353)  | 1:7:A:MET:HE1   | 1:42:A:LEU:HD23 | 7        | 0.34          |
| (1,353)  | 1:7:A:MET:HE2   | 1:42:A:LEU:HD21 | 7        | 0.34          |
| (1,353)  | 1:7:A:MET:HE2   | 1:42:A:LEU:HD22 | 7        | 0.34          |
| (1,353)  | 1:7:A:MET:HE2   | 1:42:A:LEU:HD23 | 7        | 0.34          |
| (1,353)  | 1:7:A:MET:HE3   | 1:42:A:LEU:HD21 | 7        | 0.34          |
| (1,353)  | 1:7:A:MET:HE3   | 1:42:A:LEU:HD22 | 7        | 0.34          |
| (1,353)  | 1:7:A:MET:HE3   | 1:42:A:LEU:HD23 | 7        | 0.34          |
| (1,320)  | 1:53:A:MET:HE1  | 1:57:A:MET:HA   | 1        | 0.34          |
| (1,320)  | 1:53:A:MET:HE2  | 1:57:A:MET:HA   | 1        | 0.34          |
| (1,320)  | 1:53:A:MET:HE3  | 1:57:A:MET:HA   | 1        | 0.34          |
| (1,288)  | 1:53:A:MET:HE1  | 1:61:A:LYS:HE3  | 8        | 0.34          |
| (1,288)  | 1:53:A:MET:HE2  | 1:61:A:LYS:HE3  | 8        | 0.34          |
| (1,288)  | 1:53:A:MET:HE3  | 1:61:A:LYS:HE3  | 8        | 0.34          |
| (1,180)  | 1:15:A:LEU:HA   | 1:46:A:THR:HG21 | 10       | 0.34          |
| (1,180)  | 1:15:A:LEU:HA   | 1:46:A:THR:HG22 | 10       | 0.34          |
| (1,180)  | 1:15:A:LEU:HA   | 1:46:A:THR:HG23 | 10       | 0.34          |
| (1,179)  | 1:15:A:LEU:HA   | 1:46:A:THR:HG21 | 10       | 0.34          |
| (1,179)  | 1:15:A:LEU:HA   | 1:46:A:THR:HG22 | 10       | 0.34          |
| (1,179)  | 1:15:A:LEU:HA   | 1:46:A:THR:HG23 | 10       | 0.34          |
| (1,1344) | 1:9:A:ILE:HG12  | 1:32:A:LYS:HB3  | 6        | 0.33          |
| (1,1344) | 1:9:A:ILE:HG13  | 1:32:A:LYS:HB3  | 6        | 0.33          |
| (1,1062) | 1:7:A:MET:H     | 1:32:A:LYS:H    | 5        | 0.33          |
| (1,1052) | 1:63:A:ALA:H    | 1:65:A:VAL:HG11 | 2        | 0.33          |
| (1,1052) | 1:63:A:ALA:H    | 1:65:A:VAL:HG12 | 2        | 0.33          |
| (1,1052) | 1:63:A:ALA:H    | 1:65:A:VAL:HG13 | 2        | 0.33          |
| (1,1051) | 1:63:A:ALA:H    | 1:65:A:VAL:HG11 | 2        | 0.33          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1051) | 1:63:A:ALA:H    | 1:65:A:VAL:HG12 | 2        | 0.33          |
| (1,1051) | 1:63:A:ALA:H    | 1:65:A:VAL:HG13 | 2        | 0.33          |
| (1,935)  | 1:76:A:VAL:H    | 1:76:A:VAL:HB   | 1        | 0.33          |
| (1,935)  | 1:76:A:VAL:H    | 1:76:A:VAL:HB   | 3        | 0.33          |
| (1,935)  | 1:76:A:VAL:H    | 1:76:A:VAL:HB   | 5        | 0.33          |
| (1,935)  | 1:76:A:VAL:H    | 1:76:A:VAL:HB   | 7        | 0.33          |
| (1,935)  | 1:76:A:VAL:H    | 1:76:A:VAL:HB   | 9        | 0.33          |
| (1,935)  | 1:76:A:VAL:H    | 1:76:A:VAL:HB   | 10       | 0.33          |
| (1,665)  | 1:65:A:VAL:HG11 | 1:97:A:ALA:H    | 3        | 0.33          |
| (1,665)  | 1:65:A:VAL:HG12 | 1:97:A:ALA:H    | 3        | 0.33          |
| (1,665)  | 1:65:A:VAL:HG13 | 1:97:A:ALA:H    | 3        | 0.33          |
| (1,665)  | 1:65:A:VAL:HG11 | 1:97:A:ALA:H    | 4        | 0.33          |
| (1,665)  | 1:65:A:VAL:HG12 | 1:97:A:ALA:H    | 4        | 0.33          |
| (1,665)  | 1:65:A:VAL:HG13 | 1:97:A:ALA:H    | 4        | 0.33          |
| (1,320)  | 1:53:A:MET:HE1  | 1:57:A:MET:HA   | 5        | 0.33          |
| (1,320)  | 1:53:A:MET:HE2  | 1:57:A:MET:HA   | 5        | 0.33          |
| (1,320)  | 1:53:A:MET:HE3  | 1:57:A:MET:HA   | 5        | 0.33          |
| (1,1485) | 1:52:A:LYS:HD2  | 1:54:A:SER:H    | 2        | 0.32          |
| (1,1485) | 1:52:A:LYS:HD3  | 1:54:A:SER:H    | 2        | 0.32          |
| (1,935)  | 1:76:A:VAL:H    | 1:76:A:VAL:HB   | 2        | 0.32          |
| (1,935)  | 1:76:A:VAL:H    | 1:76:A:VAL:HB   | 4        | 0.32          |
| (1,935)  | 1:76:A:VAL:H    | 1:76:A:VAL:HB   | 6        | 0.32          |
| (1,935)  | 1:76:A:VAL:H    | 1:76:A:VAL:HB   | 8        | 0.32          |
| (1,926)  | 1:74:A:GLN:HG2  | 1:75:A:ASP:H    | 9        | 0.32          |
| (1,799)  | 1:70:A:GLU:H    | 1:70:A:GLU:HB3  | 8        | 0.32          |
| (1,1447) | 1:45:A:SER:HB2  | 1:46:A:THR:H    | 7        | 0.31          |
| (1,1447) | 1:45:A:SER:HB3  | 1:46:A:THR:H    | 7        | 0.31          |
| (1,1344) | 1:9:A:ILE:HG12  | 1:32:A:LYS:HB3  | 5        | 0.31          |
| (1,1344) | 1:9:A:ILE:HG13  | 1:32:A:LYS:HB3  | 5        | 0.31          |
| (1,1047) | 1:10:A:LEU:HD11 | 1:34:A:THR:H    | 2        | 0.31          |
| (1,1047) | 1:10:A:LEU:HD12 | 1:34:A:THR:H    | 2        | 0.31          |
| (1,1047) | 1:10:A:LEU:HD13 | 1:34:A:THR:H    | 2        | 0.31          |
| (1,799)  | 1:70:A:GLU:H    | 1:70:A:GLU:HB3  | 6        | 0.31          |
| (1,320)  | 1:53:A:MET:HE1  | 1:57:A:MET:HA   | 4        | 0.31          |
| (1,320)  | 1:53:A:MET:HE2  | 1:57:A:MET:HA   | 4        | 0.31          |
| (1,320)  | 1:53:A:MET:HE3  | 1:57:A:MET:HA   | 4        | 0.31          |
| (1,320)  | 1:53:A:MET:HE1  | 1:57:A:MET:HA   | 7        | 0.31          |
| (1,320)  | 1:53:A:MET:HE2  | 1:57:A:MET:HA   | 7        | 0.31          |
| (1,320)  | 1:53:A:MET:HE3  | 1:57:A:MET:HA   | 7        | 0.31          |
| (1,1446) | 1:45:A:SER:H    | 1:70:A:GLU:HG2  | 9        | 0.3           |
| (1,1446) | 1:45:A:SER:H    | 1:70:A:GLU:HG3  | 9        | 0.3           |
| (1,683)  | 1:12:A:LEU:H    | 1:43:A:CYS:HA   | 10       | 0.3           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,648)  | 1:65:A:VAL:HB   | 1:67:A:VAL:H    | 3        | 0.3           |
| (1,1606) | 1:91:A:SER:HB2  | 1:92:A:LEU:HG   | 10       | 0.29          |
| (1,1606) | 1:91:A:SER:HB3  | 1:92:A:LEU:HG   | 10       | 0.29          |
| (1,1419) | 1:25:A:MET:HG2  | 1:74:A:GLN:HE21 | 9        | 0.29          |
| (1,1419) | 1:25:A:MET:HG2  | 1:74:A:GLN:HE22 | 9        | 0.29          |
| (1,1137) | 1:41:A:SER:H    | 1:42:A:LEU:HD21 | 8        | 0.29          |
| (1,1137) | 1:41:A:SER:H    | 1:42:A:LEU:HD22 | 8        | 0.29          |
| (1,1137) | 1:41:A:SER:H    | 1:42:A:LEU:HD23 | 8        | 0.29          |
| (1,1136) | 1:41:A:SER:H    | 1:42:A:LEU:HD21 | 8        | 0.29          |
| (1,1136) | 1:41:A:SER:H    | 1:42:A:LEU:HD22 | 8        | 0.29          |
| (1,1136) | 1:41:A:SER:H    | 1:42:A:LEU:HD23 | 8        | 0.29          |
| (1,926)  | 1:74:A:GLN:HG2  | 1:75:A:ASP:H    | 6        | 0.29          |
| (1,799)  | 1:70:A:GLU:H    | 1:70:A:GLU:HB3  | 10       | 0.29          |
| (1,737)  | 1:15:A:LEU:HD11 | 1:22:A:ALA:H    | 8        | 0.29          |
| (1,737)  | 1:15:A:LEU:HD12 | 1:22:A:ALA:H    | 8        | 0.29          |
| (1,737)  | 1:15:A:LEU:HD13 | 1:22:A:ALA:H    | 8        | 0.29          |
| (1,736)  | 1:15:A:LEU:HD11 | 1:22:A:ALA:H    | 8        | 0.29          |
| (1,736)  | 1:15:A:LEU:HD12 | 1:22:A:ALA:H    | 8        | 0.29          |
| (1,736)  | 1:15:A:LEU:HD13 | 1:22:A:ALA:H    | 8        | 0.29          |
| (1,649)  | 1:9:A:ILE:H     | 1:33:A:LEU:HG   | 9        | 0.29          |
| (1,607)  | 1:66:A:ARG:H    | 1:97:A:ALA:H    | 9        | 0.29          |
| (1,347)  | 1:25:A:MET:HE1  | 1:29:A:LEU:HD21 | 6        | 0.29          |
| (1,347)  | 1:25:A:MET:HE1  | 1:29:A:LEU:HD22 | 6        | 0.29          |
| (1,347)  | 1:25:A:MET:HE1  | 1:29:A:LEU:HD23 | 6        | 0.29          |
| (1,347)  | 1:25:A:MET:HE2  | 1:29:A:LEU:HD21 | 6        | 0.29          |
| (1,347)  | 1:25:A:MET:HE2  | 1:29:A:LEU:HD22 | 6        | 0.29          |
| (1,347)  | 1:25:A:MET:HE2  | 1:29:A:LEU:HD23 | 6        | 0.29          |
| (1,347)  | 1:25:A:MET:HE3  | 1:29:A:LEU:HD21 | 6        | 0.29          |
| (1,347)  | 1:25:A:MET:HE3  | 1:29:A:LEU:HD22 | 6        | 0.29          |
| (1,347)  | 1:25:A:MET:HE3  | 1:29:A:LEU:HD23 | 6        | 0.29          |
| (1,129)  | 1:42:A:LEU:HD11 | 1:43:A:CYS:H    | 5        | 0.29          |
| (1,129)  | 1:42:A:LEU:HD12 | 1:43:A:CYS:H    | 5        | 0.29          |
| (1,129)  | 1:42:A:LEU:HD13 | 1:43:A:CYS:H    | 5        | 0.29          |
| (1,109)  | 1:28:A:LYS:HG3  | 1:29:A:LEU:HA   | 10       | 0.29          |
| (1,1093) | 1:90:A:HIS:HB3  | 1:91:A:SER:H    | 2        | 0.28          |
| (1,1052) | 1:63:A:ALA:H    | 1:65:A:VAL:HG11 | 5        | 0.28          |
| (1,1052) | 1:63:A:ALA:H    | 1:65:A:VAL:HG12 | 5        | 0.28          |
| (1,1052) | 1:63:A:ALA:H    | 1:65:A:VAL:HG13 | 5        | 0.28          |
| (1,1051) | 1:63:A:ALA:H    | 1:65:A:VAL:HG11 | 5        | 0.28          |
| (1,1051) | 1:63:A:ALA:H    | 1:65:A:VAL:HG12 | 5        | 0.28          |
| (1,1051) | 1:63:A:ALA:H    | 1:65:A:VAL:HG13 | 5        | 0.28          |
| (1,983)  | 1:11:A:THR:H    | 1:43:A:CYS:HA   | 9        | 0.28          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,907)  | 1:72:A:PHE:HB2  | 1:76:A:VAL:H    | 6        | 0.28          |
| (1,621)  | 1:38:A:ASN:HD22 | 1:97:A:ALA:H    | 8        | 0.28          |
| (1,505)  | 1:22:A:ALA:HA   | 1:25:A:MET:HA   | 10       | 0.28          |
| (1,1344) | 1:9:A:ILE:HG12  | 1:32:A:LYS:HB3  | 7        | 0.27          |
| (1,1344) | 1:9:A:ILE:HG13  | 1:32:A:LYS:HB3  | 7        | 0.27          |
| (1,1252) | 1:92:A:LEU:HD11 | 1:93:A:SER:H    | 9        | 0.27          |
| (1,1252) | 1:92:A:LEU:HD12 | 1:93:A:SER:H    | 9        | 0.27          |
| (1,1252) | 1:92:A:LEU:HD13 | 1:93:A:SER:H    | 9        | 0.27          |
| (1,1028) | 1:23:A:LYS:H    | 1:23:A:LYS:HB3  | 10       | 0.27          |
| (1,799)  | 1:70:A:GLU:H    | 1:70:A:GLU:HB3  | 4        | 0.27          |
| (1,765)  | 1:38:A:ASN:HD22 | 1:98:A:GLU:H    | 3        | 0.27          |
| (1,590)  | 1:42:A:LEU:HA   | 1:44:A:ILE:H    | 6        | 0.27          |
| (1,109)  | 1:28:A:LYS:HG3  | 1:29:A:LEU:HA   | 1        | 0.27          |
| (1,1447) | 1:45:A:SER:HB2  | 1:46:A:THR:H    | 8        | 0.26          |
| (1,1447) | 1:45:A:SER:HB3  | 1:46:A:THR:H    | 8        | 0.26          |
| (1,1396) | 1:19:A:LYS:HD2  | 1:21:A:GLU:H    | 10       | 0.26          |
| (1,1396) | 1:19:A:LYS:HD3  | 1:21:A:GLU:H    | 10       | 0.26          |
| (1,1346) | 1:12:A:LEU:H    | 1:45:A:SER:HB2  | 4        | 0.26          |
| (1,1346) | 1:12:A:LEU:H    | 1:45:A:SER:HB3  | 4        | 0.26          |
| (1,1344) | 1:9:A:ILE:HG12  | 1:32:A:LYS:HB3  | 9        | 0.26          |
| (1,1344) | 1:9:A:ILE:HG13  | 1:32:A:LYS:HB3  | 9        | 0.26          |
| (1,1252) | 1:92:A:LEU:HD11 | 1:93:A:SER:H    | 6        | 0.26          |
| (1,1252) | 1:92:A:LEU:HD12 | 1:93:A:SER:H    | 6        | 0.26          |
| (1,1252) | 1:92:A:LEU:HD13 | 1:93:A:SER:H    | 6        | 0.26          |
| (1,1052) | 1:63:A:ALA:H    | 1:65:A:VAL:HG11 | 3        | 0.26          |
| (1,1052) | 1:63:A:ALA:H    | 1:65:A:VAL:HG12 | 3        | 0.26          |
| (1,1052) | 1:63:A:ALA:H    | 1:65:A:VAL:HG13 | 3        | 0.26          |
| (1,1051) | 1:63:A:ALA:H    | 1:65:A:VAL:HG11 | 3        | 0.26          |
| (1,1051) | 1:63:A:ALA:H    | 1:65:A:VAL:HG12 | 3        | 0.26          |
| (1,1051) | 1:63:A:ALA:H    | 1:65:A:VAL:HG13 | 3        | 0.26          |
| (1,1028) | 1:23:A:LYS:H    | 1:23:A:LYS:HB3  | 6        | 0.26          |
| (1,683)  | 1:12:A:LEU:H    | 1:43:A:CYS:HA   | 3        | 0.26          |
| (1,458)  | 1:25:A:MET:HA   | 1:28:A:LYS:HG2  | 6        | 0.26          |
| (1,446)  | 1:4:A:LEU:HD11  | 1:7:A:MET:HB2   | 9        | 0.26          |
| (1,446)  | 1:4:A:LEU:HD12  | 1:7:A:MET:HB2   | 9        | 0.26          |
| (1,446)  | 1:4:A:LEU:HD13  | 1:7:A:MET:HB2   | 9        | 0.26          |
| (1,1606) | 1:91:A:SER:HB2  | 1:92:A:LEU:HG   | 4        | 0.25          |
| (1,1606) | 1:91:A:SER:HB3  | 1:92:A:LEU:HG   | 4        | 0.25          |
| (1,1047) | 1:10:A:LEU:HD11 | 1:34:A:THR:H    | 8        | 0.25          |
| (1,1047) | 1:10:A:LEU:HD12 | 1:34:A:THR:H    | 8        | 0.25          |
| (1,1047) | 1:10:A:LEU:HD13 | 1:34:A:THR:H    | 8        | 0.25          |
| (1,1028) | 1:23:A:LYS:H    | 1:23:A:LYS:HB3  | 4        | 0.25          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,983)  | 1:11:A:THR:H    | 1:43:A:CYS:HA   | 2        | 0.25          |
| (1,983)  | 1:11:A:THR:H    | 1:43:A:CYS:HA   | 8        | 0.25          |
| (1,666)  | 1:65:A:VAL:HG21 | 1:97:A:ALA:H    | 7        | 0.25          |
| (1,666)  | 1:65:A:VAL:HG22 | 1:97:A:ALA:H    | 7        | 0.25          |
| (1,666)  | 1:65:A:VAL:HG23 | 1:97:A:ALA:H    | 7        | 0.25          |
| (1,634)  | 1:69:A:CYS:HB2  | 1:92:A:LEU:H    | 7        | 0.25          |
| (1,621)  | 1:38:A:ASN:HD22 | 1:97:A:ALA:H    | 10       | 0.25          |
| (1,310)  | 1:53:A:MET:HE1  | 1:61:A:LYS:H    | 9        | 0.25          |
| (1,310)  | 1:53:A:MET:HE2  | 1:61:A:LYS:H    | 9        | 0.25          |
| (1,310)  | 1:53:A:MET:HE3  | 1:61:A:LYS:H    | 9        | 0.25          |
| (1,281)  | 1:72:A:PHE:HB2  | 1:86:A:LEU:HB3  | 5        | 0.25          |
| (1,1028) | 1:23:A:LYS:H    | 1:23:A:LYS:HB3  | 2        | 0.24          |
| (1,1028) | 1:23:A:LYS:H    | 1:23:A:LYS:HB3  | 7        | 0.24          |
| (1,983)  | 1:11:A:THR:H    | 1:43:A:CYS:HA   | 1        | 0.24          |
| (1,900)  | 1:45:A:SER:HB3  | 1:68:A:VAL:H    | 6        | 0.24          |
| (1,790)  | 1:50:A:VAL:H    | 1:57:A:MET:HG3  | 3        | 0.24          |
| (1,768)  | 1:11:A:THR:HA   | 1:45:A:SER:H    | 3        | 0.24          |
| (1,768)  | 1:11:A:THR:HA   | 1:45:A:SER:H    | 7        | 0.24          |
| (1,602)  | 1:15:A:LEU:H    | 1:15:A:LEU:HD21 | 1        | 0.24          |
| (1,602)  | 1:15:A:LEU:H    | 1:15:A:LEU:HD22 | 1        | 0.24          |
| (1,602)  | 1:15:A:LEU:H    | 1:15:A:LEU:HD23 | 1        | 0.24          |
| (1,601)  | 1:15:A:LEU:H    | 1:15:A:LEU:HD21 | 1        | 0.24          |
| (1,601)  | 1:15:A:LEU:H    | 1:15:A:LEU:HD22 | 1        | 0.24          |
| (1,601)  | 1:15:A:LEU:H    | 1:15:A:LEU:HD23 | 1        | 0.24          |
| (1,590)  | 1:42:A:LEU:HA   | 1:44:A:ILE:H    | 7        | 0.24          |
| (1,288)  | 1:53:A:MET:HE1  | 1:61:A:LYS:HE3  | 7        | 0.24          |
| (1,288)  | 1:53:A:MET:HE2  | 1:61:A:LYS:HE3  | 7        | 0.24          |
| (1,288)  | 1:53:A:MET:HE3  | 1:61:A:LYS:HE3  | 7        | 0.24          |
| (1,281)  | 1:72:A:PHE:HB2  | 1:86:A:LEU:HB3  | 4        | 0.24          |
| (1,1606) | 1:91:A:SER:HB2  | 1:92:A:LEU:HG   | 6        | 0.23          |
| (1,1606) | 1:91:A:SER:HB3  | 1:92:A:LEU:HG   | 6        | 0.23          |
| (1,1028) | 1:23:A:LYS:H    | 1:23:A:LYS:HB3  | 3        | 0.23          |
| (1,1028) | 1:23:A:LYS:H    | 1:23:A:LYS:HB3  | 5        | 0.23          |
| (1,1028) | 1:23:A:LYS:H    | 1:23:A:LYS:HB3  | 8        | 0.23          |
| (1,900)  | 1:45:A:SER:HB3  | 1:68:A:VAL:H    | 10       | 0.23          |
| (1,893)  | 1:79:A:SER:HB2  | 1:81:A:LYS:H    | 7        | 0.23          |
| (1,304)  | 1:50:A:VAL:H    | 1:53:A:MET:HE1  | 4        | 0.23          |
| (1,304)  | 1:50:A:VAL:H    | 1:53:A:MET:HE2  | 4        | 0.23          |
| (1,304)  | 1:50:A:VAL:H    | 1:53:A:MET:HE3  | 4        | 0.23          |
| (1,304)  | 1:50:A:VAL:H    | 1:53:A:MET:HE1  | 7        | 0.23          |
| (1,304)  | 1:50:A:VAL:H    | 1:53:A:MET:HE2  | 7        | 0.23          |
| (1,304)  | 1:50:A:VAL:H    | 1:53:A:MET:HE3  | 7        | 0.23          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1606) | 1:91:A:SER:HB2  | 1:92:A:LEU:HG   | 8        | 0.22          |
| (1,1606) | 1:91:A:SER:HB3  | 1:92:A:LEU:HG   | 8        | 0.22          |
| (1,1426) | 1:28:A:LYS:HD2  | 1:29:A:LEU:H    | 6        | 0.22          |
| (1,1426) | 1:28:A:LYS:HD3  | 1:29:A:LEU:H    | 6        | 0.22          |
| (1,1127) | 1:28:A:LYS:HD2  | 1:29:A:LEU:H    | 6        | 0.22          |
| (1,907)  | 1:72:A:PHE:HB2  | 1:76:A:VAL:H    | 4        | 0.22          |
| (1,790)  | 1:50:A:VAL:H    | 1:57:A:MET:HG3  | 5        | 0.22          |
| (1,683)  | 1:12:A:LEU:H    | 1:43:A:CYS:HA   | 2        | 0.22          |
| (1,607)  | 1:66:A:ARG:H    | 1:97:A:ALA:H    | 4        | 0.22          |
| (1,157)  | 1:68:A:VAL:H    | 1:92:A:LEU:HD21 | 10       | 0.22          |
| (1,157)  | 1:68:A:VAL:H    | 1:92:A:LEU:HD22 | 10       | 0.22          |
| (1,157)  | 1:68:A:VAL:H    | 1:92:A:LEU:HD23 | 10       | 0.22          |
| (1,156)  | 1:68:A:VAL:H    | 1:92:A:LEU:HD21 | 10       | 0.22          |
| (1,156)  | 1:68:A:VAL:H    | 1:92:A:LEU:HD22 | 10       | 0.22          |
| (1,156)  | 1:68:A:VAL:H    | 1:92:A:LEU:HD23 | 10       | 0.22          |
| (1,129)  | 1:42:A:LEU:HD11 | 1:43:A:CYS:H    | 6        | 0.22          |
| (1,129)  | 1:42:A:LEU:HD12 | 1:43:A:CYS:H    | 6        | 0.22          |
| (1,129)  | 1:42:A:LEU:HD13 | 1:43:A:CYS:H    | 6        | 0.22          |
| (1,1446) | 1:45:A:SER:H    | 1:70:A:GLU:HG2  | 7        | 0.21          |
| (1,1446) | 1:45:A:SER:H    | 1:70:A:GLU:HG3  | 7        | 0.21          |
| (1,1028) | 1:23:A:LYS:H    | 1:23:A:LYS:HB3  | 1        | 0.21          |
| (1,983)  | 1:11:A:THR:H    | 1:43:A:CYS:HA   | 6        | 0.21          |
| (1,983)  | 1:11:A:THR:H    | 1:43:A:CYS:HA   | 7        | 0.21          |
| (1,907)  | 1:72:A:PHE:HB2  | 1:76:A:VAL:H    | 8        | 0.21          |
| (1,505)  | 1:22:A:ALA:HA   | 1:25:A:MET:HA   | 9        | 0.21          |
| (1,481)  | 1:49:A:GLU:HB3  | 1:57:A:MET:HG3  | 10       | 0.21          |
| (1,476)  | 1:69:A:CYS:HB3  | 1:71:A:ASP:HA   | 6        | 0.21          |
| (1,1606) | 1:91:A:SER:HB2  | 1:92:A:LEU:HG   | 1        | 0.2           |
| (1,1606) | 1:91:A:SER:HB3  | 1:92:A:LEU:HG   | 1        | 0.2           |
| (1,1485) | 1:52:A:LYS:HD2  | 1:54:A:SER:H    | 1        | 0.2           |
| (1,1485) | 1:52:A:LYS:HD3  | 1:54:A:SER:H    | 1        | 0.2           |
| (1,1447) | 1:45:A:SER:HB2  | 1:46:A:THR:H    | 9        | 0.2           |
| (1,1447) | 1:45:A:SER:HB3  | 1:46:A:THR:H    | 9        | 0.2           |
| (1,1215) | 1:5:A:SER:H     | 1:31:A:GLY:HA2  | 6        | 0.2           |
| (1,1052) | 1:63:A:ALA:H    | 1:65:A:VAL:HG11 | 7        | 0.2           |
| (1,1052) | 1:63:A:ALA:H    | 1:65:A:VAL:HG12 | 7        | 0.2           |
| (1,1052) | 1:63:A:ALA:H    | 1:65:A:VAL:HG13 | 7        | 0.2           |
| (1,1051) | 1:63:A:ALA:H    | 1:65:A:VAL:HG11 | 7        | 0.2           |
| (1,1051) | 1:63:A:ALA:H    | 1:65:A:VAL:HG12 | 7        | 0.2           |
| (1,1051) | 1:63:A:ALA:H    | 1:65:A:VAL:HG13 | 7        | 0.2           |
| (1,907)  | 1:72:A:PHE:HB2  | 1:76:A:VAL:H    | 10       | 0.2           |
| (1,783)  | 1:57:A:MET:HG3  | 1:58:A:GLU:H    | 4        | 0.2           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,648)  | 1:65:A:VAL:HB   | 1:67:A:VAL:H    | 10       | 0.2           |
| (1,1606) | 1:91:A:SER:HB2  | 1:92:A:LEU:HG   | 2        | 0.19          |
| (1,1606) | 1:91:A:SER:HB3  | 1:92:A:LEU:HG   | 2        | 0.19          |
| (1,1547) | 1:73:A:LEU:HB3  | 1:77:A:SER:HB2  | 2        | 0.19          |
| (1,1547) | 1:73:A:LEU:HB3  | 1:77:A:SER:HB3  | 2        | 0.19          |
| (1,1384) | 1:18:A:ASN:HD21 | 1:20:A:ASP:H    | 9        | 0.19          |
| (1,1384) | 1:18:A:ASN:HD22 | 1:20:A:ASP:H    | 9        | 0.19          |
| (1,1241) | 1:66:A:ARG:HA   | 1:93:A:SER:H    | 5        | 0.19          |
| (1,1224) | 1:38:A:ASN:HD21 | 1:97:A:ALA:HB1  | 3        | 0.19          |
| (1,1224) | 1:38:A:ASN:HD21 | 1:97:A:ALA:HB2  | 3        | 0.19          |
| (1,1224) | 1:38:A:ASN:HD21 | 1:97:A:ALA:HB3  | 3        | 0.19          |
| (1,1125) | 1:83:A:LEU:HG   | 1:84:A:GLN:H    | 5        | 0.19          |
| (1,893)  | 1:79:A:SER:HB2  | 1:81:A:LYS:H    | 5        | 0.19          |
| (1,790)  | 1:50:A:VAL:H    | 1:57:A:MET:HG3  | 8        | 0.19          |
| (1,790)  | 1:50:A:VAL:H    | 1:57:A:MET:HG3  | 10       | 0.19          |
| (1,768)  | 1:11:A:THR:HA   | 1:45:A:SER:H    | 8        | 0.19          |
| (1,621)  | 1:38:A:ASN:HD22 | 1:97:A:ALA:H    | 2        | 0.19          |
| (1,590)  | 1:42:A:LEU:HA   | 1:44:A:ILE:H    | 4        | 0.19          |
| (1,292)  | 1:9:A:ILE:HG21  | 1:42:A:LEU:HD21 | 4        | 0.19          |
| (1,292)  | 1:9:A:ILE:HG21  | 1:42:A:LEU:HD22 | 4        | 0.19          |
| (1,292)  | 1:9:A:ILE:HG21  | 1:42:A:LEU:HD23 | 4        | 0.19          |
| (1,292)  | 1:9:A:ILE:HG22  | 1:42:A:LEU:HD21 | 4        | 0.19          |
| (1,292)  | 1:9:A:ILE:HG22  | 1:42:A:LEU:HD22 | 4        | 0.19          |
| (1,292)  | 1:9:A:ILE:HG22  | 1:42:A:LEU:HD23 | 4        | 0.19          |
| (1,292)  | 1:9:A:ILE:HG23  | 1:42:A:LEU:HD21 | 4        | 0.19          |
| (1,292)  | 1:9:A:ILE:HG23  | 1:42:A:LEU:HD22 | 4        | 0.19          |
| (1,292)  | 1:9:A:ILE:HG23  | 1:42:A:LEU:HD23 | 4        | 0.19          |
| (1,291)  | 1:9:A:ILE:HG21  | 1:42:A:LEU:HD21 | 4        | 0.19          |
| (1,291)  | 1:9:A:ILE:HG21  | 1:42:A:LEU:HD22 | 4        | 0.19          |
| (1,291)  | 1:9:A:ILE:HG21  | 1:42:A:LEU:HD23 | 4        | 0.19          |
| (1,291)  | 1:9:A:ILE:HG22  | 1:42:A:LEU:HD21 | 4        | 0.19          |
| (1,291)  | 1:9:A:ILE:HG22  | 1:42:A:LEU:HD22 | 4        | 0.19          |
| (1,291)  | 1:9:A:ILE:HG22  | 1:42:A:LEU:HD23 | 4        | 0.19          |
| (1,291)  | 1:9:A:ILE:HG23  | 1:42:A:LEU:HD21 | 4        | 0.19          |
| (1,291)  | 1:9:A:ILE:HG23  | 1:42:A:LEU:HD22 | 4        | 0.19          |
| (1,291)  | 1:9:A:ILE:HG23  | 1:42:A:LEU:HD23 | 4        | 0.19          |
| (1,1301) | 1:4:A:LEU:HB3   | 1:30:A:GLY:H    | 7        | 0.18          |
| (1,1127) | 1:28:A:LYS:HD2  | 1:29:A:LEU:H    | 3        | 0.18          |
| (1,1062) | 1:7:A:MET:H     | 1:32:A:LYS:H    | 6        | 0.18          |
| (1,764)  | 1:38:A:ASN:HD21 | 1:40:A:ALA:H    | 7        | 0.18          |
| (1,737)  | 1:15:A:LEU:HD11 | 1:22:A:ALA:H    | 9        | 0.18          |
| (1,737)  | 1:15:A:LEU:HD12 | 1:22:A:ALA:H    | 9        | 0.18          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,737)  | 1:15:A:LEU:HD13 | 1:22:A:ALA:H    | 9        | 0.18          |
| (1,736)  | 1:15:A:LEU:HD11 | 1:22:A:ALA:H    | 9        | 0.18          |
| (1,736)  | 1:15:A:LEU:HD12 | 1:22:A:ALA:H    | 9        | 0.18          |
| (1,736)  | 1:15:A:LEU:HD13 | 1:22:A:ALA:H    | 9        | 0.18          |
| (1,590)  | 1:42:A:LEU:HA   | 1:44:A:ILE:H    | 8        | 0.18          |
| (1,304)  | 1:50:A:VAL:H    | 1:53:A:MET:HE1  | 9        | 0.18          |
| (1,304)  | 1:50:A:VAL:H    | 1:53:A:MET:HE2  | 9        | 0.18          |
| (1,304)  | 1:50:A:VAL:H    | 1:53:A:MET:HE3  | 9        | 0.18          |
| (1,296)  | 1:53:A:MET:HE1  | 1:54:A:SER:H    | 4        | 0.18          |
| (1,296)  | 1:53:A:MET:HE2  | 1:54:A:SER:H    | 4        | 0.18          |
| (1,296)  | 1:53:A:MET:HE3  | 1:54:A:SER:H    | 4        | 0.18          |
| (1,1617) | 1:97:A:ALA:HA   | 1:98:A:GLU:HB2  | 9        | 0.17          |
| (1,1617) | 1:97:A:ALA:HA   | 1:98:A:GLU:HB3  | 9        | 0.17          |
| (1,1359) | 1:16:A:SER:H    | 1:70:A:GLU:HG2  | 2        | 0.17          |
| (1,1359) | 1:16:A:SER:H    | 1:70:A:GLU:HG3  | 2        | 0.17          |
| (1,1346) | 1:12:A:LEU:H    | 1:45:A:SER:HB2  | 3        | 0.17          |
| (1,1346) | 1:12:A:LEU:H    | 1:45:A:SER:HB3  | 3        | 0.17          |
| (1,1301) | 1:4:A:LEU:HB3   | 1:30:A:GLY:H    | 9        | 0.17          |
| (1,1215) | 1:5:A:SER:H     | 1:31:A:GLY:HA2  | 10       | 0.17          |
| (1,1166) | 1:4:A:LEU:H     | 1:30:A:GLY:HA3  | 3        | 0.17          |
| (1,1027) | 1:23:A:LYS:H    | 1:23:A:LYS:HB2  | 9        | 0.17          |
| (1,926)  | 1:74:A:GLN:HG2  | 1:75:A:ASP:H    | 5        | 0.17          |
| (1,907)  | 1:72:A:PHE:HB2  | 1:76:A:VAL:H    | 1        | 0.17          |
| (1,783)  | 1:57:A:MET:HG3  | 1:58:A:GLU:H    | 5        | 0.17          |
| (1,649)  | 1:9:A:ILE:H     | 1:33:A:LEU:HG   | 4        | 0.17          |
| (1,602)  | 1:15:A:LEU:H    | 1:15:A:LEU:HD21 | 3        | 0.17          |
| (1,602)  | 1:15:A:LEU:H    | 1:15:A:LEU:HD22 | 3        | 0.17          |
| (1,602)  | 1:15:A:LEU:H    | 1:15:A:LEU:HD23 | 3        | 0.17          |
| (1,601)  | 1:15:A:LEU:H    | 1:15:A:LEU:HD21 | 3        | 0.17          |
| (1,601)  | 1:15:A:LEU:H    | 1:15:A:LEU:HD22 | 3        | 0.17          |
| (1,601)  | 1:15:A:LEU:H    | 1:15:A:LEU:HD23 | 3        | 0.17          |
| (1,590)  | 1:42:A:LEU:HA   | 1:44:A:ILE:H    | 3        | 0.17          |
| (1,310)  | 1:53:A:MET:HE1  | 1:61:A:LYS:H    | 8        | 0.17          |
| (1,310)  | 1:53:A:MET:HE2  | 1:61:A:LYS:H    | 8        | 0.17          |
| (1,310)  | 1:53:A:MET:HE3  | 1:61:A:LYS:H    | 8        | 0.17          |
| (1,109)  | 1:28:A:LYS:HG3  | 1:29:A:LEU:HA   | 7        | 0.17          |
| (1,1447) | 1:45:A:SER:HB2  | 1:46:A:THR:H    | 1        | 0.16          |
| (1,1447) | 1:45:A:SER:HB3  | 1:46:A:THR:H    | 1        | 0.16          |
| (1,1301) | 1:4:A:LEU:HB3   | 1:30:A:GLY:H    | 3        | 0.16          |
| (1,790)  | 1:50:A:VAL:H    | 1:57:A:MET:HG3  | 2        | 0.16          |
| (1,607)  | 1:66:A:ARG:H    | 1:97:A:ALA:H    | 5        | 0.16          |
| (1,310)  | 1:53:A:MET:HE1  | 1:61:A:LYS:H    | 1        | 0.16          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,310)  | 1:53:A:MET:HE2  | 1:61:A:LYS:H    | 1        | 0.16          |
| (1,310)  | 1:53:A:MET:HE3  | 1:61:A:LYS:H    | 1        | 0.16          |
| (1,180)  | 1:15:A:LEU:HA   | 1:46:A:THR:HG21 | 7        | 0.16          |
| (1,180)  | 1:15:A:LEU:HA   | 1:46:A:THR:HG22 | 7        | 0.16          |
| (1,180)  | 1:15:A:LEU:HA   | 1:46:A:THR:HG23 | 7        | 0.16          |
| (1,179)  | 1:15:A:LEU:HA   | 1:46:A:THR:HG21 | 7        | 0.16          |
| (1,179)  | 1:15:A:LEU:HA   | 1:46:A:THR:HG22 | 7        | 0.16          |
| (1,179)  | 1:15:A:LEU:HA   | 1:46:A:THR:HG23 | 7        | 0.16          |
| (1,7)    | 1:15:A:LEU:HG   | 1:70:A:GLU:HB3  | 9        | 0.16          |
| (1,1426) | 1:28:A:LYS:HD2  | 1:29:A:LEU:H    | 2        | 0.15          |
| (1,1426) | 1:28:A:LYS:HD3  | 1:29:A:LEU:H    | 2        | 0.15          |
| (1,1293) | 1:30:A:GLY:H    | 1:31:A:GLY:H    | 4        | 0.15          |
| (1,1276) | 1:4:A:LEU:HG    | 1:31:A:GLY:H    | 10       | 0.15          |
| (1,1166) | 1:4:A:LEU:H     | 1:30:A:GLY:HA3  | 6        | 0.15          |
| (1,963)  | 1:6:A:ASN:H     | 1:7:A:MET:H     | 10       | 0.15          |
| (1,930)  | 1:68:A:VAL:H    | 1:92:A:LEU:HG   | 9        | 0.15          |
| (1,789)  | 1:71:A:ASP:H    | 1:72:A:PHE:HB3  | 4        | 0.15          |
| (1,783)  | 1:57:A:MET:HG3  | 1:58:A:GLU:H    | 7        | 0.15          |
| (1,768)  | 1:11:A:THR:HA   | 1:45:A:SER:H    | 9        | 0.15          |
| (1,619)  | 1:38:A:ASN:HD21 | 1:97:A:ALA:H    | 4        | 0.15          |
| (1,1617) | 1:97:A:ALA:HA   | 1:98:A:GLU:HB2  | 7        | 0.14          |
| (1,1617) | 1:97:A:ALA:HA   | 1:98:A:GLU:HB3  | 7        | 0.14          |
| (1,1479) | 1:51:A:GLU:HB2  | 1:52:A:LYS:HD2  | 7        | 0.14          |
| (1,1479) | 1:51:A:GLU:HB2  | 1:52:A:LYS:HD3  | 7        | 0.14          |
| (1,1479) | 1:51:A:GLU:HB3  | 1:52:A:LYS:HD2  | 7        | 0.14          |
| (1,1479) | 1:51:A:GLU:HB3  | 1:52:A:LYS:HD3  | 7        | 0.14          |
| (1,1395) | 1:19:A:LYS:HD2  | 1:20:A:ASP:HA   | 8        | 0.14          |
| (1,1395) | 1:19:A:LYS:HD3  | 1:20:A:ASP:HA   | 8        | 0.14          |
| (1,1344) | 1:9:A:ILE:HG12  | 1:32:A:LYS:HB3  | 3        | 0.14          |
| (1,1344) | 1:9:A:ILE:HG13  | 1:32:A:LYS:HB3  | 3        | 0.14          |
| (1,1047) | 1:10:A:LEU:HD11 | 1:34:A:THR:H    | 5        | 0.14          |
| (1,1047) | 1:10:A:LEU:HD12 | 1:34:A:THR:H    | 5        | 0.14          |
| (1,1047) | 1:10:A:LEU:HD13 | 1:34:A:THR:H    | 5        | 0.14          |
| (1,784)  | 1:57:A:MET:HG2  | 1:58:A:GLU:H    | 9        | 0.14          |
| (1,783)  | 1:57:A:MET:HG3  | 1:58:A:GLU:H    | 2        | 0.14          |
| (1,783)  | 1:57:A:MET:HG3  | 1:58:A:GLU:H    | 6        | 0.14          |
| (1,590)  | 1:42:A:LEU:HA   | 1:44:A:ILE:H    | 5        | 0.14          |
| (1,1623) | 1:99:A:VAL:H    | 1:100:A:LYS:HD2 | 8        | 0.13          |
| (1,1623) | 1:99:A:VAL:H    | 1:100:A:LYS:HD3 | 8        | 0.13          |
| (1,1426) | 1:28:A:LYS:HD2  | 1:29:A:LEU:H    | 8        | 0.13          |
| (1,1426) | 1:28:A:LYS:HD3  | 1:29:A:LEU:H    | 8        | 0.13          |
| (1,1166) | 1:4:A:LEU:H     | 1:30:A:GLY:HA3  | 2        | 0.13          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1034) | 1:33:A:LEU:HG   | 1:34:A:THR:H    | 8        | 0.13          |
| (1,790)  | 1:50:A:VAL:H    | 1:57:A:MET:HG3  | 7        | 0.13          |
| (1,783)  | 1:57:A:MET:HG3  | 1:58:A:GLU:H    | 1        | 0.13          |
| (1,683)  | 1:12:A:LEU:H    | 1:43:A:CYS:HA   | 6        | 0.13          |
| (1,602)  | 1:15:A:LEU:H    | 1:15:A:LEU:HD21 | 5        | 0.13          |
| (1,602)  | 1:15:A:LEU:H    | 1:15:A:LEU:HD22 | 5        | 0.13          |
| (1,602)  | 1:15:A:LEU:H    | 1:15:A:LEU:HD23 | 5        | 0.13          |
| (1,601)  | 1:15:A:LEU:H    | 1:15:A:LEU:HD21 | 5        | 0.13          |
| (1,601)  | 1:15:A:LEU:H    | 1:15:A:LEU:HD22 | 5        | 0.13          |
| (1,601)  | 1:15:A:LEU:H    | 1:15:A:LEU:HD23 | 5        | 0.13          |
| (1,476)  | 1:69:A:CYS:HB3  | 1:71:A:ASP:HA   | 5        | 0.13          |
| (1,304)  | 1:50:A:VAL:H    | 1:53:A:MET:HE1  | 6        | 0.13          |
| (1,304)  | 1:50:A:VAL:H    | 1:53:A:MET:HE2  | 6        | 0.13          |
| (1,304)  | 1:50:A:VAL:H    | 1:53:A:MET:HE3  | 6        | 0.13          |
| (1,129)  | 1:42:A:LEU:HD11 | 1:43:A:CYS:H    | 7        | 0.13          |
| (1,129)  | 1:42:A:LEU:HD12 | 1:43:A:CYS:H    | 7        | 0.13          |
| (1,129)  | 1:42:A:LEU:HD13 | 1:43:A:CYS:H    | 7        | 0.13          |
| (1,1549) | 1:74:A:GLN:H    | 1:74:A:GLN:HE21 | 2        | 0.12          |
| (1,1549) | 1:74:A:GLN:H    | 1:74:A:GLN:HE22 | 2        | 0.12          |
| (1,1426) | 1:28:A:LYS:HD2  | 1:29:A:LEU:H    | 3        | 0.12          |
| (1,1426) | 1:28:A:LYS:HD3  | 1:29:A:LEU:H    | 3        | 0.12          |
| (1,1396) | 1:19:A:LYS:HD2  | 1:21:A:GLU:H    | 1        | 0.12          |
| (1,1396) | 1:19:A:LYS:HD3  | 1:21:A:GLU:H    | 1        | 0.12          |
| (1,1293) | 1:30:A:GLY:H    | 1:31:A:GLY:H    | 1        | 0.12          |
| (1,1293) | 1:30:A:GLY:H    | 1:31:A:GLY:H    | 5        | 0.12          |
| (1,1052) | 1:63:A:ALA:H    | 1:65:A:VAL:HG11 | 4        | 0.12          |
| (1,1052) | 1:63:A:ALA:H    | 1:65:A:VAL:HG12 | 4        | 0.12          |
| (1,1052) | 1:63:A:ALA:H    | 1:65:A:VAL:HG13 | 4        | 0.12          |
| (1,1052) | 1:63:A:ALA:H    | 1:65:A:VAL:HG11 | 9        | 0.12          |
| (1,1052) | 1:63:A:ALA:H    | 1:65:A:VAL:HG12 | 9        | 0.12          |
| (1,1052) | 1:63:A:ALA:H    | 1:65:A:VAL:HG13 | 9        | 0.12          |
| (1,1051) | 1:63:A:ALA:H    | 1:65:A:VAL:HG11 | 4        | 0.12          |
| (1,1051) | 1:63:A:ALA:H    | 1:65:A:VAL:HG12 | 4        | 0.12          |
| (1,1051) | 1:63:A:ALA:H    | 1:65:A:VAL:HG13 | 4        | 0.12          |
| (1,1051) | 1:63:A:ALA:H    | 1:65:A:VAL:HG11 | 9        | 0.12          |
| (1,1051) | 1:63:A:ALA:H    | 1:65:A:VAL:HG12 | 9        | 0.12          |
| (1,1051) | 1:63:A:ALA:H    | 1:65:A:VAL:HG13 | 9        | 0.12          |
| (1,900)  | 1:45:A:SER:HB3  | 1:68:A:VAL:H    | 4        | 0.12          |
| (1,784)  | 1:57:A:MET:HG2  | 1:58:A:GLU:H    | 5        | 0.12          |
| (1,612)  | 1:96:A:GLY:H    | 1:97:A:ALA:H    | 7        | 0.12          |
| (1,590)  | 1:42:A:LEU:HA   | 1:44:A:ILE:H    | 1        | 0.12          |
| (1,129)  | 1:42:A:LEU:HD11 | 1:43:A:CYS:H    | 9        | 0.12          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,129)  | 1:42:A:LEU:HD12 | 1:43:A:CYS:H    | 9        | 0.12          |
| (1,129)  | 1:42:A:LEU:HD13 | 1:43:A:CYS:H    | 9        | 0.12          |
| (1,1344) | 1:9:A:ILE:HG12  | 1:32:A:LYS:HB3  | 4        | 0.11          |
| (1,1344) | 1:9:A:ILE:HG13  | 1:32:A:LYS:HB3  | 4        | 0.11          |
| (1,1301) | 1:4:A:LEU:HB3   | 1:30:A:GLY:H    | 10       | 0.11          |
| (1,1293) | 1:30:A:GLY:H    | 1:31:A:GLY:H    | 3        | 0.11          |
| (1,1293) | 1:30:A:GLY:H    | 1:31:A:GLY:H    | 7        | 0.11          |
| (1,1293) | 1:30:A:GLY:H    | 1:31:A:GLY:H    | 9        | 0.11          |
| (1,1252) | 1:92:A:LEU:HD11 | 1:93:A:SER:H    | 4        | 0.11          |
| (1,1252) | 1:92:A:LEU:HD12 | 1:93:A:SER:H    | 4        | 0.11          |
| (1,1252) | 1:92:A:LEU:HD13 | 1:93:A:SER:H    | 4        | 0.11          |
| (1,1215) | 1:5:A:SER:H     | 1:31:A:GLY:HA2  | 9        | 0.11          |
| (1,1052) | 1:63:A:ALA:H    | 1:65:A:VAL:HG11 | 1        | 0.11          |
| (1,1052) | 1:63:A:ALA:H    | 1:65:A:VAL:HG12 | 1        | 0.11          |
| (1,1052) | 1:63:A:ALA:H    | 1:65:A:VAL:HG13 | 1        | 0.11          |
| (1,1051) | 1:63:A:ALA:H    | 1:65:A:VAL:HG11 | 1        | 0.11          |
| (1,1051) | 1:63:A:ALA:H    | 1:65:A:VAL:HG12 | 1        | 0.11          |
| (1,1051) | 1:63:A:ALA:H    | 1:65:A:VAL:HG13 | 1        | 0.11          |
| (1,1034) | 1:33:A:LEU:HG   | 1:34:A:THR:H    | 1        | 0.11          |
| (1,1034) | 1:33:A:LEU:HG   | 1:34:A:THR:H    | 4        | 0.11          |
| (1,837)  | 1:12:A:LEU:HD21 | 1:61:A:LYS:H    | 1        | 0.11          |
| (1,837)  | 1:12:A:LEU:HD22 | 1:61:A:LYS:H    | 1        | 0.11          |
| (1,837)  | 1:12:A:LEU:HD23 | 1:61:A:LYS:H    | 1        | 0.11          |
| (1,790)  | 1:50:A:VAL:H    | 1:57:A:MET:HG3  | 9        | 0.11          |
| (1,784)  | 1:57:A:MET:HG2  | 1:58:A:GLU:H    | 2        | 0.11          |
| (1,784)  | 1:57:A:MET:HG2  | 1:58:A:GLU:H    | 3        | 0.11          |
| (1,784)  | 1:57:A:MET:HG2  | 1:58:A:GLU:H    | 7        | 0.11          |
| (1,737)  | 1:15:A:LEU:HD11 | 1:22:A:ALA:H    | 6        | 0.11          |
| (1,737)  | 1:15:A:LEU:HD12 | 1:22:A:ALA:H    | 6        | 0.11          |
| (1,737)  | 1:15:A:LEU:HD13 | 1:22:A:ALA:H    | 6        | 0.11          |
| (1,736)  | 1:15:A:LEU:HD11 | 1:22:A:ALA:H    | 6        | 0.11          |
| (1,736)  | 1:15:A:LEU:HD12 | 1:22:A:ALA:H    | 6        | 0.11          |
| (1,736)  | 1:15:A:LEU:HD13 | 1:22:A:ALA:H    | 6        | 0.11          |
| (1,694)  | 1:69:A:CYS:HB3  | 1:92:A:LEU:H    | 2        | 0.11          |
| (1,634)  | 1:69:A:CYS:HB2  | 1:92:A:LEU:H    | 2        | 0.11          |
| (1,634)  | 1:69:A:CYS:HB2  | 1:92:A:LEU:H    | 4        | 0.11          |
| (1,590)  | 1:42:A:LEU:HA   | 1:44:A:ILE:H    | 2        | 0.11          |
| (1,521)  | 1:14:A:LYS:HA   | 1:15:A:LEU:HD21 | 8        | 0.11          |
| (1,521)  | 1:14:A:LYS:HA   | 1:15:A:LEU:HD22 | 8        | 0.11          |
| (1,521)  | 1:14:A:LYS:HA   | 1:15:A:LEU:HD23 | 8        | 0.11          |
| (1,520)  | 1:14:A:LYS:HA   | 1:15:A:LEU:HD21 | 8        | 0.11          |
| (1,520)  | 1:14:A:LYS:HA   | 1:15:A:LEU:HD22 | 8        | 0.11          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,520) | 1:14:A:LYS:HA   | 1:15:A:LEU:HD23 | 8        | 0.11          |
| (1,330) | 1:25:A:MET:HE1  | 1:77:A:SER:HA   | 6        | 0.11          |
| (1,330) | 1:25:A:MET:HE2  | 1:77:A:SER:HA   | 6        | 0.11          |
| (1,330) | 1:25:A:MET:HE3  | 1:77:A:SER:HA   | 6        | 0.11          |
| (1,310) | 1:53:A:MET:HE1  | 1:61:A:LYS:H    | 5        | 0.11          |
| (1,310) | 1:53:A:MET:HE2  | 1:61:A:LYS:H    | 5        | 0.11          |
| (1,310) | 1:53:A:MET:HE3  | 1:61:A:LYS:H    | 5        | 0.11          |
| (1,292) | 1:9:A:ILE:HG21  | 1:42:A:LEU:HD21 | 6        | 0.11          |
| (1,292) | 1:9:A:ILE:HG21  | 1:42:A:LEU:HD22 | 6        | 0.11          |
| (1,292) | 1:9:A:ILE:HG21  | 1:42:A:LEU:HD23 | 6        | 0.11          |
| (1,292) | 1:9:A:ILE:HG22  | 1:42:A:LEU:HD21 | 6        | 0.11          |
| (1,292) | 1:9:A:ILE:HG22  | 1:42:A:LEU:HD22 | 6        | 0.11          |
| (1,292) | 1:9:A:ILE:HG22  | 1:42:A:LEU:HD23 | 6        | 0.11          |
| (1,292) | 1:9:A:ILE:HG23  | 1:42:A:LEU:HD21 | 6        | 0.11          |
| (1,292) | 1:9:A:ILE:HG23  | 1:42:A:LEU:HD22 | 6        | 0.11          |
| (1,292) | 1:9:A:ILE:HG23  | 1:42:A:LEU:HD23 | 6        | 0.11          |
| (1,291) | 1:9:A:ILE:HG21  | 1:42:A:LEU:HD21 | 6        | 0.11          |
| (1,291) | 1:9:A:ILE:HG21  | 1:42:A:LEU:HD22 | 6        | 0.11          |
| (1,291) | 1:9:A:ILE:HG21  | 1:42:A:LEU:HD23 | 6        | 0.11          |
| (1,291) | 1:9:A:ILE:HG22  | 1:42:A:LEU:HD21 | 6        | 0.11          |
| (1,291) | 1:9:A:ILE:HG22  | 1:42:A:LEU:HD22 | 6        | 0.11          |
| (1,291) | 1:9:A:ILE:HG22  | 1:42:A:LEU:HD23 | 6        | 0.11          |
| (1,291) | 1:9:A:ILE:HG23  | 1:42:A:LEU:HD21 | 6        | 0.11          |
| (1,291) | 1:9:A:ILE:HG23  | 1:42:A:LEU:HD22 | 6        | 0.11          |
| (1,291) | 1:9:A:ILE:HG23  | 1:42:A:LEU:HD23 | 6        | 0.11          |
| (1,180) | 1:15:A:LEU:HA   | 1:46:A:THR:HG21 | 6        | 0.11          |
| (1,180) | 1:15:A:LEU:HA   | 1:46:A:THR:HG22 | 6        | 0.11          |
| (1,180) | 1:15:A:LEU:HA   | 1:46:A:THR:HG23 | 6        | 0.11          |
| (1,179) | 1:15:A:LEU:HA   | 1:46:A:THR:HG21 | 6        | 0.11          |
| (1,179) | 1:15:A:LEU:HA   | 1:46:A:THR:HG22 | 6        | 0.11          |
| (1,179) | 1:15:A:LEU:HA   | 1:46:A:THR:HG23 | 6        | 0.11          |
| (1,129) | 1:42:A:LEU:HD11 | 1:43:A:CYS:H    | 4        | 0.11          |
| (1,129) | 1:42:A:LEU:HD12 | 1:43:A:CYS:H    | 4        | 0.11          |
| (1,129) | 1:42:A:LEU:HD13 | 1:43:A:CYS:H    | 4        | 0.11          |
| (1,86)  | 1:9:A:ILE:HD11  | 1:42:A:LEU:HD21 | 10       | 0.11          |
| (1,86)  | 1:9:A:ILE:HD11  | 1:42:A:LEU:HD22 | 10       | 0.11          |
| (1,86)  | 1:9:A:ILE:HD11  | 1:42:A:LEU:HD23 | 10       | 0.11          |
| (1,86)  | 1:9:A:ILE:HD12  | 1:42:A:LEU:HD21 | 10       | 0.11          |
| (1,86)  | 1:9:A:ILE:HD12  | 1:42:A:LEU:HD22 | 10       | 0.11          |
| (1,86)  | 1:9:A:ILE:HD12  | 1:42:A:LEU:HD23 | 10       | 0.11          |
| (1,86)  | 1:9:A:ILE:HD13  | 1:42:A:LEU:HD21 | 10       | 0.11          |
| (1,86)  | 1:9:A:ILE:HD13  | 1:42:A:LEU:HD22 | 10       | 0.11          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,86)   | 1:9:A:ILE:HD13  | 1:42:A:LEU:HD23 | 10       | 0.11          |
| (1,85)   | 1:9:A:ILE:HD11  | 1:42:A:LEU:HD21 | 10       | 0.11          |
| (1,85)   | 1:9:A:ILE:HD11  | 1:42:A:LEU:HD22 | 10       | 0.11          |
| (1,85)   | 1:9:A:ILE:HD11  | 1:42:A:LEU:HD23 | 10       | 0.11          |
| (1,85)   | 1:9:A:ILE:HD12  | 1:42:A:LEU:HD21 | 10       | 0.11          |
| (1,85)   | 1:9:A:ILE:HD12  | 1:42:A:LEU:HD22 | 10       | 0.11          |
| (1,85)   | 1:9:A:ILE:HD12  | 1:42:A:LEU:HD23 | 10       | 0.11          |
| (1,85)   | 1:9:A:ILE:HD13  | 1:42:A:LEU:HD21 | 10       | 0.11          |
| (1,85)   | 1:9:A:ILE:HD13  | 1:42:A:LEU:HD22 | 10       | 0.11          |
| (1,85)   | 1:9:A:ILE:HD13  | 1:42:A:LEU:HD23 | 10       | 0.11          |
| (1,1606) | 1:91:A:SER:HB2  | 1:92:A:LEU:HG   | 3        | 0.1           |
| (1,1606) | 1:91:A:SER:HB3  | 1:92:A:LEU:HG   | 3        | 0.1           |
| (1,1419) | 1:25:A:MET:HG2  | 1:74:A:GLN:HE21 | 6        | 0.1           |
| (1,1419) | 1:25:A:MET:HG2  | 1:74:A:GLN:HE22 | 6        | 0.1           |
| (1,1293) | 1:30:A:GLY:H    | 1:31:A:GLY:H    | 8        | 0.1           |
| (1,1252) | 1:92:A:LEU:HD11 | 1:93:A:SER:H    | 8        | 0.1           |
| (1,1252) | 1:92:A:LEU:HD12 | 1:93:A:SER:H    | 8        | 0.1           |
| (1,1252) | 1:92:A:LEU:HD13 | 1:93:A:SER:H    | 8        | 0.1           |
| (1,1166) | 1:4:A:LEU:H     | 1:30:A:GLY:HA3  | 4        | 0.1           |
| (1,1127) | 1:28:A:LYS:HD2  | 1:29:A:LEU:H    | 2        | 0.1           |
| (1,983)  | 1:11:A:THR:H    | 1:43:A:CYS:HA   | 3        | 0.1           |
| (1,790)  | 1:50:A:VAL:H    | 1:57:A:MET:HG3  | 1        | 0.1           |
| (1,784)  | 1:57:A:MET:HG2  | 1:58:A:GLU:H    | 1        | 0.1           |

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

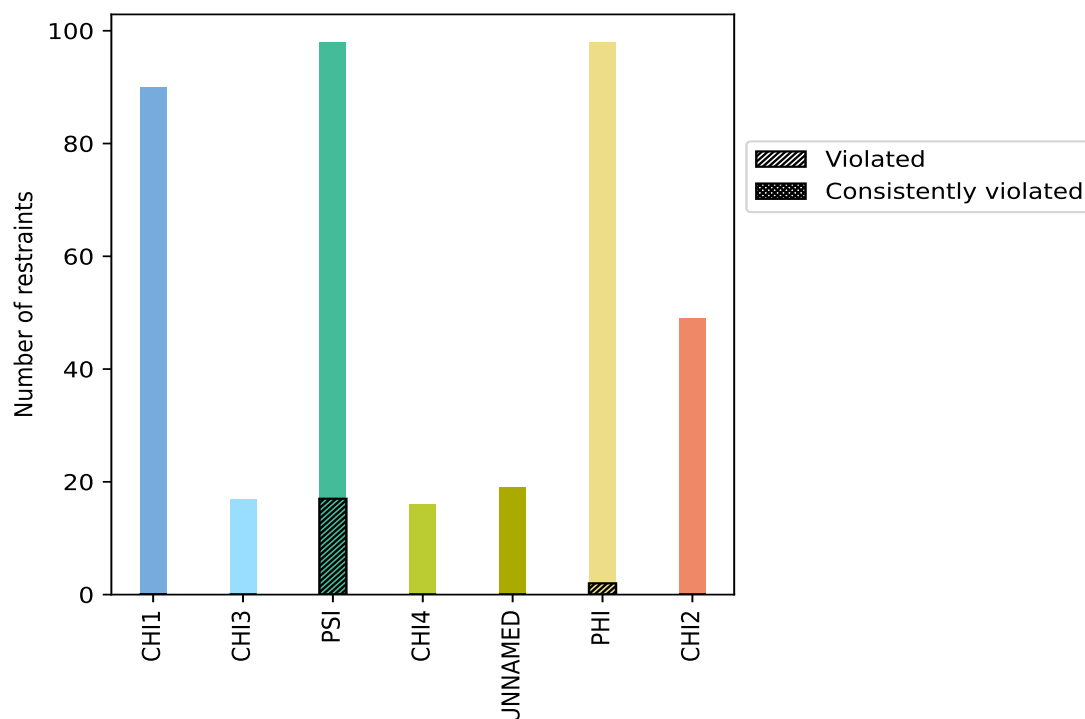
### 10.1 Summary of dihedral-angle violations [i](#)

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

| Angle type | Count | % <sup>1</sup> | Violated <sup>3</sup> |                |                | Consistently Violated <sup>4</sup> |                |                |
|------------|-------|----------------|-----------------------|----------------|----------------|------------------------------------|----------------|----------------|
|            |       |                | Count                 | % <sup>2</sup> | % <sup>1</sup> | Count                              | % <sup>2</sup> | % <sup>1</sup> |
| CHI1       | 90    | 23.3           | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| CHI3       | 17    | 4.4            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| PSI        | 98    | 25.3           | 17                    | 17.3           | 4.4            | 0                                  | 0.0            | 0.0            |
| CHI4       | 16    | 4.1            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| UNNAMED    | 19    | 4.9            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| PHI        | 98    | 25.3           | 2                     | 2.0            | 0.5            | 0                                  | 0.0            | 0.0            |
| CHI2       | 49    | 12.7           | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Total      | 387   | 100.0          | 19                    | 4.9            | 4.9            | 0                                  | 0.0            | 0.0            |

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

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



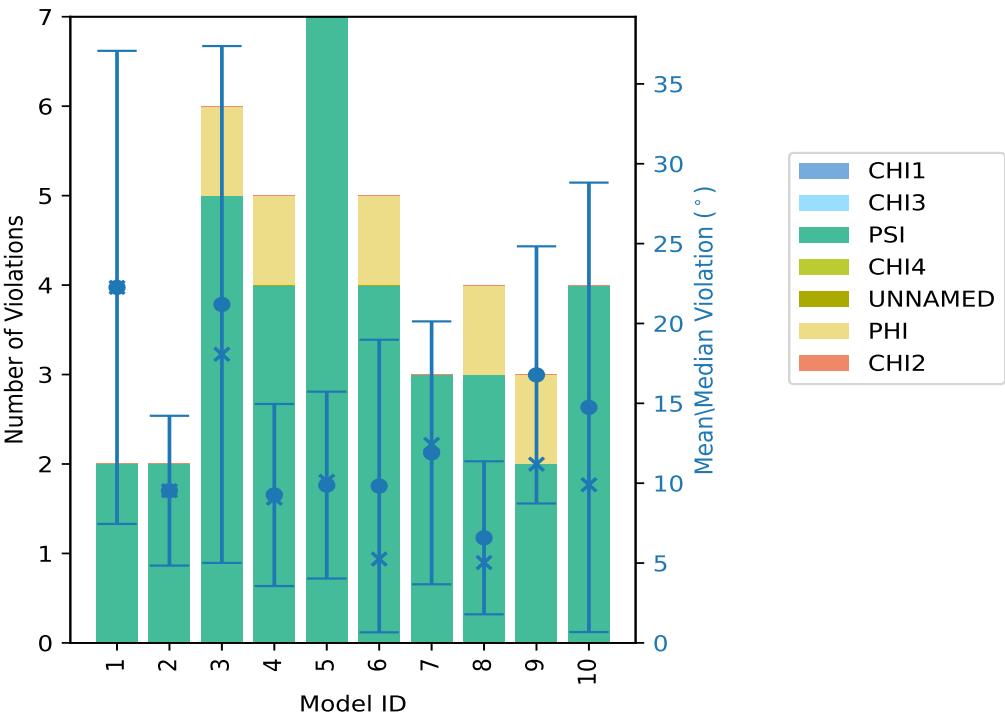
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model ⓘ

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

| Model ID | Number of violations |      |     |      |         |     |      | Total | Mean (°) | Max (°) | SD (°) | Median (°) |
|----------|----------------------|------|-----|------|---------|-----|------|-------|----------|---------|--------|------------|
|          | CHI1                 | CHI3 | PSI | CHI4 | UNNAMED | PHI | CHI2 |       |          |         |        |            |
| 1        | 0                    | 0    | 2   | 0    | 0       | 0   | 0    | 2     | 22.26    | 37.06   | 14.81  | 22.26      |
| 2        | 0                    | 0    | 2   | 0    | 0       | 0   | 0    | 2     | 9.53     | 14.22   | 4.69   | 9.53       |
| 3        | 0                    | 0    | 5   | 0    | 0       | 1   | 0    | 6     | 21.19    | 48.28   | 16.18  | 18.07      |
| 4        | 0                    | 0    | 4   | 0    | 0       | 1   | 0    | 5     | 9.26     | 19.01   | 5.7    | 9.06       |
| 5        | 0                    | 0    | 7   | 0    | 0       | 0   | 0    | 7     | 9.88     | 18.64   | 5.85   | 10.12      |
| 6        | 0                    | 0    | 4   | 0    | 0       | 1   | 0    | 5     | 9.82     | 27.46   | 9.16   | 5.25       |
| 7        | 0                    | 0    | 3   | 0    | 0       | 0   | 0    | 3     | 11.9     | 21.7    | 8.23   | 12.43      |
| 8        | 0                    | 0    | 3   | 0    | 0       | 1   | 0    | 4     | 6.58     | 14.33   | 4.79   | 5.03       |
| 9        | 0                    | 0    | 2   | 0    | 0       | 1   | 0    | 3     | 16.78    | 28.16   | 8.05   | 11.19      |
| 10       | 0                    | 0    | 4   | 0    | 0       | 0   | 0    | 4     | 14.75    | 37.92   | 14.07  | 9.9        |

10.2.1 Bar graph : Dihedral violation statistics for each model ⓘ



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

10.3 Dihedral-angle violation statistics for the ensemble ⓘ

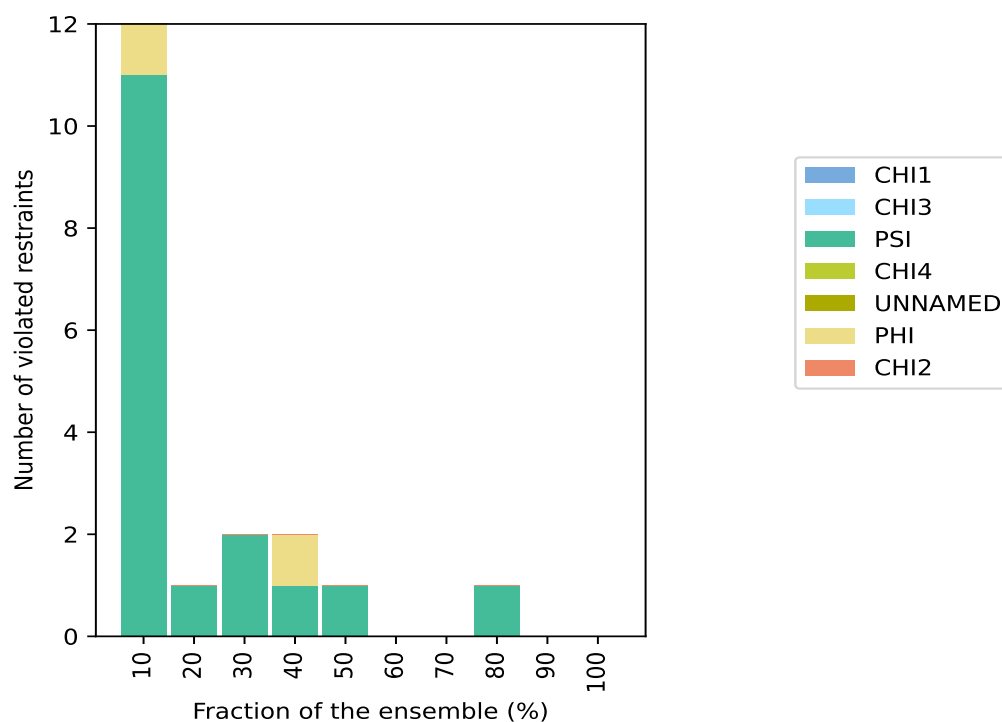
Violation analysis may find that some restraints are violated in very few models and some are violated in most of models. The following table provides this information as number of violated

restraints for a given fraction of ensemble.

| Number of violated restraints |      |     |      |         |     |      |       | Fraction of the ensemble |       |
|-------------------------------|------|-----|------|---------|-----|------|-------|--------------------------|-------|
| CHI1                          | CHI3 | PSI | CHI4 | UNNAMED | PHI | CHI2 | Total | Count <sup>1</sup>       | %     |
| 0                             | 0    | 11  | 0    | 0       | 1   | 0    | 12    | 1                        | 10.0  |
| 0                             | 0    | 1   | 0    | 0       | 0   | 0    | 1     | 2                        | 20.0  |
| 0                             | 0    | 2   | 0    | 0       | 0   | 0    | 2     | 3                        | 30.0  |
| 0                             | 0    | 1   | 0    | 0       | 1   | 0    | 2     | 4                        | 40.0  |
| 0                             | 0    | 1   | 0    | 0       | 0   | 0    | 1     | 5                        | 50.0  |
| 0                             | 0    | 0   | 0    | 0       | 0   | 0    | 0     | 6                        | 60.0  |
| 0                             | 0    | 0   | 0    | 0       | 0   | 0    | 0     | 7                        | 70.0  |
| 0                             | 0    | 1   | 0    | 0       | 0   | 0    | 1     | 8                        | 80.0  |
| 0                             | 0    | 0   | 0    | 0       | 0   | 0    | 0     | 9                        | 90.0  |
| 0                             | 0    | 0   | 0    | 0       | 0   | 0    | 0     | 10                       | 100.0 |

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

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

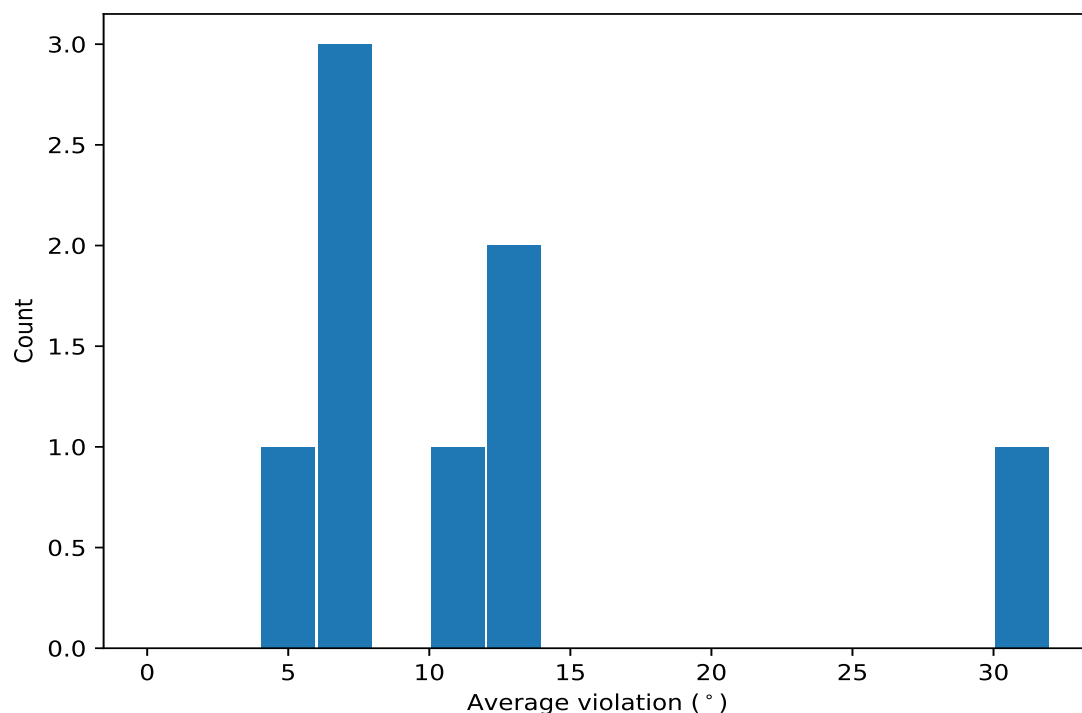


## 10.4 Most violated dihedral-angle restraints in the ensemble [i](#)

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

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

in the ensemble



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

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

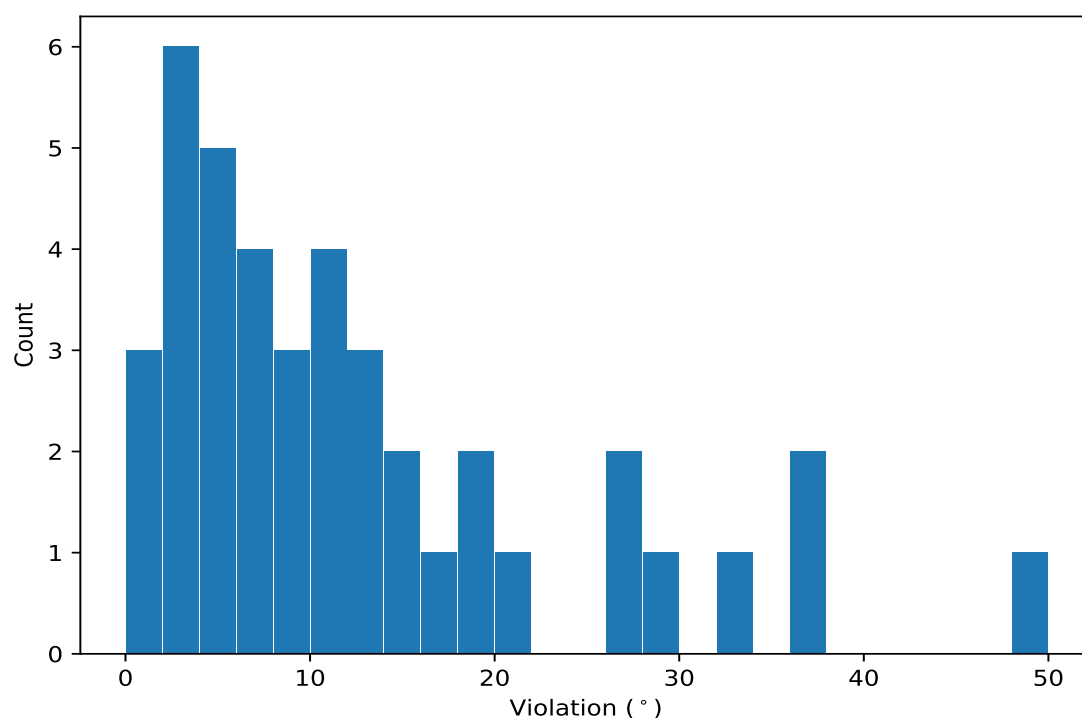
| Key     | Atom-1        | Atom-2         | Atom-3        | Atom-4        | Models <sup>1</sup> | Mean  | SD <sup>2</sup> | Median |
|---------|---------------|----------------|---------------|---------------|---------------------|-------|-----------------|--------|
| (1,149) | 1:81:A:LYS:N  | 1:81:A:LYS:CA  | 1:81:A:LYS:C  | 1:82:A:SER:N  | 8                   | 13.81 | 7.02            | 12.6   |
| (1,29)  | 1:18:A:ASN:N  | 1:18:A:ASN:CA  | 1:18:A:ASN:C  | 1:19:A:LYS:N  | 5                   | 11.05 | 9.27            | 9.4    |
| (1,59)  | 1:36:A:SER:N  | 1:36:A:SER:CA  | 1:36:A:SER:C  | 1:37:A:ALA:N  | 4                   | 31.13 | 13.62           | 32.61  |
| (1,178) | 1:96:A:GLY:C  | 1:97:A:ALA:N   | 1:97:A:ALA:CA | 1:97:A:ALA:C  | 4                   | 6.57  | 3.64            | 6.24   |
| (1,178) | 1:96:A:GLY:C  | 1:97:A:ALA:N   | 1:97:A:ALA:CA | 1:97:A:ALA:C  | 4                   | 6.57  | 3.64            | 6.24   |
| (1,61)  | 1:37:A:ALA:N  | 1:37:A:ALA:CA  | 1:37:A:ALA:C  | 1:38:A:ASN:N  | 3                   | 7.96  | 4.52            | 5.25   |
| (1,181) | 1:98:A:GLU:N  | 1:98:A:GLU:CA  | 1:98:A:GLU:C  | 1:99:A:VAL:N  | 3                   | 4.65  | 2.14            | 4.37   |
| (1,185) | 1:100:A:LYS:N | 1:100:A:LYS:CA | 1:100:A:LYS:C | 1:101:A:HIS:N | 2                   | 12.35 | 0.08            | 12.35  |

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

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

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

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



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

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

| Key     | Atom-1        | Atom-2         | Atom-3        | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|---------------|---------------|----------|---------------|
| (1,59)  | 1:36:A:SER:N  | 1:36:A:SER:CA  | 1:36:A:SER:C  | 1:37:A:ALA:N  | 3        | 48.28         |
| (1,1)   | 1:1:A:MET:N   | 1:1:A:MET:CA   | 1:1:A:MET:C   | 1:2:A:LYS:N   | 10       | 37.92         |
| (1,59)  | 1:36:A:SER:N  | 1:36:A:SER:CA  | 1:36:A:SER:C  | 1:37:A:ALA:N  | 1        | 37.06         |
| (1,193) | 1:104:A:HIS:N | 1:104:A:HIS:CA | 1:104:A:HIS:C | 1:105:A:HIS:N | 3        | 32.7          |
| (1,59)  | 1:36:A:SER:N  | 1:36:A:SER:CA  | 1:36:A:SER:C  | 1:37:A:ALA:N  | 9        | 28.16         |
| (1,29)  | 1:18:A:ASN:N  | 1:18:A:ASN:CA  | 1:18:A:ASN:C  | 1:19:A:LYS:N  | 6        | 27.46         |
| (1,149) | 1:81:A:LYS:N  | 1:81:A:LYS:CA  | 1:81:A:LYS:C  | 1:82:A:SER:N  | 3        | 26.73         |
| (1,149) | 1:81:A:LYS:N  | 1:81:A:LYS:CA  | 1:81:A:LYS:C  | 1:82:A:SER:N  | 7        | 21.7          |
| (1,27)  | 1:17:A:GLN:N  | 1:17:A:GLN:CA  | 1:17:A:GLN:C  | 1:18:A:ASN:N  | 4        | 19.01         |
| (1,195) | 1:105:A:HIS:N | 1:105:A:HIS:CA | 1:105:A:HIS:C | 1:106:A:HIS:N | 5        | 18.64         |
| (1,149) | 1:81:A:LYS:N  | 1:81:A:LYS:CA  | 1:81:A:LYS:C  | 1:82:A:SER:N  | 5        | 16.51         |
| (1,61)  | 1:37:A:ALA:N  | 1:37:A:ALA:CA  | 1:37:A:ALA:C  | 1:38:A:ASN:N  | 8        | 14.33         |
| (1,149) | 1:81:A:LYS:N  | 1:81:A:LYS:CA  | 1:81:A:LYS:C  | 1:82:A:SER:N  | 2        | 14.22         |
| (1,29)  | 1:18:A:ASN:N  | 1:18:A:ASN:CA  | 1:18:A:ASN:C  | 1:19:A:LYS:N  | 10       | 13.59         |
| (1,185) | 1:100:A:LYS:N | 1:100:A:LYS:CA | 1:100:A:LYS:C | 1:101:A:HIS:N | 7        | 12.43         |
| (1,185) | 1:100:A:LYS:N | 1:100:A:LYS:CA | 1:100:A:LYS:C | 1:101:A:HIS:N | 5        | 12.27         |
| (1,178) | 1:96:A:GLY:C  | 1:97:A:ALA:N   | 1:97:A:ALA:CA | 1:97:A:ALA:C  | 9        | 11.19         |
| (1,59)  | 1:36:A:SER:N  | 1:36:A:SER:CA  | 1:36:A:SER:C  | 1:37:A:ALA:N  | 4        | 11.02         |
| (1,149) | 1:81:A:LYS:N  | 1:81:A:LYS:CA  | 1:81:A:LYS:C  | 1:82:A:SER:N  | 9        | 10.99         |
| (1,177) | 1:95:A:TRP:N  | 1:95:A:TRP:CA  | 1:95:A:TRP:C  | 1:96:A:GLY:N  | 5        | 10.12         |
| (1,6)   | 1:5:A:SER:C   | 1:6:A:ASN:N    | 1:6:A:ASN:CA  | 1:6:A:ASN:C   | 6        | 9.78          |

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| Key     | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Model ID | Violation (°) |
|---------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,29)  | 1:18:A:ASN:N | 1:18:A:ASN:CA | 1:18:A:ASN:C  | 1:19:A:LYS:N | 3        | 9.4           |
| (1,178) | 1:96:A:GLY:C | 1:97:A:ALA:N  | 1:97:A:ALA:CA | 1:97:A:ALA:C | 4        | 9.06          |
| (1,149) | 1:81:A:LYS:N | 1:81:A:LYS:CA | 1:81:A:LYS:C  | 1:82:A:SER:N | 1        | 7.45          |
| (1,181) | 1:98:A:GLU:N | 1:98:A:GLU:CA | 1:98:A:GLU:C  | 1:99:A:VAL:N | 3        | 7.4           |
| (1,149) | 1:81:A:LYS:N | 1:81:A:LYS:CA | 1:81:A:LYS:C  | 1:82:A:SER:N | 8        | 6.65          |
| (1,149) | 1:81:A:LYS:N | 1:81:A:LYS:CA | 1:81:A:LYS:C  | 1:82:A:SER:N | 10       | 6.22          |
| (1,61)  | 1:37:A:ALA:N | 1:37:A:ALA:CA | 1:37:A:ALA:C  | 1:38:A:ASN:N | 6        | 5.25          |
| (1,23)  | 1:15:A:LEU:N | 1:15:A:LEU:CA | 1:15:A:LEU:C  | 1:16:A:SER:N | 5        | 5.17          |
| (1,25)  | 1:16:A:SER:N | 1:16:A:SER:CA | 1:16:A:SER:C  | 1:17:A:GLN:N | 2        | 4.84          |
| (1,181) | 1:98:A:GLU:N | 1:98:A:GLU:CA | 1:98:A:GLU:C  | 1:99:A:VAL:N | 6        | 4.37          |
| (1,61)  | 1:37:A:ALA:N | 1:37:A:ALA:CA | 1:37:A:ALA:C  | 1:38:A:ASN:N | 5        | 4.29          |
| (1,95)  | 1:54:A:SER:N | 1:54:A:SER:CA | 1:54:A:SER:C  | 1:55:A:LYS:N | 4        | 3.95          |
| (1,178) | 1:96:A:GLY:C | 1:97:A:ALA:N  | 1:97:A:ALA:CA | 1:97:A:ALA:C | 8        | 3.41          |
| (1,29)  | 1:18:A:ASN:N | 1:18:A:ASN:CA | 1:18:A:ASN:C  | 1:19:A:LYS:N | 4        | 3.24          |
| (1,178) | 1:96:A:GLY:C | 1:97:A:ALA:N  | 1:97:A:ALA:CA | 1:97:A:ALA:C | 3        | 2.62          |
| (1,19)  | 1:12:A:LEU:N | 1:12:A:LEU:CA | 1:12:A:LEU:C  | 1:13:A:GLY:N | 6        | 2.22          |
| (1,181) | 1:98:A:GLU:N | 1:98:A:GLU:CA | 1:98:A:GLU:C  | 1:99:A:VAL:N | 5        | 2.18          |
| (1,69)  | 1:41:A:SER:N | 1:41:A:SER:CA | 1:41:A:SER:C  | 1:42:A:LEU:N | 8        | 1.92          |
| (1,29)  | 1:18:A:ASN:N | 1:18:A:ASN:CA | 1:18:A:ASN:C  | 1:19:A:LYS:N | 7        | 1.57          |
| (1,67)  | 1:40:A:ALA:N | 1:40:A:ALA:CA | 1:40:A:ALA:C  | 1:41:A:SER:N | 10       | 1.28          |