



# Full wwPDB NMR Structure Validation Report ⓘ

Sep 15, 2025 – 10:16 AM EDT

PDB ID : 9DCJ / pdb\_00009dcj  
BMRB ID : 31198  
Title : Pentameric Structure of MERS-CoV Envelope Protein Transmembrane Domain Determined by Solid-State NMR  
Authors : Sucec, I.; Hong, M.  
Deposited on : 2024-08-26

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 Phenix2.0rc1  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
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) : 2.45.1

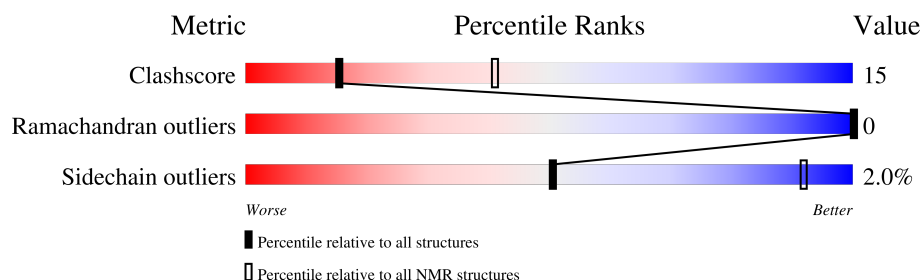
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLID-STATE NMR*

The overall completeness of chemical shifts assignment is 7%.

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            | 210492                      | 14027                     |
| Ramachandran outliers | 207382                      | 12486                     |
| Sidechain outliers    | 206894                      | 12463                     |

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     | 38     | 61% 16% 24%      |
| 1   | B     | 38     | 61% 16% 24%      |
| 1   | C     | 38     | 61% 16% 24%      |
| 1   | D     | 38     | 61% 16% 24%      |
| 1   | E     | 38     | 63% 16% 21%      |

## 2 Ensemble composition and analysis

This entry contains 10 models. Model 5 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:9-A:37, B:9-B:37, C:9-C:37, D:9-D:37, E:9-E:38 (146) | 0.59              | 5            |

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. No single-model clusters were found.

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

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3155 atoms, of which 1635 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Envelope small membrane protein.

| Mol | Chain | Residues | Atoms |     |     |    |    |   | Trace |
|-----|-------|----------|-------|-----|-----|----|----|---|-------|
| 1   | A     | 38       | Total | C   | H   | N  | O  | S | 0     |
|     |       |          | 631   | 207 | 327 | 46 | 49 | 2 |       |
| 1   | B     | 38       | Total | C   | H   | N  | O  | S | 0     |
|     |       |          | 631   | 207 | 327 | 46 | 49 | 2 |       |
| 1   | C     | 38       | Total | C   | H   | N  | O  | S | 0     |
|     |       |          | 631   | 207 | 327 | 46 | 49 | 2 |       |
| 1   | D     | 38       | Total | C   | H   | N  | O  | S | 0     |
|     |       |          | 631   | 207 | 327 | 46 | 49 | 2 |       |
| 1   | E     | 38       | Total | C   | H   | N  | O  | S | 0     |
|     |       |          | 631   | 207 | 327 | 46 | 49 | 2 |       |

There are 10 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| A     | 23      | SER      | CYS    | engineered mutation | UNP K9N5R3 |
| A     | 30      | SER      | CYS    | engineered mutation | UNP K9N5R3 |
| B     | 23      | SER      | CYS    | engineered mutation | UNP K9N5R3 |
| B     | 30      | SER      | CYS    | engineered mutation | UNP K9N5R3 |
| C     | 23      | SER      | CYS    | engineered mutation | UNP K9N5R3 |
| C     | 30      | SER      | CYS    | engineered mutation | UNP K9N5R3 |
| D     | 23      | SER      | CYS    | engineered mutation | UNP K9N5R3 |
| D     | 30      | SER      | CYS    | engineered mutation | UNP K9N5R3 |
| E     | 23      | SER      | CYS    | engineered mutation | UNP K9N5R3 |
| E     | 30      | SER      | CYS    | engineered mutation | UNP K9N5R3 |

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

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

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

- Molecule 1: Envelope small membrane protein



- Molecule 1: Envelope small membrane protein



- Molecule 1: Envelope small membrane protein



- Molecule 1: Envelope small membrane protein



- Molecule 1: Envelope small membrane protein



## 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: Envelope small membrane protein

Chain A:  58% 18% 24%



- Molecule 1: Envelope small membrane protein

Chain B:  58% 18% 24%



- Molecule 1: Envelope small membrane protein

Chain C:  58% 18% 24%



- Molecule 1: Envelope small membrane protein

Chain D:  58% 18% 24%



- Molecule 1: Envelope small membrane protein

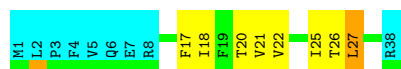
Chain E:  58% 21% 21%



### 4.2.2 Score per residue for model 2

- Molecule 1: Envelope small membrane protein

Chain A:  55% 18% 24%



- Molecule 1: Envelope small membrane protein



- Molecule 1: Envelope small membrane protein



- Molecule 1: Envelope small membrane protein

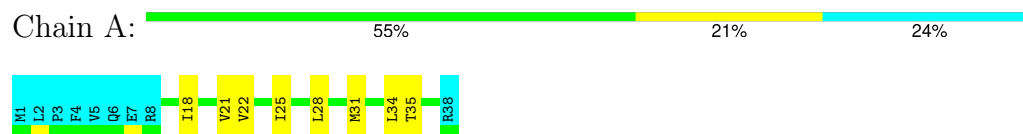


- Molecule 1: Envelope small membrane protein

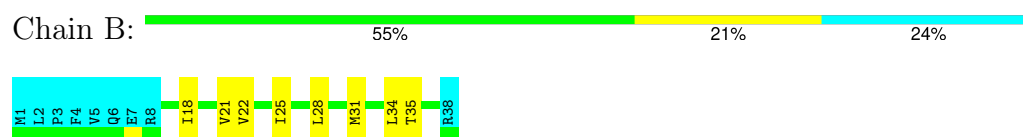


#### 4.2.3 Score per residue for model 3

- Molecule 1: Envelope small membrane protein



- Molecule 1: Envelope small membrane protein



- Molecule 1: Envelope small membrane protein



- Molecule 1: Envelope small membrane protein

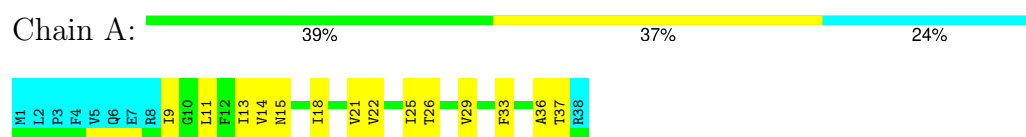


- Molecule 1: Envelope small membrane protein

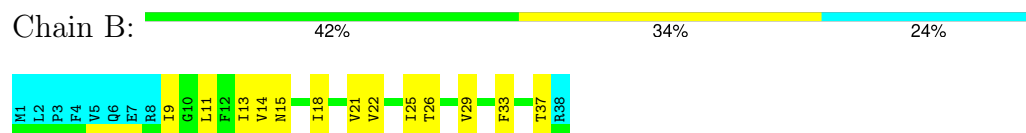


#### 4.2.4 Score per residue for model 4

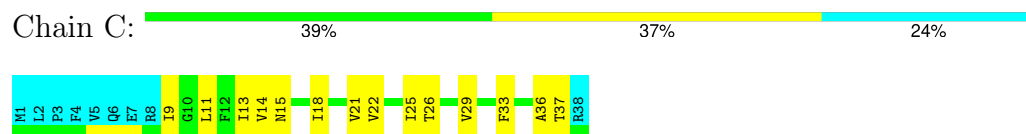
- Molecule 1: Envelope small membrane protein



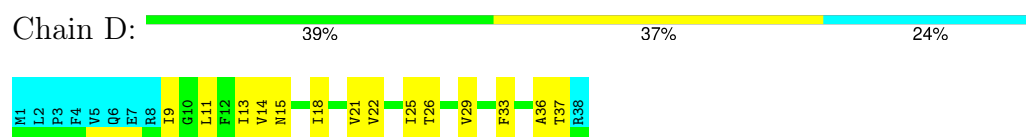
- Molecule 1: Envelope small membrane protein



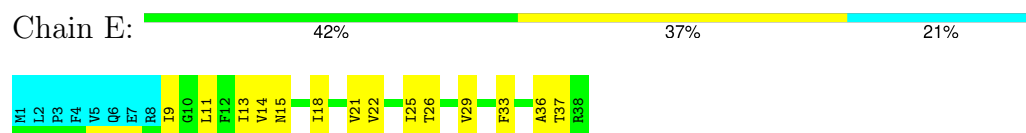
- Molecule 1: Envelope small membrane protein



- Molecule 1: Envelope small membrane protein



- Molecule 1: Envelope small membrane protein





#### 4.2.5 Score per residue for model 5 (medoid)

- Molecule 1: Envelope small membrane protein



- Molecule 1: Envelope small membrane protein



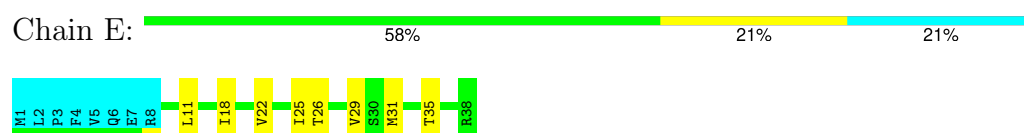
- Molecule 1: Envelope small membrane protein



- Molecule 1: Envelope small membrane protein

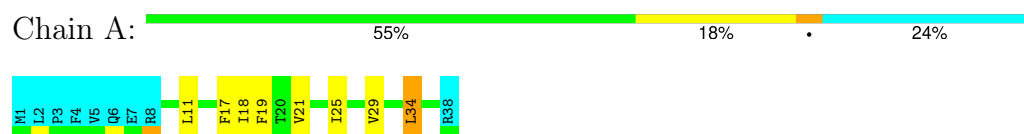


- Molecule 1: Envelope small membrane protein



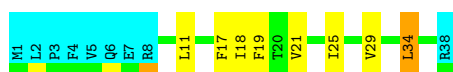
#### 4.2.6 Score per residue for model 6

- Molecule 1: Envelope small membrane protein

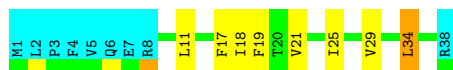


- Molecule 1: Envelope small membrane protein

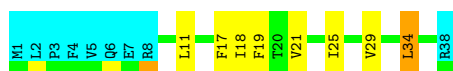




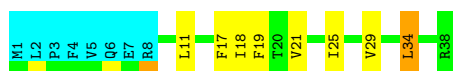
- Molecule 1: Envelope small membrane protein



- Molecule 1: Envelope small membrane protein

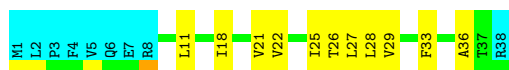


- Molecule 1: Envelope small membrane protein

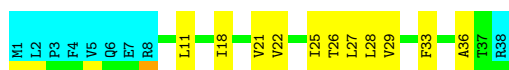


#### 4.2.7 Score per residue for model 7

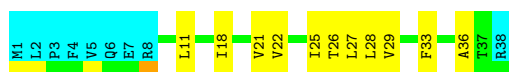
- Molecule 1: Envelope small membrane protein



- Molecule 1: Envelope small membrane protein

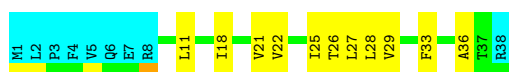


- Molecule 1: Envelope small membrane protein



- Molecule 1: Envelope small membrane protein





- Molecule 1: Envelope small membrane protein



#### 4.2.8 Score per residue for model 8

- Molecule 1: Envelope small membrane protein



- Molecule 1: Envelope small membrane protein



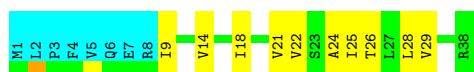
- Molecule 1: Envelope small membrane protein



- Molecule 1: Envelope small membrane protein



- Molecule 1: Envelope small membrane protein



### 4.2.9 Score per residue for model 9

- Molecule 1: Envelope small membrane protein



- Molecule 1: Envelope small membrane protein



- Molecule 1: Envelope small membrane protein



- Molecule 1: Envelope small membrane protein



- Molecule 1: Envelope small membrane protein



### 4.2.10 Score per residue for model 10

- Molecule 1: Envelope small membrane protein

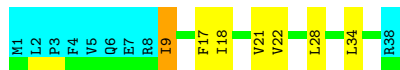


- Molecule 1: Envelope small membrane protein

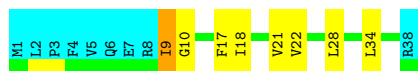




- Molecule 1: Envelope small membrane protein



- Molecule 1: Envelope small membrane protein



- Molecule 1: Envelope small membrane protein



## 5 Refinement protocol and experimental data overview

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

Of the 200 calculated structures, 10 were deposited, based on the following criterion: *structures with the lowest energy*.

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

| Software name | Classification        | Version |
|---------------|-----------------------|---------|
| X-PLOR NIH    | structure calculation |         |

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                       | 170            |
| Number of shifts mapped to atoms             | 170            |
| Number of unparsed shifts                    | 0              |
| Number of shifts with mapping errors         | 0              |
| Number of shifts with mapping warnings       | 0              |
| Assignment completeness (well-defined parts) | 7%             |

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

## 6 Model quality

### 6.1 Standard geometry

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 6.2 Too-close contacts

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     | 222   | 240      | 240      | 9±4     |
| 1   | B     | 222   | 240      | 240      | 9±4     |
| 1   | C     | 222   | 240      | 240      | 9±4     |
| 1   | D     | 222   | 240      | 240      | 9±4     |
| 1   | E     | 234   | 253      | 253      | 10±4    |
| All | All   | 11220 | 12130    | 12130    | 339     |

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 15.

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

| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:C:25:ILE:HD11 | 1:D:22:VAL:CG2  | 0.73     | 2.14        | 5      | 1     |
| 1:B:25:ILE:HD11 | 1:C:22:VAL:CG2  | 0.73     | 2.14        | 5      | 1     |
| 1:A:25:ILE:HD11 | 1:B:22:VAL:CG2  | 0.72     | 2.14        | 5      | 1     |
| 1:A:22:VAL:CG2  | 1:E:25:ILE:HD11 | 0.72     | 2.14        | 5      | 1     |
| 1:A:15:ASN:O    | 1:A:18:ILE:HG22 | 0.71     | 1.85        | 4      | 1     |
| 1:D:25:ILE:HD11 | 1:E:22:VAL:CG2  | 0.71     | 2.14        | 5      | 1     |
| 1:B:15:ASN:O    | 1:B:18:ILE:HG22 | 0.71     | 1.85        | 4      | 1     |
| 1:C:15:ASN:O    | 1:C:18:ILE:HG22 | 0.71     | 1.85        | 4      | 1     |
| 1:E:15:ASN:O    | 1:E:18:ILE:HG22 | 0.71     | 1.86        | 4      | 1     |
| 1:D:15:ASN:O    | 1:D:18:ILE:HG22 | 0.69     | 1.85        | 4      | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:C:25:ILE:HD11 | 1:D:22:VAL:CG1  | 0.68     | 2.19        | 7      | 1     |
| 1:A:25:ILE:HD11 | 1:B:22:VAL:CG1  | 0.67     | 2.19        | 7      | 1     |
| 1:B:25:ILE:HD11 | 1:C:22:VAL:CG1  | 0.67     | 2.19        | 7      | 1     |
| 1:D:25:ILE:HD11 | 1:E:22:VAL:CG1  | 0.67     | 2.19        | 7      | 1     |
| 1:A:22:VAL:CG1  | 1:E:25:ILE:HD11 | 0.67     | 2.19        | 7      | 1     |
| 1:A:21:VAL:HG11 | 1:B:22:VAL:HG11 | 0.66     | 1.67        | 10     | 1     |
| 1:A:22:VAL:HG11 | 1:E:21:VAL:HG11 | 0.66     | 1.67        | 10     | 1     |
| 1:C:21:VAL:HG11 | 1:D:22:VAL:HG11 | 0.66     | 1.67        | 10     | 1     |
| 1:D:18:ILE:HD12 | 1:D:19:PHE:N    | 0.65     | 2.07        | 6      | 1     |
| 1:D:21:VAL:HG11 | 1:E:22:VAL:HG11 | 0.65     | 1.67        | 10     | 1     |
| 1:B:21:VAL:HG11 | 1:C:22:VAL:HG11 | 0.65     | 1.67        | 10     | 1     |
| 1:E:18:ILE:HD12 | 1:E:19:PHE:N    | 0.65     | 2.07        | 6      | 1     |
| 1:A:18:ILE:HD12 | 1:A:19:PHE:N    | 0.64     | 2.07        | 6      | 1     |
| 1:C:18:ILE:HD12 | 1:C:19:PHE:N    | 0.64     | 2.07        | 6      | 1     |
| 1:B:18:ILE:HD12 | 1:B:19:PHE:N    | 0.64     | 2.07        | 6      | 1     |
| 1:D:33:PHE:O    | 1:D:37:THR:HG22 | 0.64     | 1.93        | 9      | 2     |
| 1:E:18:ILE:O    | 1:E:22:VAL:HG23 | 0.63     | 1.93        | 7      | 3     |
| 1:A:18:ILE:O    | 1:A:22:VAL:HG23 | 0.63     | 1.93        | 7      | 3     |
| 1:B:18:ILE:O    | 1:B:22:VAL:HG23 | 0.63     | 1.93        | 7      | 3     |
| 1:B:33:PHE:O    | 1:B:37:THR:HG22 | 0.63     | 1.93        | 9      | 2     |
| 1:C:33:PHE:O    | 1:C:37:THR:HG22 | 0.63     | 1.93        | 9      | 2     |
| 1:E:33:PHE:O    | 1:E:37:THR:HG22 | 0.63     | 1.93        | 9      | 2     |
| 1:E:25:ILE:O    | 1:E:29:VAL:HG22 | 0.63     | 1.94        | 5      | 3     |
| 1:D:18:ILE:O    | 1:D:22:VAL:HG23 | 0.63     | 1.93        | 7      | 3     |
| 1:B:25:ILE:O    | 1:B:29:VAL:HG22 | 0.63     | 1.94        | 5      | 3     |
| 1:A:33:PHE:O    | 1:A:37:THR:HG22 | 0.63     | 1.93        | 9      | 2     |
| 1:C:18:ILE:O    | 1:C:22:VAL:HG23 | 0.62     | 1.93        | 7      | 3     |
| 1:B:18:ILE:O    | 1:B:22:VAL:HG22 | 0.62     | 1.95        | 4      | 2     |
| 1:A:25:ILE:O    | 1:A:29:VAL:HG22 | 0.62     | 1.94        | 5      | 3     |
| 1:C:25:ILE:O    | 1:C:29:VAL:HG22 | 0.62     | 1.94        | 5      | 3     |
| 1:D:25:ILE:O    | 1:D:29:VAL:HG22 | 0.62     | 1.94        | 5      | 3     |
| 1:C:18:ILE:O    | 1:C:22:VAL:HG22 | 0.62     | 1.95        | 4      | 2     |
| 1:E:18:ILE:O    | 1:E:22:VAL:HG22 | 0.62     | 1.95        | 4      | 2     |
| 1:A:18:ILE:O    | 1:A:22:VAL:HG22 | 0.61     | 1.95        | 4      | 2     |
| 1:D:18:ILE:O    | 1:D:22:VAL:HG22 | 0.60     | 1.95        | 4      | 2     |
| 1:C:33:PHE:O    | 1:C:37:THR:HG23 | 0.59     | 1.98        | 4      | 1     |
| 1:E:33:PHE:O    | 1:E:37:THR:HG23 | 0.59     | 1.98        | 4      | 1     |
| 1:A:33:PHE:O    | 1:A:37:THR:HG23 | 0.58     | 1.98        | 4      | 1     |
| 1:B:33:PHE:O    | 1:B:37:THR:HG23 | 0.58     | 1.98        | 4      | 1     |
| 1:D:33:PHE:O    | 1:D:37:THR:HG23 | 0.58     | 1.98        | 4      | 1     |
| 1:C:25:ILE:HD11 | 1:D:22:VAL:HG22 | 0.58     | 1.76        | 5      | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:25:ILE:HD11 | 1:B:22:VAL:HG23 | 0.57     | 1.77        | 5      | 1     |
| 1:B:25:ILE:HD11 | 1:C:22:VAL:HG22 | 0.57     | 1.76        | 5      | 1     |
| 1:A:22:VAL:HG22 | 1:E:25:ILE:HD11 | 0.56     | 1.76        | 5      | 1     |
| 1:B:25:ILE:HD11 | 1:C:22:VAL:HG23 | 0.56     | 1.77        | 5      | 1     |
| 1:D:25:ILE:HD11 | 1:E:22:VAL:HG22 | 0.56     | 1.76        | 5      | 1     |
| 1:A:25:ILE:HD11 | 1:B:22:VAL:HG22 | 0.56     | 1.77        | 5      | 1     |
| 1:C:25:ILE:HD11 | 1:D:22:VAL:HG23 | 0.56     | 1.77        | 5      | 1     |
| 1:E:17:PHE:O    | 1:E:21:VAL:HG23 | 0.55     | 2.02        | 6      | 2     |
| 1:D:25:ILE:HD11 | 1:E:22:VAL:HG23 | 0.55     | 1.77        | 5      | 1     |
| 1:D:17:PHE:O    | 1:D:21:VAL:HG23 | 0.54     | 2.02        | 6      | 2     |
| 1:A:17:PHE:O    | 1:A:21:VAL:HG23 | 0.54     | 2.02        | 6      | 2     |
| 1:A:25:ILE:HG23 | 1:B:26:THR:HB   | 0.54     | 1.80        | 8      | 4     |
| 1:B:29:VAL:HG23 | 1:B:33:PHE:CE2  | 0.54     | 2.38        | 1      | 1     |
| 1:A:29:VAL:HG23 | 1:A:33:PHE:CE2  | 0.54     | 2.38        | 1      | 1     |
| 1:D:29:VAL:HG23 | 1:D:33:PHE:CE2  | 0.54     | 2.38        | 1      | 1     |
| 1:B:34:LEU:HD13 | 1:B:34:LEU:O    | 0.54     | 2.03        | 6      | 1     |
| 1:B:17:PHE:O    | 1:B:21:VAL:HG23 | 0.53     | 2.02        | 6      | 2     |
| 1:C:17:PHE:O    | 1:C:21:VAL:HG23 | 0.53     | 2.02        | 6      | 2     |
| 1:D:18:ILE:O    | 1:D:22:VAL:HG12 | 0.53     | 2.03        | 3      | 3     |
| 1:A:22:VAL:HG23 | 1:E:25:ILE:HD11 | 0.53     | 1.77        | 5      | 1     |
| 1:E:18:ILE:O    | 1:E:22:VAL:HG12 | 0.53     | 2.03        | 3      | 3     |
| 1:D:25:ILE:HG23 | 1:E:26:THR:HB   | 0.53     | 1.80        | 5      | 4     |
| 1:A:18:ILE:O    | 1:A:22:VAL:HG12 | 0.53     | 2.03        | 3      | 3     |
| 1:A:34:LEU:HD13 | 1:A:34:LEU:O    | 0.53     | 2.04        | 6      | 1     |
| 1:C:34:LEU:O    | 1:C:34:LEU:HD13 | 0.53     | 2.03        | 6      | 1     |
| 1:A:26:THR:HB   | 1:E:25:ILE:HG23 | 0.53     | 1.81        | 5      | 4     |
| 1:C:22:VAL:O    | 1:C:26:THR:HG22 | 0.53     | 2.04        | 4      | 1     |
| 1:B:25:ILE:HG23 | 1:C:26:THR:HB   | 0.53     | 1.81        | 5      | 4     |
| 1:C:18:ILE:O    | 1:C:22:VAL:HG12 | 0.53     | 2.03        | 3      | 3     |
| 1:E:29:VAL:HG23 | 1:E:33:PHE:CE2  | 0.52     | 2.38        | 1      | 1     |
| 1:B:18:ILE:O    | 1:B:22:VAL:HG12 | 0.52     | 2.03        | 3      | 3     |
| 1:E:22:VAL:O    | 1:E:26:THR:HG22 | 0.52     | 2.04        | 4      | 1     |
| 1:C:25:ILE:HG23 | 1:D:26:THR:HB   | 0.52     | 1.81        | 5      | 4     |
| 1:D:22:VAL:O    | 1:D:26:THR:HG22 | 0.52     | 2.04        | 4      | 1     |
| 1:E:34:LEU:HD13 | 1:E:34:LEU:O    | 0.52     | 2.03        | 6      | 1     |
| 1:C:29:VAL:HG23 | 1:C:33:PHE:CE2  | 0.52     | 2.38        | 1      | 1     |
| 1:A:25:ILE:HD11 | 1:B:22:VAL:HB   | 0.52     | 1.82        | 4      | 2     |
| 1:A:14:VAL:O    | 1:A:18:ILE:HG22 | 0.52     | 2.05        | 8      | 1     |
| 1:B:25:ILE:HD11 | 1:C:22:VAL:HB   | 0.52     | 1.82        | 4      | 2     |
| 1:A:22:VAL:O    | 1:A:26:THR:HG22 | 0.52     | 2.04        | 4      | 1     |
| 1:B:22:VAL:O    | 1:B:26:THR:HG22 | 0.52     | 2.04        | 4      | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:D:34:LEU:O    | 1:D:34:LEU:HD13 | 0.51     | 2.04        | 6      | 1     |
| 1:D:25:ILE:HD11 | 1:E:22:VAL:HB   | 0.51     | 1.82        | 4      | 2     |
| 1:E:25:ILE:O    | 1:E:29:VAL:HG23 | 0.51     | 2.05        | 7      | 2     |
| 1:A:25:ILE:O    | 1:A:29:VAL:HG23 | 0.51     | 2.05        | 7      | 2     |
| 1:A:22:VAL:HB   | 1:E:25:ILE:HD11 | 0.51     | 1.82        | 4      | 2     |
| 1:D:21:VAL:CG1  | 1:E:22:VAL:HG21 | 0.51     | 2.36        | 4      | 1     |
| 1:C:25:ILE:O    | 1:C:29:VAL:HG23 | 0.51     | 2.05        | 7      | 2     |
| 1:D:25:ILE:O    | 1:D:29:VAL:HG23 | 0.51     | 2.05        | 7      | 2     |
| 1:C:21:VAL:CG1  | 1:D:22:VAL:HG21 | 0.51     | 2.36        | 4      | 1     |
| 1:C:14:VAL:O    | 1:C:18:ILE:HG22 | 0.51     | 2.05        | 8      | 1     |
| 1:D:14:VAL:O    | 1:D:18:ILE:HG22 | 0.51     | 2.05        | 8      | 1     |
| 1:B:14:VAL:O    | 1:B:18:ILE:HG22 | 0.51     | 2.05        | 8      | 1     |
| 1:E:14:VAL:O    | 1:E:18:ILE:HG22 | 0.50     | 2.05        | 8      | 1     |
| 1:C:25:ILE:HD11 | 1:D:22:VAL:HB   | 0.50     | 1.82        | 4      | 2     |
| 1:B:25:ILE:O    | 1:B:29:VAL:HG23 | 0.50     | 2.05        | 7      | 2     |
| 1:A:21:VAL:CG1  | 1:B:22:VAL:HG21 | 0.50     | 2.36        | 4      | 1     |
| 1:C:14:VAL:HG22 | 1:D:15:ASN:HB2  | 0.50     | 1.84        | 4      | 1     |
| 1:A:21:VAL:O    | 1:A:25:ILE:HD12 | 0.50     | 2.07        | 7      | 1     |
| 1:C:21:VAL:O    | 1:C:25:ILE:HD12 | 0.50     | 2.07        | 7      | 1     |
| 1:A:22:VAL:HG21 | 1:E:21:VAL:CG1  | 0.50     | 2.36        | 4      | 1     |
| 1:B:21:VAL:O    | 1:B:25:ILE:HD12 | 0.50     | 2.07        | 7      | 1     |
| 1:D:21:VAL:O    | 1:D:25:ILE:HD12 | 0.50     | 2.07        | 7      | 1     |
| 1:A:14:VAL:CG2  | 1:B:11:LEU:HD21 | 0.49     | 2.37        | 4      | 1     |
| 1:B:14:VAL:CG2  | 1:C:11:LEU:HD21 | 0.49     | 2.37        | 4      | 1     |
| 1:B:21:VAL:CG1  | 1:C:22:VAL:HG21 | 0.49     | 2.36        | 4      | 1     |
| 1:A:15:ASN:HB2  | 1:E:14:VAL:HG22 | 0.49     | 1.84        | 4      | 1     |
| 1:D:14:VAL:CG2  | 1:E:11:LEU:HD21 | 0.49     | 2.37        | 4      | 1     |
| 1:A:22:VAL:HG23 | 1:E:21:VAL:CG1  | 0.49     | 2.38        | 8      | 1     |
| 1:C:21:VAL:CG1  | 1:D:22:VAL:HG23 | 0.49     | 2.38        | 8      | 1     |
| 1:A:11:LEU:HD21 | 1:E:14:VAL:CG2  | 0.49     | 2.37        | 4      | 1     |
| 1:A:22:VAL:HG21 | 1:E:21:VAL:HG11 | 0.49     | 1.85        | 2      | 2     |
| 1:B:14:VAL:HG22 | 1:C:15:ASN:HB2  | 0.49     | 1.83        | 4      | 1     |
| 1:B:21:VAL:CG1  | 1:C:22:VAL:HG23 | 0.49     | 2.38        | 8      | 1     |
| 1:D:14:VAL:HG22 | 1:E:15:ASN:HB2  | 0.49     | 1.83        | 4      | 1     |
| 1:B:21:VAL:HG11 | 1:C:22:VAL:HG21 | 0.48     | 1.85        | 2      | 2     |
| 1:E:21:VAL:O    | 1:E:25:ILE:HD12 | 0.48     | 2.07        | 7      | 1     |
| 1:D:21:VAL:CG1  | 1:E:22:VAL:HG23 | 0.48     | 2.38        | 8      | 1     |
| 1:C:21:VAL:HG11 | 1:D:22:VAL:CG1  | 0.48     | 2.39        | 10     | 1     |
| 1:C:14:VAL:CG2  | 1:D:11:LEU:HD21 | 0.48     | 2.37        | 4      | 1     |
| 1:A:14:VAL:HG22 | 1:B:15:ASN:HB2  | 0.48     | 1.83        | 4      | 1     |
| 1:A:21:VAL:CG1  | 1:B:22:VAL:HG23 | 0.48     | 2.38        | 8      | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:C:21:VAL:HG11 | 1:D:22:VAL:HG21 | 0.48     | 1.85        | 2      | 2     |
| 1:B:31:MET:O    | 1:B:35:THR:HG23 | 0.48     | 2.09        | 3      | 2     |
| 1:E:31:MET:O    | 1:E:35:THR:HG23 | 0.47     | 2.09        | 3      | 2     |
| 1:D:21:VAL:HG11 | 1:E:22:VAL:HG21 | 0.47     | 1.85        | 2      | 2     |
| 1:D:31:MET:O    | 1:D:35:THR:HG23 | 0.47     | 2.09        | 3      | 2     |
| 1:C:31:MET:O    | 1:C:35:THR:HG23 | 0.47     | 2.09        | 3      | 2     |
| 1:D:25:ILE:O    | 1:D:29:VAL:HG13 | 0.47     | 2.10        | 8      | 1     |
| 1:A:33:PHE:HE2  | 1:E:36:ALA:HB3  | 0.47     | 1.70        | 7      | 1     |
| 1:A:21:VAL:HG11 | 1:B:22:VAL:CG1  | 0.47     | 2.39        | 10     | 1     |
| 1:B:21:VAL:HG11 | 1:C:22:VAL:CG1  | 0.47     | 2.39        | 10     | 1     |
| 1:A:31:MET:O    | 1:A:35:THR:HG23 | 0.47     | 2.10        | 5      | 2     |
| 1:C:25:ILE:O    | 1:C:29:VAL:HG13 | 0.47     | 2.10        | 8      | 1     |
| 1:E:25:ILE:O    | 1:E:29:VAL:HG13 | 0.47     | 2.10        | 8      | 1     |
| 1:A:22:VAL:CG1  | 1:E:21:VAL:HG11 | 0.47     | 2.39        | 10     | 1     |
| 1:A:21:VAL:HG11 | 1:B:22:VAL:HG21 | 0.46     | 1.85        | 2      | 2     |
| 1:C:36:ALA:HB3  | 1:D:33:PHE:HE2  | 0.46     | 1.70        | 7      | 1     |
| 1:A:25:ILE:O    | 1:A:29:VAL:HG12 | 0.46     | 2.10        | 4      | 2     |
| 1:C:25:ILE:O    | 1:C:29:VAL:HG12 | 0.46     | 2.10        | 4      | 2     |
| 1:A:25:ILE:O    | 1:A:29:VAL:HG13 | 0.46     | 2.10        | 8      | 1     |
| 1:E:25:ILE:O    | 1:E:29:VAL:HG12 | 0.46     | 2.10        | 4      | 2     |
| 1:B:36:ALA:HB3  | 1:C:33:PHE:HE2  | 0.46     | 1.70        | 7      | 1     |
| 1:B:25:ILE:O    | 1:B:29:VAL:HG13 | 0.46     | 2.10        | 8      | 1     |
| 1:D:25:ILE:O    | 1:D:29:VAL:HG12 | 0.46     | 2.10        | 4      | 1     |
| 1:D:24:ALA:O    | 1:D:28:LEU:HD13 | 0.46     | 2.11        | 8      | 1     |
| 1:A:11:LEU:HD12 | 1:B:11:LEU:HD21 | 0.46     | 1.88        | 7      | 1     |
| 1:A:11:LEU:HD21 | 1:E:11:LEU:HD12 | 0.46     | 1.88        | 7      | 1     |
| 1:C:24:ALA:O    | 1:C:28:LEU:HD13 | 0.45     | 2.11        | 8      | 1     |
| 1:B:25:ILE:O    | 1:B:29:VAL:HG12 | 0.45     | 2.10        | 4      | 2     |
| 1:A:25:ILE:HG21 | 1:B:22:VAL:HG22 | 0.45     | 1.88        | 3      | 1     |
| 1:C:11:LEU:HD12 | 1:D:11:LEU:HD21 | 0.45     | 1.88        | 7      | 1     |
| 1:D:36:ALA:HB3  | 1:E:33:PHE:HE2  | 0.45     | 1.70        | 7      | 1     |
| 1:B:24:ALA:O    | 1:B:28:LEU:HD13 | 0.45     | 2.11        | 8      | 1     |
| 1:A:24:ALA:O    | 1:A:28:LEU:HD13 | 0.45     | 2.11        | 8      | 1     |
| 1:A:22:VAL:HG22 | 1:E:25:ILE:HG21 | 0.45     | 1.89        | 3      | 1     |
| 1:C:25:ILE:HG21 | 1:D:22:VAL:HG22 | 0.45     | 1.89        | 3      | 1     |
| 1:B:28:LEU:C    | 1:B:28:LEU:HD23 | 0.45     | 2.37        | 3      | 3     |
| 1:E:28:LEU:C    | 1:E:28:LEU:HD23 | 0.45     | 2.37        | 3      | 3     |
| 1:C:28:LEU:C    | 1:C:28:LEU:HD23 | 0.44     | 2.37        | 3      | 3     |
| 1:A:36:ALA:HB3  | 1:B:33:PHE:HE2  | 0.44     | 1.70        | 7      | 1     |
| 1:B:11:LEU:HD12 | 1:C:11:LEU:HD21 | 0.44     | 1.87        | 7      | 1     |
| 1:B:25:ILE:HG21 | 1:C:22:VAL:HG22 | 0.44     | 1.88        | 3      | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:D:28:LEU:C    | 1:D:28:LEU:HD23 | 0.44     | 2.37        | 3      | 3     |
| 1:D:11:LEU:HD12 | 1:E:11:LEU:HD21 | 0.44     | 1.88        | 7      | 1     |
| 1:A:28:LEU:C    | 1:A:28:LEU:HD23 | 0.44     | 2.37        | 3      | 3     |
| 1:E:24:ALA:O    | 1:E:28:LEU:HD13 | 0.44     | 2.11        | 8      | 1     |
| 1:D:21:VAL:HG11 | 1:E:22:VAL:CG1  | 0.44     | 2.39        | 10     | 1     |
| 1:E:9:ILE:H     | 1:E:9:ILE:HD13  | 0.44     | 1.73        | 10     | 1     |
| 1:A:18:ILE:HD12 | 1:A:18:ILE:C    | 0.44     | 2.38        | 6      | 1     |
| 1:A:22:VAL:HG22 | 1:E:25:ILE:CG2  | 0.43     | 2.43        | 3      | 1     |
| 1:E:34:LEU:O    | 1:E:34:LEU:HD23 | 0.43     | 2.14        | 3      | 1     |
| 1:D:25:ILE:HG21 | 1:E:22:VAL:HG22 | 0.43     | 1.89        | 3      | 1     |
| 1:D:25:ILE:CG2  | 1:E:22:VAL:HG22 | 0.43     | 2.43        | 3      | 1     |
| 1:B:21:VAL:HG12 | 1:C:22:VAL:HG23 | 0.43     | 1.90        | 8      | 1     |
| 1:C:9:ILE:H     | 1:C:9:ILE:HD13  | 0.43     | 1.73        | 10     | 1     |
| 1:A:25:ILE:CG2  | 1:B:22:VAL:HG22 | 0.43     | 2.43        | 3      | 1     |
| 1:D:34:LEU:O    | 1:D:34:LEU:HD23 | 0.43     | 2.14        | 3      | 1     |
| 1:A:9:ILE:O     | 1:A:13:ILE:HD12 | 0.43     | 2.14        | 4      | 1     |
| 1:E:18:ILE:HD12 | 1:E:18:ILE:C    | 0.43     | 2.38        | 6      | 1     |
| 1:E:9:ILE:O     | 1:E:13:ILE:HD12 | 0.43     | 2.14        | 4      | 1     |
| 1:B:34:LEU:HD23 | 1:B:34:LEU:O    | 0.43     | 2.14        | 3      | 1     |
| 1:B:18:ILE:HD12 | 1:B:18:ILE:C    | 0.43     | 2.38        | 6      | 1     |
| 1:A:34:LEU:O    | 1:A:34:LEU:HD23 | 0.43     | 2.14        | 3      | 1     |
| 1:C:18:ILE:HD12 | 1:C:18:ILE:C    | 0.43     | 2.38        | 6      | 1     |
| 1:D:25:ILE:HG22 | 1:E:26:THR:CG2  | 0.43     | 2.44        | 1      | 1     |
| 1:B:25:ILE:CG2  | 1:C:22:VAL:HG22 | 0.43     | 2.43        | 3      | 1     |
| 1:B:9:ILE:O     | 1:B:13:ILE:HD12 | 0.43     | 2.14        | 4      | 1     |
| 1:A:25:ILE:HG22 | 1:B:26:THR:CG2  | 0.42     | 2.44        | 1      | 1     |
| 1:C:17:PHE:O    | 1:C:20:THR:HG22 | 0.42     | 2.15        | 2      | 1     |
| 1:D:9:ILE:O     | 1:D:13:ILE:HD12 | 0.42     | 2.14        | 4      | 1     |
| 1:D:9:ILE:H     | 1:D:9:ILE:HD13  | 0.42     | 1.73        | 10     | 1     |
| 1:A:26:THR:CG2  | 1:E:25:ILE:HG22 | 0.42     | 2.44        | 1      | 1     |
| 1:C:25:ILE:CG2  | 1:D:22:VAL:HG22 | 0.42     | 2.44        | 3      | 1     |
| 1:C:34:LEU:HD23 | 1:C:34:LEU:O    | 0.42     | 2.13        | 3      | 1     |
| 1:C:21:VAL:HG12 | 1:D:22:VAL:HG23 | 0.42     | 1.90        | 8      | 1     |
| 1:A:9:ILE:H     | 1:A:9:ILE:HD13  | 0.42     | 1.73        | 10     | 1     |
| 1:E:37:THR:HG23 | 1:E:38:ARG:N    | 0.42     | 2.29        | 1      | 1     |
| 1:D:18:ILE:HD12 | 1:D:18:ILE:C    | 0.42     | 2.38        | 6      | 1     |
| 1:A:22:VAL:HG23 | 1:E:21:VAL:HG12 | 0.42     | 1.90        | 8      | 1     |
| 1:B:9:ILE:HD13  | 1:B:9:ILE:H     | 0.42     | 1.73        | 10     | 1     |
| 1:C:9:ILE:O     | 1:C:13:ILE:HD12 | 0.42     | 2.14        | 4      | 1     |
| 1:A:21:VAL:HG12 | 1:B:22:VAL:HG23 | 0.42     | 1.90        | 8      | 1     |
| 1:B:17:PHE:O    | 1:B:20:THR:HG22 | 0.41     | 2.15        | 2      | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:C:36:ALA:HB3  | 1:D:33:PHE:HE1  | 0.41     | 1.75        | 4      | 1     |
| 1:B:25:ILE:HG22 | 1:C:26:THR:CG2  | 0.41     | 2.44        | 1      | 1     |
| 1:C:25:ILE:HG22 | 1:D:26:THR:CG2  | 0.41     | 2.44        | 1      | 1     |
| 1:A:17:PHE:O    | 1:A:20:THR:HG22 | 0.41     | 2.15        | 2      | 1     |
| 1:A:9:ILE:HD12  | 1:A:9:ILE:H     | 0.41     | 1.76        | 8      | 1     |
| 1:A:34:LEU:C    | 1:A:34:LEU:HD23 | 0.41     | 2.41        | 10     | 1     |
| 1:C:27:LEU:O    | 1:C:27:LEU:HD13 | 0.41     | 2.16        | 2      | 1     |
| 1:E:27:LEU:HD13 | 1:E:27:LEU:O    | 0.41     | 2.16        | 2      | 1     |
| 1:E:9:ILE:H     | 1:E:9:ILE:HD12  | 0.41     | 1.76        | 8      | 1     |
| 1:D:17:PHE:O    | 1:D:20:THR:HG22 | 0.41     | 2.14        | 2      | 1     |
| 1:E:17:PHE:O    | 1:E:20:THR:HG22 | 0.41     | 2.14        | 2      | 1     |
| 1:A:33:PHE:HE1  | 1:E:36:ALA:HB3  | 0.41     | 1.75        | 4      | 1     |
| 1:A:36:ALA:HB3  | 1:B:33:PHE:HE1  | 0.41     | 1.75        | 4      | 1     |
| 1:D:36:ALA:HB3  | 1:E:33:PHE:HE1  | 0.41     | 1.75        | 4      | 1     |
| 1:C:9:ILE:H     | 1:C:9:ILE:HD12  | 0.41     | 1.76        | 8      | 1     |
| 1:D:21:VAL:HG12 | 1:E:22:VAL:HG23 | 0.41     | 1.90        | 8      | 1     |
| 1:B:34:LEU:C    | 1:B:34:LEU:HD23 | 0.41     | 2.41        | 10     | 1     |
| 1:C:34:LEU:C    | 1:C:34:LEU:HD23 | 0.41     | 2.41        | 10     | 1     |
| 1:E:34:LEU:C    | 1:E:34:LEU:HD23 | 0.41     | 2.41        | 10     | 1     |
| 1:B:21:VAL:HG23 | 1:B:22:VAL:N    | 0.41     | 2.31        | 3      | 2     |
| 1:D:25:ILE:HD11 | 1:E:22:VAL:HG12 | 0.41     | 1.93        | 7      | 1     |
| 1:D:10:GLY:O    | 1:E:11:LEU:HD11 | 0.40     | 2.16        | 10     | 1     |
| 1:C:21:VAL:HG23 | 1:C:22:VAL:N    | 0.40     | 2.32        | 4      | 1     |
| 1:A:27:LEU:HD13 | 1:A:27:LEU:O    | 0.40     | 2.16        | 2      | 1     |
| 1:C:11:LEU:HD12 | 1:C:11:LEU:C    | 0.40     | 2.42        | 2      | 1     |
| 1:A:21:VAL:HG23 | 1:A:22:VAL:N    | 0.40     | 2.31        | 3      | 2     |
| 1:E:21:VAL:HG23 | 1:E:22:VAL:N    | 0.40     | 2.32        | 4      | 1     |
| 1:D:34:LEU:HD23 | 1:D:34:LEU:C    | 0.40     | 2.41        | 10     | 1     |

## 6.3 Torsion angles ⓘ

### 6.3.1 Protein backbone ⓘ

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

| Mol | Chain | Analysed    | Favoured     | Allowed    | Outliers   | Percentiles |     |
|-----|-------|-------------|--------------|------------|------------|-------------|-----|
| 1   | A     | 29/38 (76%) | 28±0 (98±2%) | 1±0 (2±2%) | 0±0 (0±0%) | 100         | 100 |

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| Mol | Chain | Analysed        | Favoured     | Allowed    | Outliers   | Percentiles |     |
|-----|-------|-----------------|--------------|------------|------------|-------------|-----|
| 1   | B     | 29/38 (76%)     | 28±0 (98±2%) | 1±0 (2±2%) | 0±0 (0±0%) | 100         | 100 |
| 1   | C     | 29/38 (76%)     | 28±0 (98±2%) | 1±0 (2±2%) | 0±0 (0±0%) | 100         | 100 |
| 1   | D     | 29/38 (76%)     | 28±0 (98±2%) | 1±0 (2±2%) | 0±0 (0±0%) | 100         | 100 |
| 1   | E     | 29/38 (76%)     | 28±0 (98±2%) | 1±0 (2±2%) | 0±0 (0±0%) | 100         | 100 |
| All | All   | 1450/1900 (76%) | 1415 (98%)   | 35 (2%)    | 0 (0%)     | 100         | 100 |

There are no Ramachandran outliers.

### 6.3.2 Protein sidechains ⓘ

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

| Mol | Chain | Analysed        | Rotameric    | Outliers   | Percentiles |    |
|-----|-------|-----------------|--------------|------------|-------------|----|
| 1   | A     | 25/34 (74%)     | 24±1 (98±3%) | 0±1 (2±3%) | 50          | 92 |
| 1   | B     | 25/34 (74%)     | 24±1 (98±3%) | 0±1 (2±3%) | 50          | 92 |
| 1   | C     | 25/34 (74%)     | 24±1 (98±3%) | 0±1 (2±3%) | 50          | 92 |
| 1   | D     | 25/34 (74%)     | 24±1 (98±3%) | 0±1 (2±3%) | 50          | 92 |
| 1   | E     | 26/34 (76%)     | 26±1 (98±3%) | 0±1 (2±3%) | 52          | 92 |
| All | All   | 1260/1700 (74%) | 1235 (98%)   | 25 (2%)    | 50          | 92 |

All 20 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     | 27  | LEU  | 2              |
| 1   | B     | 27  | LEU  | 2              |
| 1   | C     | 27  | LEU  | 2              |
| 1   | D     | 27  | LEU  | 2              |
| 1   | E     | 27  | LEU  | 2              |
| 1   | A     | 11  | LEU  | 1              |
| 1   | A     | 34  | LEU  | 1              |
| 1   | B     | 11  | LEU  | 1              |
| 1   | B     | 34  | LEU  | 1              |
| 1   | C     | 11  | LEU  | 1              |
| 1   | C     | 34  | LEU  | 1              |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | D     | 11  | LEU  | 1              |
| 1   | D     | 34  | LEU  | 1              |
| 1   | E     | 11  | LEU  | 1              |
| 1   | E     | 34  | LEU  | 1              |
| 1   | A     | 9   | ILE  | 1              |
| 1   | B     | 9   | ILE  | 1              |
| 1   | C     | 9   | ILE  | 1              |
| 1   | D     | 9   | ILE  | 1              |
| 1   | E     | 9   | 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 [i](#)

The completeness of assignment taking into account all chemical shift lists is 7% for the well-defined parts and 6% for the entire structure.

### 7.1 Chemical shift list 1

File name: `working_cs.cif`

Chemical shift list name: *starch\_output*

#### 7.1.1 Bookkeeping [i](#)

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                  | 170 |
| Number of shifts mapped to atoms        | 170 |
| Number of unparsed shifts               | 0   |
| Number of shifts with mapping errors    | 0   |
| Number of shifts with mapping warnings  | 0   |
| Number of shift outliers (ShiftChecker) | 51  |

#### 7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

| Nucleus                | # values | Correction $\pm$ precision, ppm | Suggested action        |
|------------------------|----------|---------------------------------|-------------------------|
| $^{13}\text{C}_\alpha$ | 31       | $-1.61 \pm 1.22$                | None needed (imprecise) |
| $^{13}\text{C}_\beta$  | 30       | $0.91 \pm 0.55$                 | None needed (imprecise) |
| $^{13}\text{C}'$       | 29       | $-1.09 \pm 0.56$                | None needed (imprecise) |
| $^{15}\text{N}$        | 30       | $-2.22 \pm 0.87$                | Should be applied       |

#### 7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 7%, i.e. 149 atoms were assigned a chemical shift out of a possible 2093. 0 out of 40 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total        | $^1\text{H}$ | $^{13}\text{C}$ | $^{15}\text{N}$ |
|-----------|--------------|--------------|-----------------|-----------------|
| Backbone  | 83/735 (11%) | 0/297 (0%)   | 55/292 (19%)    | 28/146 (19%)    |
| Sidechain | 58/1108 (5%) | 0/761 (0%)   | 58/339 (17%)    | 0/8 (0%)        |

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|          | <b>Total</b>  | <b><sup>1</sup>H</b> | <b><sup>13</sup>C</b> | <b><sup>15</sup>N</b> |
|----------|---------------|----------------------|-----------------------|-----------------------|
| Aromatic | 8/250 (3%)    | 0/125 (0%)           | 8/125 (6%)            | 0/0 (—%)              |
| Overall  | 149/2093 (7%) | 0/1183 (0%)          | 121/756 (16%)         | 28/154 (18%)          |

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

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 6%, i.e. 166 atoms were assigned a chemical shift out of a possible 2825. 0 out of 50 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  | 90/945 (10%)  | 0/380 (0%)           | 60/380 (16%)          | 30/185 (16%)          |
| Sidechain | 68/1580 (4%)  | 0/1065 (0%)          | 68/475 (14%)          | 0/40 (0%)             |
| Aromatic  | 8/300 (3%)    | 0/150 (0%)           | 8/150 (5%)            | 0/0 (—%)              |
| Overall   | 166/2825 (6%) | 0/1595 (0%)          | 136/1005 (14%)        | 30/225 (13%)          |

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

#### 7.1.4 Statistically unusual chemical shifts ⓘ

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

| List Id | Chain | Res | Type | Atom | Shift, ppm | Expected range, ppm | Z-score |
|---------|-------|-----|------|------|------------|---------------------|---------|
| 1       | A     | 11  | LEU  | CG   | 122.17     | 21.37 – 32.19       | 88.2    |
| 1       | A     | 15  | ASN  | CB   | 171.51     | 30.50 – 46.89       | 81.0    |
| 1       | A     | 9   | ILE  | CG2  | 119.98     | 10.93 – 24.12       | 77.7    |
| 1       | A     | 18  | ILE  | CG2  | 119.97     | 10.93 – 24.12       | 77.7    |
| 1       | A     | 13  | ILE  | CG2  | 119.78     | 10.93 – 24.12       | 77.5    |
| 1       | A     | 10  | GLY  | C    | 47.59      | 164.92 – 182.89     | -70.3   |
| 1       | A     | 15  | ASN  | C    | 55.70      | 166.56 – 184.06     | -68.3   |
| 1       | A     | 14  | VAL  | CG2  | 122.15     | 13.71 – 28.88       | 66.5    |
| 1       | A     | 11  | LEU  | C    | 57.96      | 167.56 – 186.66     | -62.4   |
| 1       | A     | 13  | ILE  | C    | 62.50      | 166.59 – 185.34     | -60.5   |
| 1       | A     | 14  | VAL  | C    | 64.62      | 166.52 – 184.93     | -60.4   |
| 1       | A     | 17  | PHE  | C    | 60.46      | 165.76 – 185.24     | -59.1   |
| 1       | A     | 16  | PHE  | C    | 62.01      | 165.76 – 185.24     | -58.3   |
| 1       | A     | 19  | PHE  | C    | 62.04      | 165.76 – 185.24     | -58.3   |
| 1       | A     | 18  | ILE  | C    | 67.33      | 166.59 – 185.34     | -57.9   |
| 1       | A     | 10  | GLY  | CA   | 109.51     | 38.93 – 51.79       | 49.9    |

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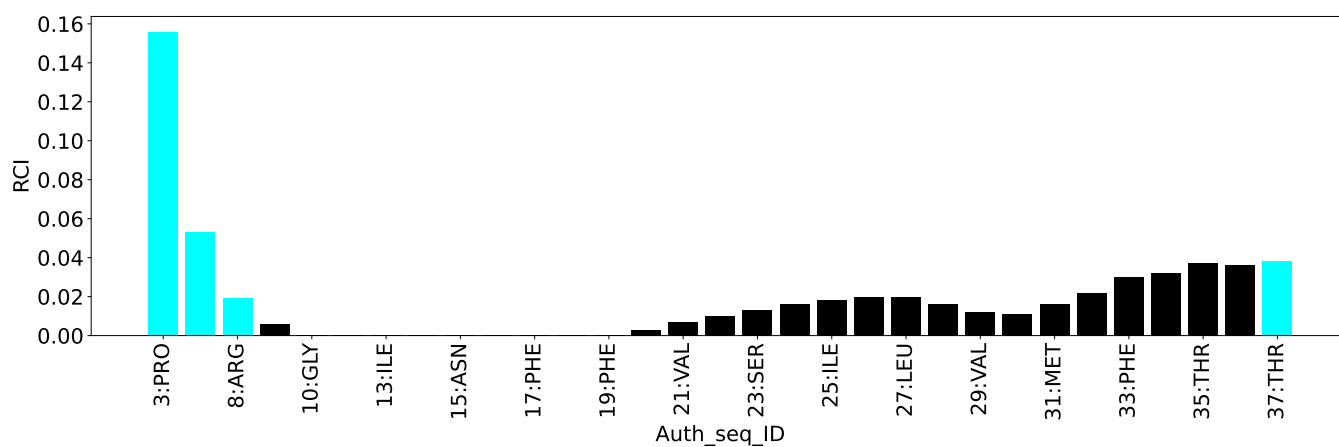
| List Id | Chain | Res | Type | Atom | Shift, ppm | Expected range, ppm | Z-score |
|---------|-------|-----|------|------|------------|---------------------|---------|
| 1       | A     | 19  | PHE  | CB   | 131.09     | 29.72 – 50.07       | 44.8    |
| 1       | A     | 17  | PHE  | CB   | 131.05     | 29.72 – 50.07       | 44.8    |
| 1       | A     | 16  | PHE  | CB   | 130.95     | 29.72 – 50.07       | 44.7    |
| 1       | A     | 15  | ASN  | CG   | 121.11     | 164.52 – 188.90     | -22.8   |
| 1       | A     | 10  | GLY  | N    | 177.88     | 91.59 – 127.52      | 19.0    |
| 1       | A     | 8   | ARG  | CD   | 26.40      | 38.57 – 47.75       | -18.2   |
| 1       | A     | 15  | ASN  | N    | 177.99     | 99.66 – 138.23      | 15.3    |
| 1       | A     | 11  | LEU  | N    | 177.89     | 102.77 – 140.89     | 14.7    |
| 1       | A     | 17  | PHE  | N    | 177.42     | 99.93 – 140.82      | 13.9    |
| 1       | A     | 16  | PHE  | N    | 175.99     | 99.93 – 140.82      | 13.6    |
| 1       | A     | 13  | ILE  | N    | 177.12     | 100.55 – 142.30     | 13.3    |
| 1       | A     | 18  | ILE  | N    | 176.50     | 100.55 – 142.30     | 13.2    |
| 1       | A     | 14  | VAL  | N    | 177.84     | 99.23 – 142.92      | 13.0    |
| 1       | A     | 9   | ILE  | N    | 174.60     | 100.55 – 142.30     | 12.7    |
| 1       | A     | 18  | ILE  | CB   | 14.11      | 28.63 – 48.45       | -12.3   |
| 1       | A     | 13  | ILE  | CB   | 14.19      | 28.63 – 48.45       | -12.3   |
| 1       | A     | 8   | ARG  | CG   | 41.50      | 21.24 – 33.19       | 11.9    |
| 1       | A     | 14  | VAL  | CA   | 30.68      | 48.38 – 76.73       | -11.2   |
| 1       | A     | 13  | ILE  | CD1  | 30.41      | 5.18 – 21.60        | 10.4    |
| 1       | A     | 18  | ILE  | CD1  | 30.37      | 5.18 – 21.60        | 10.3    |
| 1       | A     | 9   | ILE  | CD1  | 30.24      | 5.18 – 21.60        | 10.3    |
| 1       | A     | 11  | LEU  | CB   | 23.96      | 33.11 – 51.34       | -10.0   |
| 1       | A     | 18  | ILE  | CA   | 38.39      | 48.30 – 75.08       | -8.7    |
| 1       | A     | 13  | ILE  | CA   | 38.76      | 48.30 – 75.08       | -8.6    |
| 1       | A     | 15  | ASN  | CA   | 38.62      | 44.28 – 62.79       | -8.1    |
| 1       | A     | 17  | PHE  | CA   | 38.46      | 45.38 – 70.89       | -7.7    |
| 1       | A     | 19  | PHE  | CA   | 38.49      | 45.38 – 70.89       | -7.7    |
| 1       | A     | 16  | PHE  | CA   | 38.60      | 45.38 – 70.89       | -7.7    |
| 1       | A     | 16  | PHE  | CD1  | 139.87     | 125.33 – 137.83     | 6.6     |
| 1       | A     | 11  | LEU  | CA   | 42.43      | 45.17 – 66.21       | -6.3    |
| 1       | A     | 17  | PHE  | CD1  | 139.17     | 125.33 – 137.83     | 6.1     |
| 1       | A     | 9   | ILE  | CG1  | 18.04      | 19.24 – 36.26       | -5.7    |
| 1       | A     | 14  | VAL  | CB   | 22.65      | 23.86 – 41.50       | -5.7    |
| 1       | A     | 13  | ILE  | CG1  | 18.18      | 19.24 – 36.26       | -5.6    |
| 1       | A     | 18  | ILE  | CG1  | 18.21      | 19.24 – 36.26       | -5.6    |

### 7.1.5 Random Coil Index (RCI) plots

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble

composition. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:



## 8 NMR restraints analysis

### 8.1 Conformationally restricting restraints

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

| Description  | Value |
|--|-------|
| Total distance restraints                                | 1795  |
| Intra-residue ( $ i-j =0$ )                              | 26    |
| Sequential ( $ i-j =1$ )                                 | 105   |
| Medium range ( $ i-j >1$ and $ i-j <5$ )                 | 375   |
| Long range ( $ i-j \geq 5$ )                             | 18    |
| Inter-chain  | 1271  |
| Hydrogen bond restraints                                 | 0     |
| Disulfide bond restraints                                | 0     |
| Total dihedral-angle restraints                          | 290   |
| Number of unmapped restraints                            | 0     |
| Number of restraints per residue                         | 11.0  |
| Number of long range restraints per residue <sup>1</sup> | 0.1   |

<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)  | 21.3                                   | 0.2     |
| 0.2-0.5 (Medium) | 49.6                                   | 0.5     |
| >0.5 (Large)     | 48.5                                   | 2.57    |

### 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)   | 0.4                                    | 1.22    |
| 10.0-20.0 (Medium) | None                                   | None    |
| >20.0 (Large)      | None                                   | None    |

## 9 Distance violation analysis ⓘ

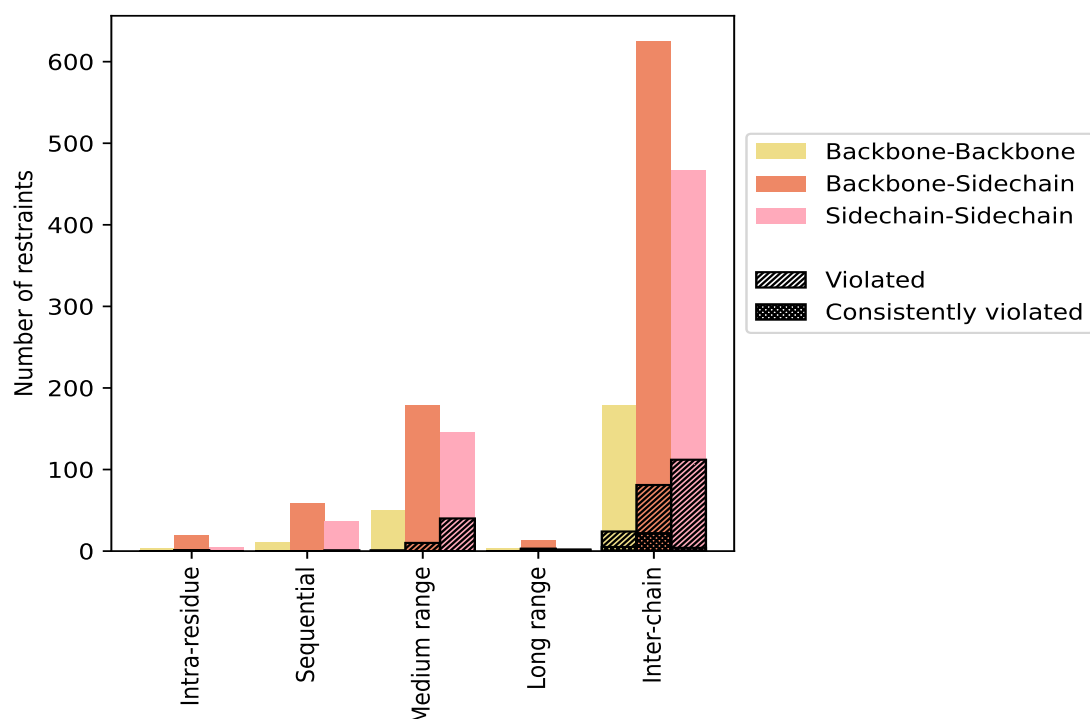
### 9.1 Summary of distance violations ⓘ

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

| Restrains type  | Count       | % <sup>1</sup> | Violated <sup>3</sup> |                |                | Consistently Violated <sup>4</sup> |                |                |
|---|-------------|----------------|-----------------------|----------------|----------------|------------------------------------|----------------|----------------|
|   |             |                | Count                 | % <sup>2</sup> | % <sup>1</sup> | Count                              | % <sup>2</sup> | % <sup>1</sup> |
| <b>Intra-residue (<math> i-j =0</math>)</b>                                 | <b>26</b>   | <b>1.4</b>     | <b>1</b>              | <b>3.8</b>     | <b>0.1</b>     | <b>1</b>                           | <b>3.8</b>     | <b>0.1</b>     |
| Backbone-Backbone   | 3           | 0.2            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain  | 19          | 1.1            | 1                     | 5.3            | 0.1            | 1                                  | 5.3            | 0.1            |
| Sidechain-Sidechain   | 4           | 0.2            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| <b>Sequential (<math> i-j =1</math>)</b>                                    | <b>105</b>  | <b>5.8</b>     | <b>1</b>              | <b>1.0</b>     | <b>0.1</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| Backbone-Backbone   | 11          | 0.6            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain  | 58          | 3.2            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Sidechain-Sidechain   | 36          | 2.0            | 1                     | 2.8            | 0.1            | 0                                  | 0.0            | 0.0            |
| <b>Medium range (<math> i-j &gt;1</math> &amp; <math> i-j &lt;5</math>)</b> | <b>375</b>  | <b>20.9</b>    | <b>51</b>             | <b>13.6</b>    | <b>2.8</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| Backbone-Backbone   | 50          | 2.8            | 1                     | 2.0            | 0.1            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain  | 179         | 10.0           | 10                    | 5.6            | 0.6            | 0                                  | 0.0            | 0.0            |
| Sidechain-Sidechain   | 146         | 8.1            | 40                    | 27.4           | 2.2            | 0                                  | 0.0            | 0.0            |
| <b>Long range (<math> i-j \geq 5</math>)</b>                                | <b>18</b>   | <b>1.0</b>     | <b>5</b>              | <b>27.8</b>    | <b>0.3</b>     | <b>3</b>                           | <b>16.7</b>    | <b>0.2</b>     |
| Backbone-Backbone   | 3           | 0.2            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain  | 13          | 0.7            | 3                     | 23.1           | 0.2            | 2                                  | 15.4           | 0.1            |
| Sidechain-Sidechain   | 2           | 0.1            | 2                     | 100.0          | 0.1            | 1                                  | 50.0           | 0.1            |
| <b>Inter-chain</b>  | <b>1271</b> | <b>70.8</b>    | <b>217</b>            | <b>17.1</b>    | <b>12.1</b>    | <b>31</b>                          | <b>2.4</b>     | <b>1.7</b>     |
| Backbone-Backbone   | 179         | 10.0           | 24                    | 13.4           | 1.3            | 5                                  | 2.8            | 0.3            |
| Backbone-Sidechain  | 625         | 34.8           | 81                    | 13.0           | 4.5            | 22                                 | 3.5            | 1.2            |
| Sidechain-Sidechain   | 467         | 26.0           | 112                   | 24.0           | 6.2            | 4                                  | 0.9            | 0.2            |
| Hydrogen bond   | 0           | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Disulfide bond  | 0           | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| <b>Total</b>  | <b>1795</b> | <b>100.0</b>   | <b>275</b>            | <b>15.3</b>    | <b>15.3</b>    | <b>35</b>                          | <b>1.9</b>     | <b>1.9</b>     |
| Backbone-Backbone   | 246         | 13.7           | 25                    | 10.2           | 1.4            | 5                                  | 2.0            | 0.3            |
| Backbone-Sidechain  | 894         | 49.8           | 95                    | 10.6           | 5.3            | 25                                 | 2.8            | 1.4            |
| Sidechain-Sidechain   | 655         | 36.5           | 155                   | 23.7           | 8.6            | 5                                  | 0.8            | 0.3            |

<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

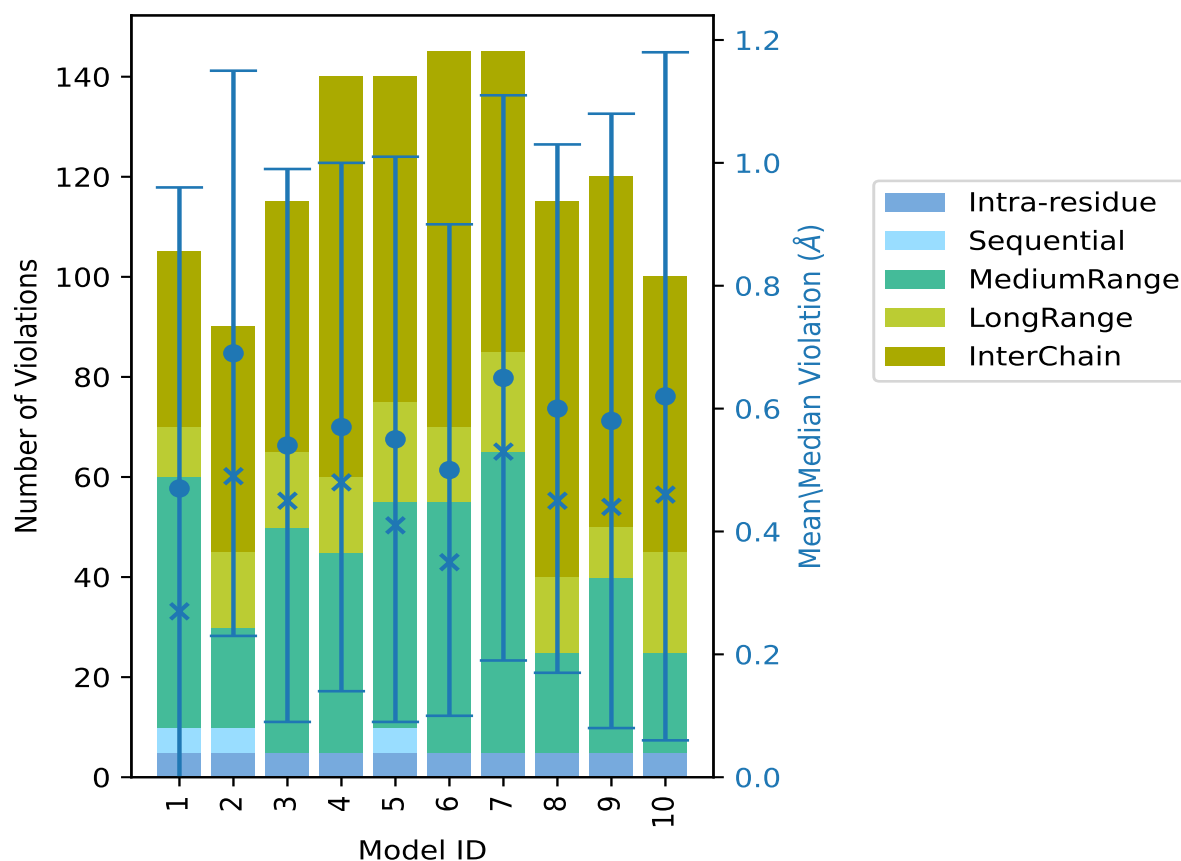
## 9.2 Distance violation statistics for each model [i](#)

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        | 5                    | 5               | 50              | 10              | 35              | 105   | 0.47     | 2.31    | 0.49                | 0.27       |
| 2        | 5                    | 5               | 20              | 15              | 45              | 90    | 0.69     | 1.79    | 0.46                | 0.49       |
| 3        | 5                    | 0               | 45              | 15              | 50              | 115   | 0.54     | 2.19    | 0.45                | 0.45       |
| 4        | 5                    | 0               | 40              | 15              | 80              | 140   | 0.57     | 2.08    | 0.43                | 0.48       |
| 5        | 5                    | 5               | 45              | 20              | 65              | 140   | 0.55     | 2.53    | 0.46                | 0.41       |
| 6        | 5                    | 0               | 50              | 15              | 75              | 145   | 0.5      | 1.68    | 0.4                 | 0.35       |
| 7        | 5                    | 0               | 60              | 20              | 60              | 145   | 0.65     | 2.24    | 0.46                | 0.53       |
| 8        | 5                    | 0               | 20              | 15              | 75              | 115   | 0.6      | 1.86    | 0.43                | 0.45       |
| 9        | 5                    | 0               | 35              | 10              | 70              | 120   | 0.58     | 2.45    | 0.5                 | 0.44       |
| 10       | 5                    | 0               | 20              | 20              | 55              | 100   | 0.62     | 2.57    | 0.56                | 0.46       |

<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, 1520(IR:25, SQ:104, MR:324, LR:13, IC:1054) restraints are not violated in the ensemble.

| Number of violated restraints |                 |                 |                 |                 |       | Fraction of the ensemble |      |
|-------------------------------|-----------------|-----------------|-----------------|-----------------|-------|--------------------------|------|
| IR <sup>1</sup>               | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total | Count <sup>6</sup>       | %    |
| 0                             | 0               | 19              | 0               | 51              | 70    | 1                        | 10.0 |
| 0                             | 1               | 13              | 0               | 31              | 45    | 2                        | 20.0 |
| 0                             | 0               | 2               | 0               | 13              | 15    | 3                        | 30.0 |

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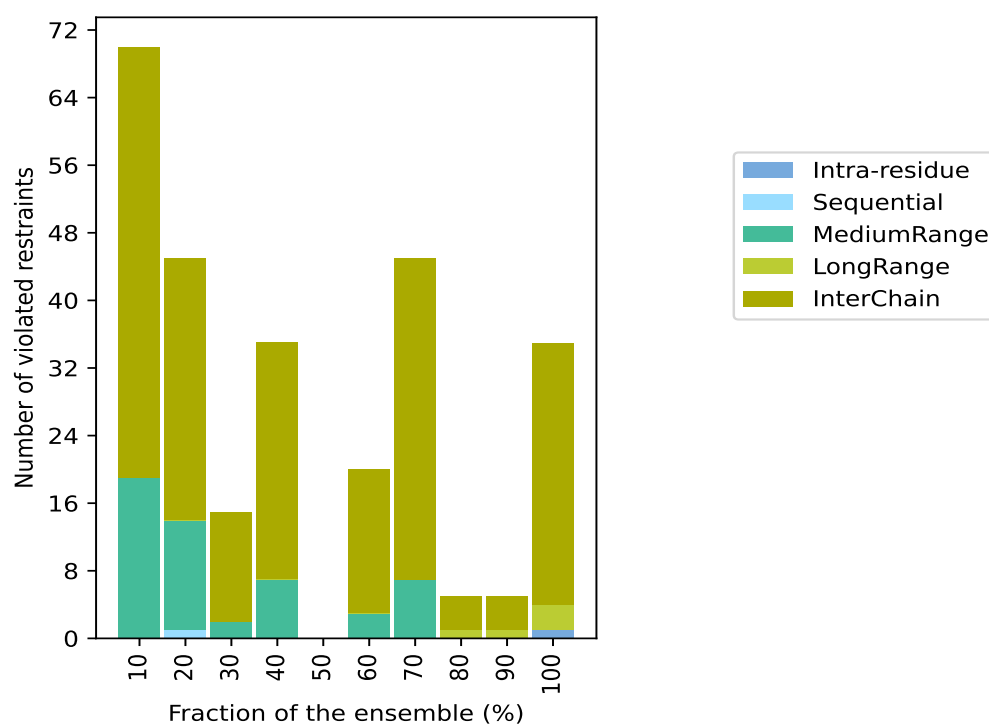


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| Number of violated restraints |                 |                 |                 |                 |       | Fraction of the ensemble |       |
|-------------------------------|-----------------|-----------------|-----------------|-----------------|-------|--------------------------|-------|
| IR <sup>1</sup>               | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total | Count <sup>6</sup>       | %     |
| 0                             | 0               | 7               | 0               | 28              | 35    | 4                        | 40.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 5                        | 50.0  |
| 0                             | 0               | 3               | 0               | 17              | 20    | 6                        | 60.0  |
| 0                             | 0               | 7               | 0               | 38              | 45    | 7                        | 70.0  |
| 0                             | 0               | 0               | 1               | 4               | 5     | 8                        | 80.0  |
| 0                             | 0               | 0               | 1               | 4               | 5     | 9                        | 90.0  |
| 1                             | 0               | 0               | 3               | 31              | 35    | 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 ⓘ

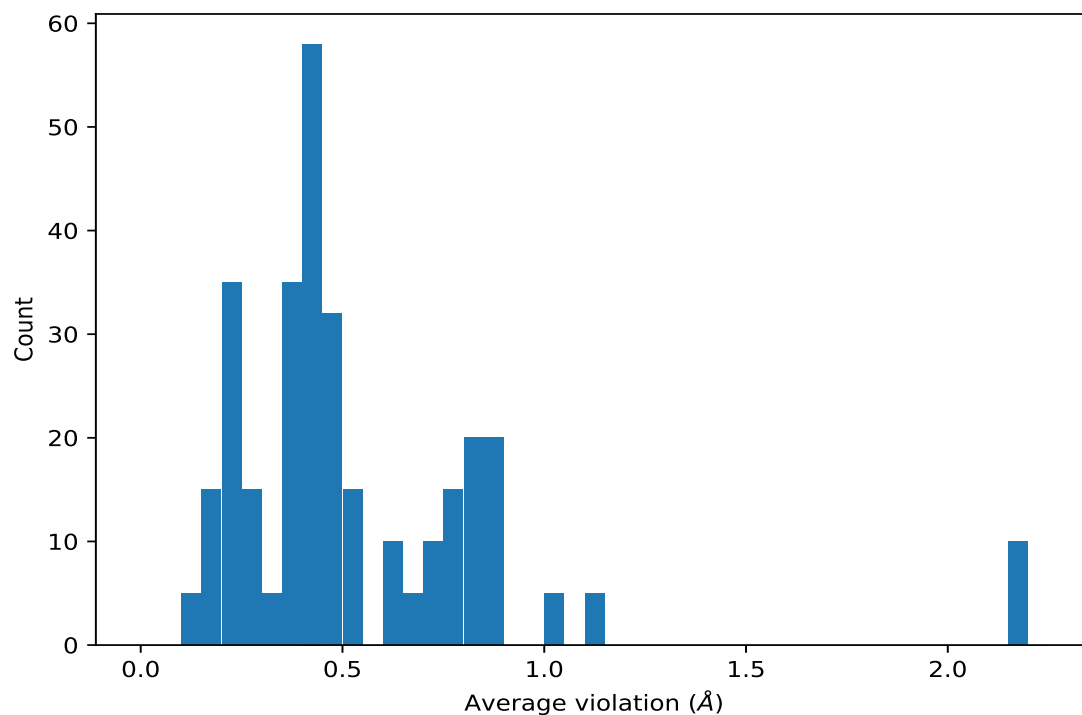


## 9.4 Most violated distance restraints in the ensemble ⓘ

### 9.4.1 Histogram : Distribution of mean distance violations ⓘ

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

in the ensemble



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

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

| Key    | Atom-1         | Atom-2         | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|--------|----------------|----------------|---------------------|----------|---------------------|------------|
| (7,7)  | 1:20:B:THR:CG2 | 1:14:B:VAL:CG2 | 10                  | 2.17     | 0.3                 | 2.22       |
| (7,7)  | 1:20:B:THR:CG2 | 1:26:B:THR:CG2 | 10                  | 2.17     | 0.3                 | 2.22       |
| (7,8)  | 1:20:C:THR:CG2 | 1:14:C:VAL:CG2 | 10                  | 2.17     | 0.3                 | 2.22       |
| (7,8)  | 1:20:C:THR:CG2 | 1:26:C:THR:CG2 | 10                  | 2.17     | 0.3                 | 2.22       |
| (7,9)  | 1:20:D:THR:CG2 | 1:14:D:VAL:CG2 | 10                  | 2.17     | 0.3                 | 2.22       |
| (7,9)  | 1:20:D:THR:CG2 | 1:26:D:THR:CG2 | 10                  | 2.17     | 0.3                 | 2.22       |
| (7,10) | 1:20:E:THR:CG2 | 1:14:E:VAL:CG2 | 10                  | 2.17     | 0.3                 | 2.22       |
| (7,10) | 1:20:E:THR:CG2 | 1:26:E:THR:CG2 | 10                  | 2.17     | 0.3                 | 2.22       |
| (7,6)  | 1:20:A:THR:CG2 | 1:14:A:VAL:CG2 | 10                  | 2.17     | 0.3                 | 2.22       |
| (7,6)  | 1:20:A:THR:CG2 | 1:26:A:THR:CG2 | 10                  | 2.17     | 0.3                 | 2.22       |
| (7,2)  | 1:37:B:THR:CA  | 1:32:B:ALA:CB  | 10                  | 1.15     | 0.16                | 1.21       |
| (7,3)  | 1:37:C:THR:CA  | 1:32:C:ALA:CB  | 10                  | 1.15     | 0.16                | 1.21       |
| (7,4)  | 1:37:D:THR:CA  | 1:32:D:ALA:CB  | 10                  | 1.15     | 0.16                | 1.21       |
| (7,5)  | 1:37:E:THR:CA  | 1:32:E:ALA:CB  | 10                  | 1.15     | 0.16                | 1.21       |
| (7,1)  | 1:37:A:THR:CA  | 1:32:A:ALA:CB  | 10                  | 1.15     | 0.15                | 1.21       |

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| Key     | Atom-1         | Atom-2        | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|----------------|---------------|---------------------|----------|---------------------|------------|
| (1,866) | 1:32:A:ALA:CB  | 1:26:B:THR:CA | 10                  | 0.51     | 0.26                | 0.4        |
| (1,867) | 1:32:B:ALA:CB  | 1:26:C:THR:CA | 10                  | 0.51     | 0.26                | 0.4        |
| (1,868) | 1:32:C:ALA:CB  | 1:26:D:THR:CA | 10                  | 0.51     | 0.26                | 0.4        |
| (1,869) | 1:32:D:ALA:CB  | 1:26:E:THR:CA | 10                  | 0.51     | 0.26                | 0.4        |
| (1,870) | 1:32:E:ALA:CB  | 1:26:A:THR:CA | 10                  | 0.51     | 0.26                | 0.4        |
| (2,177) | 1:34:B:LEU:CA  | 1:34:B:LEU:CB | 10                  | 0.46     | 0.0                 | 0.46       |
| (2,179) | 1:34:D:LEU:CA  | 1:34:D:LEU:CB | 10                  | 0.46     | 0.0                 | 0.46       |
| (2,176) | 1:34:A:LEU:CA  | 1:34:A:LEU:CB | 10                  | 0.46     | 0.0                 | 0.46       |
| (2,178) | 1:34:C:LEU:CA  | 1:34:C:LEU:CB | 10                  | 0.46     | 0.0                 | 0.46       |
| (2,180) | 1:34:E:LEU:CA  | 1:34:E:LEU:CB | 10                  | 0.46     | 0.0                 | 0.46       |
| (3,67)  | 1:27:B:LEU:CB  | 1:25:A:ILE:N  | 10                  | 0.38     | 0.05                | 0.37       |
| (3,68)  | 1:27:C:LEU:CB  | 1:25:B:ILE:N  | 10                  | 0.38     | 0.05                | 0.37       |
| (3,69)  | 1:27:D:LEU:CB  | 1:25:C:ILE:N  | 10                  | 0.38     | 0.05                | 0.37       |
| (3,70)  | 1:27:E:LEU:CB  | 1:25:D:ILE:N  | 10                  | 0.38     | 0.05                | 0.37       |
| (3,66)  | 1:27:A:LEU:CB  | 1:25:E:ILE:N  | 10                  | 0.37     | 0.05                | 0.37       |
| (3,17)  | 1:34:B:LEU:CB  | 1:35:A:THR:N  | 10                  | 0.24     | 0.03                | 0.24       |
| (3,19)  | 1:34:D:LEU:CB  | 1:35:C:THR:N  | 10                  | 0.24     | 0.03                | 0.24       |
| (3,16)  | 1:34:A:LEU:CB  | 1:35:E:THR:N  | 10                  | 0.24     | 0.03                | 0.24       |
| (3,18)  | 1:34:C:LEU:CB  | 1:35:B:THR:N  | 10                  | 0.24     | 0.03                | 0.24       |
| (3,20)  | 1:34:E:LEU:CB  | 1:35:D:THR:N  | 10                  | 0.24     | 0.03                | 0.24       |
| (3,146) | 1:13:A:ILE:CA  | 1:16:B:PHE:N  | 10                  | 0.19     | 0.03                | 0.2        |
| (3,147) | 1:13:B:ILE:CA  | 1:16:C:PHE:N  | 10                  | 0.19     | 0.03                | 0.2        |
| (3,148) | 1:13:C:ILE:CA  | 1:16:D:PHE:N  | 10                  | 0.19     | 0.03                | 0.2        |
| (3,149) | 1:13:D:ILE:CA  | 1:16:E:PHE:N  | 10                  | 0.19     | 0.03                | 0.2        |
| (3,150) | 1:13:E:ILE:CA  | 1:16:A:PHE:N  | 10                  | 0.19     | 0.03                | 0.2        |
| (7,16)  | 1:37:A:THR:CG2 | 1:32:E:ALA:CB | 9                   | 0.43     | 0.25                | 0.43       |
| (7,16)  | 1:37:A:THR:CG2 | 1:32:A:ALA:CB | 9                   | 0.43     | 0.25                | 0.43       |
| (7,18)  | 1:37:C:THR:CG2 | 1:32:B:ALA:CB | 9                   | 0.43     | 0.25                | 0.43       |
| (7,18)  | 1:37:C:THR:CG2 | 1:32:C:ALA:CB | 9                   | 0.43     | 0.25                | 0.43       |
| (7,19)  | 1:37:D:THR:CG2 | 1:32:C:ALA:CB | 9                   | 0.43     | 0.25                | 0.43       |
| (7,19)  | 1:37:D:THR:CG2 | 1:32:D:ALA:CB | 9                   | 0.43     | 0.25                | 0.43       |
| (7,20)  | 1:37:E:THR:CG2 | 1:32:D:ALA:CB | 9                   | 0.43     | 0.25                | 0.43       |
| (7,20)  | 1:37:E:THR:CG2 | 1:32:E:ALA:CB | 9                   | 0.43     | 0.25                | 0.43       |
| (7,17)  | 1:37:B:THR:CG2 | 1:32:A:ALA:CB | 9                   | 0.43     | 0.25                | 0.42       |
| (7,17)  | 1:37:B:THR:CG2 | 1:32:B:ALA:CB | 9                   | 0.43     | 0.25                | 0.42       |
| (7,11)  | 1:37:A:THR:CG2 | 1:30:A:SER:CA | 8                   | 1.02     | 0.22                | 1.02       |
| (7,12)  | 1:37:B:THR:CG2 | 1:30:B:SER:CA | 8                   | 1.02     | 0.22                | 1.02       |
| (7,15)  | 1:37:E:THR:CG2 | 1:30:E:SER:CA | 8                   | 1.02     | 0.22                | 1.02       |
| (7,13)  | 1:37:C:THR:CG2 | 1:30:C:SER:CA | 8                   | 1.02     | 0.22                | 1.02       |
| (7,14)  | 1:37:D:THR:CG2 | 1:30:D:SER:CA | 8                   | 1.02     | 0.22                | 1.02       |
| (3,27)  | 1:33:B:PHE:CA  | 1:35:C:THR:N  | 7                   | 0.88     | 0.42                | 1.08       |
| (3,27)  | 1:33:B:PHE:CA  | 1:35:A:THR:N  | 7                   | 0.88     | 0.42                | 1.08       |

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| Key     | Atom-1         | Atom-2         | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|----------------|----------------|---------------------|----------|---------------------|------------|
| (3,26)  | 1:33:A:PHE:CA  | 1:35:B:THR:N   | 7                   | 0.88     | 0.42                | 1.08       |
| (3,26)  | 1:33:A:PHE:CA  | 1:35:E:THR:N   | 7                   | 0.88     | 0.42                | 1.08       |
| (3,28)  | 1:33:C:PHE:CA  | 1:35:D:THR:N   | 7                   | 0.88     | 0.42                | 1.08       |
| (3,28)  | 1:33:C:PHE:CA  | 1:35:B:THR:N   | 7                   | 0.88     | 0.42                | 1.08       |
| (3,29)  | 1:33:D:PHE:CA  | 1:35:E:THR:N   | 7                   | 0.88     | 0.42                | 1.08       |
| (3,29)  | 1:33:D:PHE:CA  | 1:35:C:THR:N   | 7                   | 0.88     | 0.42                | 1.08       |
| (3,30)  | 1:33:E:PHE:CA  | 1:35:A:THR:N   | 7                   | 0.88     | 0.42                | 1.08       |
| (3,30)  | 1:33:E:PHE:CA  | 1:35:D:THR:N   | 7                   | 0.88     | 0.42                | 1.08       |
| (1,598) | 1:25:C:ILE:CG2 | 1:27:C:LEU:CG  | 7                   | 0.87     | 0.32                | 0.99       |
| (1,598) | 1:25:C:ILE:CG2 | 1:27:D:LEU:CG  | 7                   | 0.87     | 0.32                | 0.99       |
| (1,596) | 1:25:A:ILE:CG2 | 1:27:A:LEU:CG  | 7                   | 0.86     | 0.32                | 0.99       |
| (1,596) | 1:25:A:ILE:CG2 | 1:27:B:LEU:CG  | 7                   | 0.86     | 0.32                | 0.99       |
| (1,597) | 1:25:B:ILE:CG2 | 1:27:B:LEU:CG  | 7                   | 0.86     | 0.32                | 0.99       |
| (1,597) | 1:25:B:ILE:CG2 | 1:27:C:LEU:CG  | 7                   | 0.86     | 0.32                | 0.99       |
| (1,599) | 1:25:D:ILE:CG2 | 1:27:D:LEU:CG  | 7                   | 0.86     | 0.32                | 0.99       |
| (1,599) | 1:25:D:ILE:CG2 | 1:27:E:LEU:CG  | 7                   | 0.86     | 0.32                | 0.99       |
| (1,600) | 1:25:E:ILE:CG2 | 1:27:E:LEU:CG  | 7                   | 0.86     | 0.32                | 0.99       |
| (1,600) | 1:25:E:ILE:CG2 | 1:27:A:LEU:CG  | 7                   | 0.86     | 0.32                | 0.99       |
| (1,588) | 1:9:C:ILE:CG2  | 1:11:D:LEU:CG  | 7                   | 0.81     | 0.24                | 0.94       |
| (1,588) | 1:9:C:ILE:CG2  | 1:11:C:LEU:CG  | 7                   | 0.81     | 0.24                | 0.94       |
| (1,586) | 1:9:A:ILE:CG2  | 1:11:B:LEU:CG  | 7                   | 0.81     | 0.24                | 0.93       |
| (1,586) | 1:9:A:ILE:CG2  | 1:11:A:LEU:CG  | 7                   | 0.81     | 0.24                | 0.93       |
| (1,587) | 1:9:B:ILE:CG2  | 1:11:C:LEU:CG  | 7                   | 0.81     | 0.24                | 0.93       |
| (1,587) | 1:9:B:ILE:CG2  | 1:11:B:LEU:CG  | 7                   | 0.81     | 0.24                | 0.93       |
| (1,589) | 1:9:D:ILE:CG2  | 1:11:E:LEU:CG  | 7                   | 0.81     | 0.24                | 0.93       |
| (1,589) | 1:9:D:ILE:CG2  | 1:11:D:LEU:CG  | 7                   | 0.81     | 0.24                | 0.93       |
| (1,590) | 1:9:E:ILE:CG2  | 1:11:A:LEU:CG  | 7                   | 0.81     | 0.24                | 0.93       |
| (1,590) | 1:9:E:ILE:CG2  | 1:11:E:LEU:CG  | 7                   | 0.81     | 0.24                | 0.93       |
| (1,833) | 1:11:C:LEU:CG  | 1:9:B:ILE:CG2  | 7                   | 0.78     | 0.21                | 0.91       |
| (1,833) | 1:11:C:LEU:CG  | 1:9:C:ILE:CG2  | 7                   | 0.78     | 0.21                | 0.91       |
| (1,833) | 1:11:C:LEU:CG  | 1:13:C:ILE:CG2 | 7                   | 0.78     | 0.21                | 0.91       |
| (1,831) | 1:11:A:LEU:CG  | 1:9:E:ILE:CG2  | 7                   | 0.78     | 0.21                | 0.91       |
| (1,831) | 1:11:A:LEU:CG  | 1:9:A:ILE:CG2  | 7                   | 0.78     | 0.21                | 0.91       |
| (1,831) | 1:11:A:LEU:CG  | 1:13:A:ILE:CG2 | 7                   | 0.78     | 0.21                | 0.91       |
| (1,832) | 1:11:B:LEU:CG  | 1:9:A:ILE:CG2  | 7                   | 0.78     | 0.21                | 0.91       |
| (1,832) | 1:11:B:LEU:CG  | 1:9:B:ILE:CG2  | 7                   | 0.78     | 0.21                | 0.91       |
| (1,832) | 1:11:B:LEU:CG  | 1:13:B:ILE:CG2 | 7                   | 0.78     | 0.21                | 0.91       |
| (1,834) | 1:11:D:LEU:CG  | 1:9:C:ILE:CG2  | 7                   | 0.78     | 0.21                | 0.91       |
| (1,834) | 1:11:D:LEU:CG  | 1:9:D:ILE:CG2  | 7                   | 0.78     | 0.21                | 0.91       |
| (1,834) | 1:11:D:LEU:CG  | 1:13:D:ILE:CG2 | 7                   | 0.78     | 0.21                | 0.91       |
| (1,835) | 1:11:E:LEU:CG  | 1:9:D:ILE:CG2  | 7                   | 0.78     | 0.21                | 0.91       |
| (1,835) | 1:11:E:LEU:CG  | 1:9:E:ILE:CG2  | 7                   | 0.78     | 0.21                | 0.91       |

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| Key      | Atom-1         | Atom-2         | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|----------------|----------------|---------------------|----------|---------------------|------------|
| (1,835)  | 1:11:E:LEU:CG  | 1:13:E:ILE:CG2 | 7                   | 0.78     | 0.21                | 0.91       |
| (1,221)  | 1:29:A:VAL:CA  | 1:25:A:ILE:CD1 | 7                   | 0.68     | 0.22                | 0.74       |
| (1,222)  | 1:29:B:VAL:CA  | 1:25:B:ILE:CD1 | 7                   | 0.68     | 0.22                | 0.74       |
| (1,224)  | 1:29:D:VAL:CA  | 1:25:D:ILE:CD1 | 7                   | 0.68     | 0.22                | 0.74       |
| (1,225)  | 1:29:E:VAL:CA  | 1:25:E:ILE:CD1 | 7                   | 0.68     | 0.22                | 0.74       |
| (1,223)  | 1:29:C:VAL:CA  | 1:25:C:ILE:CD1 | 7                   | 0.68     | 0.22                | 0.74       |
| (1,1008) | 1:27:C:LEU:CB  | 1:25:C:ILE:CD1 | 7                   | 0.63     | 0.15                | 0.62       |
| (1,1008) | 1:27:C:LEU:CB  | 1:25:B:ILE:CD1 | 7                   | 0.63     | 0.15                | 0.62       |
| (1,1010) | 1:27:E:LEU:CB  | 1:25:E:ILE:CD1 | 7                   | 0.63     | 0.15                | 0.62       |
| (1,1010) | 1:27:E:LEU:CB  | 1:25:D:ILE:CD1 | 7                   | 0.63     | 0.15                | 0.62       |
| (1,1006) | 1:27:A:LEU:CB  | 1:25:A:ILE:CD1 | 7                   | 0.62     | 0.15                | 0.62       |
| (1,1006) | 1:27:A:LEU:CB  | 1:25:E:ILE:CD1 | 7                   | 0.62     | 0.15                | 0.62       |
| (1,1007) | 1:27:B:LEU:CB  | 1:25:B:ILE:CD1 | 7                   | 0.62     | 0.15                | 0.62       |
| (1,1007) | 1:27:B:LEU:CB  | 1:25:A:ILE:CD1 | 7                   | 0.62     | 0.15                | 0.62       |
| (1,1009) | 1:27:D:LEU:CB  | 1:25:D:ILE:CD1 | 7                   | 0.62     | 0.15                | 0.62       |
| (1,1009) | 1:27:D:LEU:CB  | 1:25:C:ILE:CD1 | 7                   | 0.62     | 0.15                | 0.62       |
| (1,836)  | 1:11:A:LEU:CG  | 1:13:A:ILE:CD1 | 7                   | 0.47     | 0.34                | 0.48       |
| (1,836)  | 1:11:A:LEU:CG  | 1:9:E:ILE:CD1  | 7                   | 0.47     | 0.34                | 0.48       |
| (1,837)  | 1:11:B:LEU:CG  | 1:13:B:ILE:CD1 | 7                   | 0.47     | 0.34                | 0.48       |
| (1,837)  | 1:11:B:LEU:CG  | 1:9:A:ILE:CD1  | 7                   | 0.47     | 0.34                | 0.48       |
| (1,838)  | 1:11:C:LEU:CG  | 1:13:C:ILE:CD1 | 7                   | 0.47     | 0.34                | 0.48       |
| (1,838)  | 1:11:C:LEU:CG  | 1:9:B:ILE:CD1  | 7                   | 0.47     | 0.34                | 0.48       |
| (1,839)  | 1:11:D:LEU:CG  | 1:13:D:ILE:CD1 | 7                   | 0.47     | 0.34                | 0.48       |
| (1,839)  | 1:11:D:LEU:CG  | 1:9:C:ILE:CD1  | 7                   | 0.47     | 0.34                | 0.48       |
| (2,51)   | 1:11:A:LEU:CG  | 1:13:A:ILE:CD1 | 7                   | 0.47     | 0.34                | 0.48       |
| (2,51)   | 1:11:A:LEU:CG  | 1:9:E:ILE:CD1  | 7                   | 0.47     | 0.34                | 0.48       |
| (2,52)   | 1:11:B:LEU:CG  | 1:13:B:ILE:CD1 | 7                   | 0.47     | 0.34                | 0.48       |
| (2,52)   | 1:11:B:LEU:CG  | 1:9:A:ILE:CD1  | 7                   | 0.47     | 0.34                | 0.48       |
| (2,53)   | 1:11:C:LEU:CG  | 1:13:C:ILE:CD1 | 7                   | 0.47     | 0.34                | 0.48       |
| (2,53)   | 1:11:C:LEU:CG  | 1:9:B:ILE:CD1  | 7                   | 0.47     | 0.34                | 0.48       |
| (2,54)   | 1:11:D:LEU:CG  | 1:13:D:ILE:CD1 | 7                   | 0.47     | 0.34                | 0.48       |
| (2,54)   | 1:11:D:LEU:CG  | 1:9:C:ILE:CD1  | 7                   | 0.47     | 0.34                | 0.48       |
| (1,840)  | 1:11:E:LEU:CG  | 1:13:E:ILE:CD1 | 7                   | 0.46     | 0.33                | 0.48       |
| (1,840)  | 1:11:E:LEU:CG  | 1:9:D:ILE:CD1  | 7                   | 0.46     | 0.33                | 0.48       |
| (2,55)   | 1:11:E:LEU:CG  | 1:13:E:ILE:CD1 | 7                   | 0.46     | 0.33                | 0.48       |
| (2,55)   | 1:11:E:LEU:CG  | 1:9:D:ILE:CD1  | 7                   | 0.46     | 0.33                | 0.48       |
| (3,116)  | 1:18:A:ILE:CA  | 1:16:B:PHE:N   | 7                   | 0.39     | 0.11                | 0.41       |
| (3,117)  | 1:18:B:ILE:CA  | 1:16:C:PHE:N   | 7                   | 0.39     | 0.11                | 0.41       |
| (3,118)  | 1:18:C:ILE:CA  | 1:16:D:PHE:N   | 7                   | 0.39     | 0.11                | 0.41       |
| (3,119)  | 1:18:D:ILE:CA  | 1:16:E:PHE:N   | 7                   | 0.39     | 0.11                | 0.41       |
| (3,120)  | 1:18:E:ILE:CA  | 1:16:A:PHE:N   | 7                   | 0.39     | 0.11                | 0.41       |
| (1,585)  | 1:25:E:ILE:CG1 | 1:27:E:LEU:CG  | 6                   | 0.85     | 0.26                | 0.94       |

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| Key     | Atom-1         | Atom-2         | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|----------------|----------------|---------------------|----------|---------------------|------------|
| (1,585) | 1:25:E:ILE:CG1 | 1:27:A:LEU:CG  | 6                   | 0.85     | 0.26                | 0.94       |
| (1,581) | 1:25:A:ILE:CG1 | 1:27:A:LEU:CG  | 6                   | 0.85     | 0.26                | 0.93       |
| (1,581) | 1:25:A:ILE:CG1 | 1:27:B:LEU:CG  | 6                   | 0.85     | 0.26                | 0.93       |
| (1,582) | 1:25:B:ILE:CG1 | 1:27:B:LEU:CG  | 6                   | 0.85     | 0.26                | 0.93       |
| (1,582) | 1:25:B:ILE:CG1 | 1:27:C:LEU:CG  | 6                   | 0.85     | 0.26                | 0.93       |
| (1,583) | 1:25:C:ILE:CG1 | 1:27:C:LEU:CG  | 6                   | 0.85     | 0.26                | 0.93       |
| (1,583) | 1:25:C:ILE:CG1 | 1:27:D:LEU:CG  | 6                   | 0.85     | 0.26                | 0.93       |
| (1,584) | 1:25:D:ILE:CG1 | 1:27:D:LEU:CG  | 6                   | 0.85     | 0.26                | 0.93       |
| (1,584) | 1:25:D:ILE:CG1 | 1:27:E:LEU:CG  | 6                   | 0.85     | 0.26                | 0.93       |
| (1,121) | 1:9:A:ILE:CG1  | 1:11:A:LEU:CD2 | 6                   | 0.72     | 0.34                | 0.8        |
| (1,121) | 1:9:A:ILE:CG1  | 1:11:B:LEU:CD2 | 6                   | 0.72     | 0.34                | 0.8        |
| (1,123) | 1:9:C:ILE:CG1  | 1:11:C:LEU:CD2 | 6                   | 0.72     | 0.34                | 0.8        |
| (1,123) | 1:9:C:ILE:CG1  | 1:11:D:LEU:CD2 | 6                   | 0.72     | 0.34                | 0.8        |
| (1,122) | 1:9:B:ILE:CG1  | 1:11:B:LEU:CD2 | 6                   | 0.72     | 0.34                | 0.8        |
| (1,122) | 1:9:B:ILE:CG1  | 1:11:C:LEU:CD2 | 6                   | 0.72     | 0.34                | 0.8        |
| (1,124) | 1:9:D:ILE:CG1  | 1:11:D:LEU:CD2 | 6                   | 0.72     | 0.34                | 0.8        |
| (1,124) | 1:9:D:ILE:CG1  | 1:11:E:LEU:CD2 | 6                   | 0.72     | 0.34                | 0.8        |
| (1,125) | 1:9:E:ILE:CG1  | 1:11:E:LEU:CD2 | 6                   | 0.72     | 0.34                | 0.8        |
| (1,125) | 1:9:E:ILE:CG1  | 1:11:A:LEU:CD2 | 6                   | 0.72     | 0.34                | 0.8        |
| (1,321) | 1:25:A:ILE:CB  | 1:27:A:LEU:CG  | 6                   | 0.37     | 0.12                | 0.4        |
| (1,322) | 1:25:B:ILE:CB  | 1:27:B:LEU:CG  | 6                   | 0.37     | 0.12                | 0.4        |
| (1,323) | 1:25:C:ILE:CB  | 1:27:C:LEU:CG  | 6                   | 0.37     | 0.12                | 0.4        |
| (1,324) | 1:25:D:ILE:CB  | 1:27:D:LEU:CG  | 6                   | 0.37     | 0.12                | 0.4        |
| (1,325) | 1:25:E:ILE:CB  | 1:27:E:LEU:CG  | 6                   | 0.37     | 0.12                | 0.4        |
| (4,56)  | 1:27:A:LEU:CG  | 1:24:E:ALA:N   | 6                   | 0.31     | 0.2                 | 0.22       |
| (4,57)  | 1:27:B:LEU:CG  | 1:24:A:ALA:N   | 6                   | 0.31     | 0.2                 | 0.22       |
| (4,58)  | 1:27:C:LEU:CG  | 1:24:B:ALA:N   | 6                   | 0.31     | 0.2                 | 0.22       |
| (4,59)  | 1:27:D:LEU:CG  | 1:24:C:ALA:N   | 6                   | 0.31     | 0.2                 | 0.22       |
| (4,60)  | 1:27:E:LEU:CG  | 1:24:D:ALA:N   | 6                   | 0.31     | 0.2                 | 0.22       |
| (1,776) | 1:27:C:LEU:CA  | 1:25:B:ILE:CD1 | 4                   | 0.42     | 0.08                | 0.42       |
| (1,776) | 1:27:A:LEU:CA  | 1:25:A:ILE:CD1 | 4                   | 0.42     | 0.08                | 0.42       |
| (1,777) | 1:27:D:LEU:CA  | 1:25:C:ILE:CD1 | 4                   | 0.42     | 0.08                | 0.42       |
| (1,777) | 1:27:C:LEU:CA  | 1:25:B:ILE:CD1 | 4                   | 0.42     | 0.08                | 0.42       |
| (1,777) | 1:27:C:LEU:CA  | 1:25:C:ILE:CD1 | 4                   | 0.42     | 0.08                | 0.42       |
| (1,778) | 1:27:E:LEU:CA  | 1:25:D:ILE:CD1 | 4                   | 0.42     | 0.08                | 0.42       |
| (1,778) | 1:27:C:LEU:CA  | 1:25:B:ILE:CD1 | 4                   | 0.42     | 0.08                | 0.42       |
| (1,778) | 1:27:D:LEU:CA  | 1:25:D:ILE:CD1 | 4                   | 0.42     | 0.08                | 0.42       |
| (1,779) | 1:27:E:LEU:CA  | 1:25:D:ILE:CD1 | 4                   | 0.42     | 0.08                | 0.42       |
| (1,779) | 1:27:A:LEU:CA  | 1:25:E:ILE:CD1 | 4                   | 0.42     | 0.08                | 0.42       |
| (1,779) | 1:27:D:LEU:CA  | 1:25:D:ILE:CD1 | 4                   | 0.42     | 0.08                | 0.42       |
| (1,779) | 1:27:D:LEU:CA  | 1:25:C:ILE:CD1 | 4                   | 0.42     | 0.08                | 0.42       |
| (1,780) | 1:27:E:LEU:CA  | 1:25:D:ILE:CD1 | 4                   | 0.42     | 0.08                | 0.42       |

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| Key      | Atom-1         | Atom-2         | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|----------------|----------------|---------------------|----------|---------------------|------------|
| (1,780)  | 1:27:A:LEU:CA  | 1:25:E:ILE:CD1 | 4                   | 0.42     | 0.08                | 0.42       |
| (1,780)  | 1:27:D:LEU:CA  | 1:25:D:ILE:CD1 | 4                   | 0.42     | 0.08                | 0.42       |
| (2,192)  | 1:29:A:VAL:CA  | 1:27:B:LEU:CA  | 4                   | 0.25     | 0.09                | 0.27       |
| (2,210)  | 1:29:C:VAL:CA  | 1:27:D:LEU:CA  | 4                   | 0.25     | 0.1                 | 0.27       |
| (2,219)  | 1:29:D:VAL:CA  | 1:27:E:LEU:CA  | 4                   | 0.25     | 0.09                | 0.27       |
| (2,201)  | 1:29:B:VAL:CA  | 1:27:C:LEU:CA  | 4                   | 0.25     | 0.1                 | 0.27       |
| (2,228)  | 1:29:E:VAL:CA  | 1:27:A:LEU:CA  | 4                   | 0.25     | 0.1                 | 0.27       |
| (2,21)   | 1:35:A:THR:CG2 | 1:33:A:PHE:CB  | 4                   | 0.24     | 0.06                | 0.24       |
| (2,22)   | 1:35:B:THR:CG2 | 1:33:B:PHE:CB  | 4                   | 0.24     | 0.06                | 0.24       |
| (2,23)   | 1:35:C:THR:CG2 | 1:33:C:PHE:CB  | 4                   | 0.24     | 0.06                | 0.24       |
| (2,24)   | 1:35:D:THR:CG2 | 1:33:D:PHE:CB  | 4                   | 0.24     | 0.06                | 0.24       |
| (2,25)   | 1:35:E:THR:CG2 | 1:33:E:PHE:CB  | 4                   | 0.24     | 0.06                | 0.24       |
| (3,41)   | 1:22:A:VAL:CB  | 1:26:E:THR:N   | 4                   | 0.23     | 0.06                | 0.22       |
| (3,42)   | 1:22:B:VAL:CB  | 1:26:A:THR:N   | 4                   | 0.23     | 0.06                | 0.22       |
| (3,43)   | 1:22:C:VAL:CB  | 1:26:B:THR:N   | 4                   | 0.23     | 0.06                | 0.22       |
| (3,44)   | 1:22:D:VAL:CB  | 1:26:C:THR:N   | 4                   | 0.23     | 0.06                | 0.22       |
| (3,45)   | 1:22:E:VAL:CB  | 1:26:D:THR:N   | 4                   | 0.23     | 0.06                | 0.22       |
| (1,841)  | 1:11:A:LEU:CG  | 1:9:E:ILE:CB   | 4                   | 0.22     | 0.07                | 0.22       |
| (1,841)  | 1:11:A:LEU:CG  | 1:9:A:ILE:CB   | 4                   | 0.22     | 0.07                | 0.22       |
| (1,842)  | 1:11:B:LEU:CG  | 1:9:A:ILE:CB   | 4                   | 0.22     | 0.07                | 0.22       |
| (1,842)  | 1:11:B:LEU:CG  | 1:9:B:ILE:CB   | 4                   | 0.22     | 0.07                | 0.22       |
| (1,1056) | 1:9:A:ILE:CB   | 1:11:B:LEU:CG  | 4                   | 0.22     | 0.07                | 0.22       |
| (1,1056) | 1:9:A:ILE:CB   | 1:11:A:LEU:CG  | 4                   | 0.22     | 0.07                | 0.22       |
| (1,1057) | 1:9:B:ILE:CB   | 1:11:C:LEU:CG  | 4                   | 0.22     | 0.07                | 0.22       |
| (1,1057) | 1:9:B:ILE:CB   | 1:11:B:LEU:CG  | 4                   | 0.22     | 0.07                | 0.22       |
| (1,843)  | 1:11:C:LEU:CG  | 1:9:B:ILE:CB   | 4                   | 0.21     | 0.07                | 0.22       |
| (1,843)  | 1:11:C:LEU:CG  | 1:9:C:ILE:CB   | 4                   | 0.21     | 0.07                | 0.22       |
| (1,844)  | 1:11:D:LEU:CG  | 1:9:C:ILE:CB   | 4                   | 0.21     | 0.07                | 0.22       |
| (1,844)  | 1:11:D:LEU:CG  | 1:9:D:ILE:CB   | 4                   | 0.21     | 0.07                | 0.22       |
| (1,845)  | 1:11:E:LEU:CG  | 1:9:D:ILE:CB   | 4                   | 0.21     | 0.07                | 0.22       |
| (1,845)  | 1:11:E:LEU:CG  | 1:9:E:ILE:CB   | 4                   | 0.21     | 0.07                | 0.22       |
| (1,1058) | 1:9:C:ILE:CB   | 1:11:D:LEU:CG  | 4                   | 0.21     | 0.07                | 0.22       |
| (1,1058) | 1:9:C:ILE:CB   | 1:11:C:LEU:CG  | 4                   | 0.21     | 0.07                | 0.22       |
| (1,1059) | 1:9:D:ILE:CB   | 1:11:E:LEU:CG  | 4                   | 0.21     | 0.07                | 0.22       |
| (1,1059) | 1:9:D:ILE:CB   | 1:11:D:LEU:CG  | 4                   | 0.21     | 0.07                | 0.22       |
| (1,1060) | 1:9:E:ILE:CB   | 1:11:A:LEU:CG  | 4                   | 0.21     | 0.07                | 0.22       |
| (1,1060) | 1:9:E:ILE:CB   | 1:11:E:LEU:CG  | 4                   | 0.21     | 0.07                | 0.22       |
| (1,1124) | 1:20:D:THR:CG2 | 1:24:D:ALA:CA  | 4                   | 0.16     | 0.05                | 0.14       |
| (1,1121) | 1:20:A:THR:CG2 | 1:24:A:ALA:CA  | 4                   | 0.16     | 0.05                | 0.14       |
| (1,1122) | 1:20:B:THR:CG2 | 1:24:B:ALA:CA  | 4                   | 0.16     | 0.05                | 0.14       |
| (1,1123) | 1:20:C:THR:CG2 | 1:24:C:ALA:CA  | 4                   | 0.16     | 0.05                | 0.14       |
| (1,1125) | 1:20:E:THR:CG2 | 1:24:E:ALA:CA  | 4                   | 0.16     | 0.05                | 0.14       |

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| Key      | Atom-1         | Atom-2         | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|----------------|----------------|---------------------|----------|---------------------|------------|
| (2,194)  | 1:29:A:VAL:CA  | 1:31:A:MET:CE  | 3                   | 0.51     | 0.19                | 0.47       |
| (2,203)  | 1:29:B:VAL:CA  | 1:31:B:MET:CE  | 3                   | 0.51     | 0.19                | 0.47       |
| (2,212)  | 1:29:C:VAL:CA  | 1:31:C:MET:CE  | 3                   | 0.51     | 0.19                | 0.47       |
| (2,221)  | 1:29:D:VAL:CA  | 1:31:D:MET:CE  | 3                   | 0.51     | 0.19                | 0.47       |
| (2,230)  | 1:29:E:VAL:CA  | 1:31:E:MET:CE  | 3                   | 0.51     | 0.19                | 0.47       |
| (1,511)  | 1:15:A:ASN:CA  | 1:11:A:LEU:CD1 | 3                   | 0.46     | 0.06                | 0.49       |
| (1,512)  | 1:15:B:ASN:CA  | 1:11:B:LEU:CD1 | 3                   | 0.46     | 0.06                | 0.49       |
| (1,513)  | 1:15:C:ASN:CA  | 1:11:C:LEU:CD1 | 3                   | 0.46     | 0.06                | 0.49       |
| (1,514)  | 1:15:D:ASN:CA  | 1:11:D:LEU:CD1 | 3                   | 0.46     | 0.06                | 0.49       |
| (1,515)  | 1:15:E:ASN:CA  | 1:11:E:LEU:CD1 | 3                   | 0.46     | 0.06                | 0.49       |
| (1,1111) | 1:20:A:THR:CG2 | 1:22:A:VAL:CG2 | 3                   | 0.43     | 0.21                | 0.29       |
| (1,1112) | 1:20:B:THR:CG2 | 1:22:B:VAL:CG2 | 3                   | 0.43     | 0.21                | 0.29       |
| (1,1113) | 1:20:C:THR:CG2 | 1:22:C:VAL:CG2 | 3                   | 0.43     | 0.21                | 0.29       |
| (1,1114) | 1:20:D:THR:CG2 | 1:22:D:VAL:CG2 | 3                   | 0.43     | 0.21                | 0.29       |
| (1,1115) | 1:20:E:THR:CG2 | 1:22:E:VAL:CG2 | 3                   | 0.43     | 0.21                | 0.29       |
| (2,36)   | 1:14:A:VAL:CG2 | 1:13:A:ILE:CD1 | 2                   | 0.52     | 0.01                | 0.52       |
| (2,37)   | 1:14:B:VAL:CG2 | 1:13:B:ILE:CD1 | 2                   | 0.52     | 0.01                | 0.52       |
| (2,38)   | 1:14:C:VAL:CG2 | 1:13:C:ILE:CD1 | 2                   | 0.52     | 0.01                | 0.52       |
| (2,39)   | 1:14:D:VAL:CG2 | 1:13:D:ILE:CD1 | 2                   | 0.52     | 0.01                | 0.52       |
| (2,40)   | 1:14:E:VAL:CG2 | 1:13:E:ILE:CD1 | 2                   | 0.52     | 0.01                | 0.52       |
| (1,726)  | 1:13:A:ILE:CG2 | 1:11:B:LEU:CD1 | 2                   | 0.45     | 0.19                | 0.45       |
| (1,726)  | 1:9:A:ILE:CG2  | 1:11:A:LEU:CD1 | 2                   | 0.45     | 0.19                | 0.45       |
| (1,727)  | 1:13:B:ILE:CG2 | 1:11:C:LEU:CD1 | 2                   | 0.44     | 0.2                 | 0.44       |
| (1,727)  | 1:9:A:ILE:CG2  | 1:11:A:LEU:CD1 | 2                   | 0.44     | 0.2                 | 0.44       |
| (1,728)  | 1:13:C:ILE:CG2 | 1:11:D:LEU:CD1 | 2                   | 0.44     | 0.2                 | 0.44       |
| (1,728)  | 1:9:B:ILE:CG2  | 1:11:B:LEU:CD1 | 2                   | 0.44     | 0.2                 | 0.44       |
| (1,729)  | 1:13:D:ILE:CG2 | 1:11:E:LEU:CD1 | 2                   | 0.44     | 0.2                 | 0.44       |
| (1,729)  | 1:9:D:ILE:CG2  | 1:11:D:LEU:CD1 | 2                   | 0.44     | 0.2                 | 0.44       |
| (1,730)  | 1:13:E:ILE:CG2 | 1:11:A:LEU:CD1 | 2                   | 0.44     | 0.2                 | 0.44       |
| (1,730)  | 1:9:A:ILE:CG2  | 1:11:A:LEU:CD1 | 2                   | 0.44     | 0.2                 | 0.44       |
| (1,431)  | 1:29:A:VAL:CG2 | 1:27:B:LEU:CG  | 2                   | 0.44     | 0.09                | 0.44       |
| (1,431)  | 1:29:A:VAL:CG2 | 1:27:A:LEU:CG  | 2                   | 0.44     | 0.09                | 0.44       |
| (1,432)  | 1:29:B:VAL:CG2 | 1:27:C:LEU:CG  | 2                   | 0.44     | 0.09                | 0.44       |
| (1,432)  | 1:29:B:VAL:CG2 | 1:27:B:LEU:CG  | 2                   | 0.44     | 0.09                | 0.44       |
| (1,433)  | 1:29:C:VAL:CG2 | 1:27:D:LEU:CG  | 2                   | 0.44     | 0.09                | 0.44       |
| (1,433)  | 1:29:C:VAL:CG2 | 1:27:C:LEU:CG  | 2                   | 0.44     | 0.09                | 0.44       |
| (1,434)  | 1:29:D:VAL:CG2 | 1:27:E:LEU:CG  | 2                   | 0.44     | 0.09                | 0.44       |
| (1,434)  | 1:29:D:VAL:CG2 | 1:27:D:LEU:CG  | 2                   | 0.44     | 0.09                | 0.44       |
| (1,435)  | 1:29:E:VAL:CG2 | 1:27:A:LEU:CG  | 2                   | 0.44     | 0.09                | 0.44       |
| (1,435)  | 1:29:E:VAL:CG2 | 1:27:E:LEU:CG  | 2                   | 0.44     | 0.09                | 0.44       |
| (1,991)  | 1:27:A:LEU:CG  | 1:29:E:VAL:CG2 | 2                   | 0.44     | 0.09                | 0.44       |
| (1,991)  | 1:27:A:LEU:CG  | 1:29:A:VAL:CG2 | 2                   | 0.44     | 0.09                | 0.44       |

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| Key      | Atom-1         | Atom-2         | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|----------------|----------------|---------------------|----------|---------------------|------------|
| (1,992)  | 1:27:B:LEU:CG  | 1:29:A:VAL:CG2 | 2                   | 0.44     | 0.09                | 0.44       |
| (1,992)  | 1:27:B:LEU:CG  | 1:29:B:VAL:CG2 | 2                   | 0.44     | 0.09                | 0.44       |
| (1,993)  | 1:27:C:LEU:CG  | 1:29:B:VAL:CG2 | 2                   | 0.44     | 0.09                | 0.44       |
| (1,993)  | 1:27:C:LEU:CG  | 1:29:C:VAL:CG2 | 2                   | 0.44     | 0.09                | 0.44       |
| (1,994)  | 1:27:D:LEU:CG  | 1:29:C:VAL:CG2 | 2                   | 0.44     | 0.09                | 0.44       |
| (1,994)  | 1:27:D:LEU:CG  | 1:29:D:VAL:CG2 | 2                   | 0.44     | 0.09                | 0.44       |
| (1,995)  | 1:27:E:LEU:CG  | 1:29:D:VAL:CG2 | 2                   | 0.44     | 0.09                | 0.44       |
| (1,995)  | 1:27:E:LEU:CG  | 1:29:E:VAL:CG2 | 2                   | 0.44     | 0.09                | 0.44       |
| (1,281)  | 1:11:A:LEU:CB  | 1:13:A:ILE:CG2 | 2                   | 0.36     | 0.14                | 0.36       |
| (1,281)  | 1:11:A:LEU:CB  | 1:13:E:ILE:CG2 | 2                   | 0.36     | 0.14                | 0.36       |
| (1,282)  | 1:11:B:LEU:CB  | 1:13:B:ILE:CG2 | 2                   | 0.36     | 0.14                | 0.36       |
| (1,282)  | 1:11:B:LEU:CB  | 1:13:A:ILE:CG2 | 2                   | 0.36     | 0.14                | 0.36       |
| (1,283)  | 1:11:C:LEU:CB  | 1:13:C:ILE:CG2 | 2                   | 0.36     | 0.14                | 0.36       |
| (1,283)  | 1:11:C:LEU:CB  | 1:13:B:ILE:CG2 | 2                   | 0.36     | 0.14                | 0.36       |
| (1,284)  | 1:11:D:LEU:CB  | 1:13:D:ILE:CG2 | 2                   | 0.36     | 0.14                | 0.36       |
| (1,284)  | 1:11:D:LEU:CB  | 1:13:C:ILE:CG2 | 2                   | 0.36     | 0.14                | 0.36       |
| (1,285)  | 1:11:E:LEU:CB  | 1:13:E:ILE:CG2 | 2                   | 0.36     | 0.14                | 0.36       |
| (1,285)  | 1:11:E:LEU:CB  | 1:13:D:ILE:CG2 | 2                   | 0.36     | 0.14                | 0.36       |
| (1,996)  | 1:11:A:LEU:CB  | 1:13:A:ILE:CG2 | 2                   | 0.36     | 0.14                | 0.36       |
| (1,996)  | 1:11:A:LEU:CB  | 1:13:E:ILE:CG2 | 2                   | 0.36     | 0.14                | 0.36       |
| (1,997)  | 1:11:B:LEU:CB  | 1:13:B:ILE:CG2 | 2                   | 0.36     | 0.14                | 0.36       |
| (1,997)  | 1:11:B:LEU:CB  | 1:13:A:ILE:CG2 | 2                   | 0.36     | 0.14                | 0.36       |
| (1,998)  | 1:11:C:LEU:CB  | 1:13:C:ILE:CG2 | 2                   | 0.36     | 0.14                | 0.36       |
| (1,998)  | 1:11:C:LEU:CB  | 1:13:B:ILE:CG2 | 2                   | 0.36     | 0.14                | 0.36       |
| (1,999)  | 1:11:D:LEU:CB  | 1:13:D:ILE:CG2 | 2                   | 0.36     | 0.14                | 0.36       |
| (1,999)  | 1:11:D:LEU:CB  | 1:13:C:ILE:CG2 | 2                   | 0.36     | 0.14                | 0.36       |
| (1,1000) | 1:11:E:LEU:CB  | 1:13:E:ILE:CG2 | 2                   | 0.36     | 0.14                | 0.36       |
| (1,1000) | 1:11:E:LEU:CB  | 1:13:D:ILE:CG2 | 2                   | 0.36     | 0.14                | 0.36       |
| (1,346)  | 1:13:A:ILE:CD1 | 1:11:B:LEU:CG  | 2                   | 0.26     | 0.08                | 0.26       |
| (1,346)  | 1:25:A:ILE:CD1 | 1:28:A:LEU:CG  | 2                   | 0.26     | 0.08                | 0.26       |
| (1,347)  | 1:13:A:ILE:CD1 | 1:11:B:LEU:CG  | 2                   | 0.26     | 0.08                | 0.26       |
| (1,347)  | 1:25:B:ILE:CD1 | 1:28:B:LEU:CG  | 2                   | 0.26     | 0.08                | 0.26       |
| (1,348)  | 1:13:A:ILE:CD1 | 1:11:B:LEU:CG  | 2                   | 0.26     | 0.08                | 0.26       |
| (1,348)  | 1:25:C:ILE:CD1 | 1:28:C:LEU:CG  | 2                   | 0.26     | 0.08                | 0.26       |
| (1,349)  | 1:13:A:ILE:CD1 | 1:11:B:LEU:CG  | 2                   | 0.26     | 0.08                | 0.26       |
| (1,349)  | 1:25:D:ILE:CD1 | 1:28:D:LEU:CG  | 2                   | 0.26     | 0.08                | 0.26       |
| (1,350)  | 1:13:A:ILE:CD1 | 1:11:B:LEU:CG  | 2                   | 0.26     | 0.08                | 0.26       |
| (1,350)  | 1:25:E:ILE:CD1 | 1:28:E:LEU:CG  | 2                   | 0.26     | 0.08                | 0.26       |
| (3,51)   | 1:34:A:LEU:CB  | 1:37:E:THR:N   | 2                   | 0.16     | 0.0                 | 0.16       |
| (3,52)   | 1:34:B:LEU:CB  | 1:37:A:THR:N   | 2                   | 0.16     | 0.0                 | 0.16       |
| (3,53)   | 1:34:C:LEU:CB  | 1:37:B:THR:N   | 2                   | 0.16     | 0.0                 | 0.16       |
| (3,54)   | 1:34:D:LEU:CB  | 1:37:C:THR:N   | 2                   | 0.16     | 0.0                 | 0.16       |

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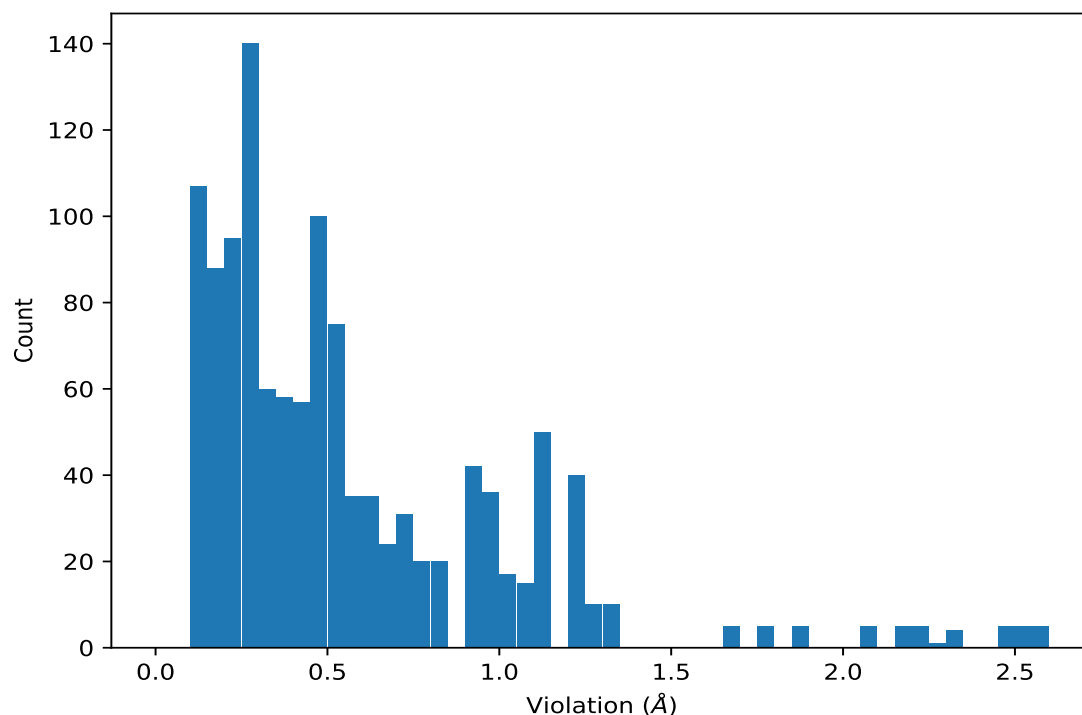
| Key     | Atom-1        | Atom-2         | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|---------------|----------------|---------------------|----------|---------------------|------------|
| (3,55)  | 1:34:E:LEU:CB | 1:37:D:THR:N   | 2                   | 0.16     | 0.0                 | 0.16       |
| (2,136) | 1:13:A:ILE:CA | 1:11:B:LEU:CD2 | 2                   | 0.14     | 0.02                | 0.14       |
| (2,137) | 1:13:B:ILE:CA | 1:11:C:LEU:CD2 | 2                   | 0.14     | 0.02                | 0.14       |
| (2,138) | 1:13:C:ILE:CA | 1:11:D:LEU:CD2 | 2                   | 0.14     | 0.02                | 0.14       |
| (2,139) | 1:13:D:ILE:CA | 1:11:E:LEU:CD2 | 2                   | 0.14     | 0.02                | 0.14       |
| (2,140) | 1:13:E:ILE:CA | 1:11:A:LEU:CD2 | 2                   | 0.14     | 0.02                | 0.14       |

<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) |
|--------|----------------|----------------|----------|---------------|
| (7,10) | 1:20:E:THR:CG2 | 1:14:E:VAL:CG2 | 10       | 2.57          |
| (7,9)  | 1:20:D:THR:CG2 | 1:14:D:VAL:CG2 | 10       | 2.57          |
| (7,8)  | 1:20:C:THR:CG2 | 1:14:C:VAL:CG2 | 10       | 2.57          |
| (7,7)  | 1:20:B:THR:CG2 | 1:14:B:VAL:CG2 | 10       | 2.57          |
| (7,6)  | 1:20:A:THR:CG2 | 1:14:A:VAL:CG2 | 10       | 2.57          |
| (7,10) | 1:20:E:THR:CG2 | 1:14:E:VAL:CG2 | 5        | 2.53          |
| (7,9)  | 1:20:D:THR:CG2 | 1:14:D:VAL:CG2 | 5        | 2.53          |
| (7,8)  | 1:20:C:THR:CG2 | 1:14:C:VAL:CG2 | 5        | 2.53          |
| (7,7)  | 1:20:B:THR:CG2 | 1:14:B:VAL:CG2 | 5        | 2.53          |
| (7,6)  | 1:20:A:THR:CG2 | 1:14:A:VAL:CG2 | 5        | 2.53          |
| (7,10) | 1:20:E:THR:CG2 | 1:26:E:THR:CG2 | 9        | 2.45          |
| (7,9)  | 1:20:D:THR:CG2 | 1:26:D:THR:CG2 | 9        | 2.45          |
| (7,8)  | 1:20:C:THR:CG2 | 1:26:C:THR:CG2 | 9        | 2.45          |
| (7,7)  | 1:20:B:THR:CG2 | 1:26:B:THR:CG2 | 9        | 2.45          |
| (7,6)  | 1:20:A:THR:CG2 | 1:26:A:THR:CG2 | 9        | 2.45          |
| (7,10) | 1:20:E:THR:CG2 | 1:14:E:VAL:CG2 | 1        | 2.31          |
| (7,9)  | 1:20:D:THR:CG2 | 1:14:D:VAL:CG2 | 1        | 2.31          |
| (7,8)  | 1:20:C:THR:CG2 | 1:14:C:VAL:CG2 | 1        | 2.31          |
| (7,7)  | 1:20:B:THR:CG2 | 1:14:B:VAL:CG2 | 1        | 2.31          |
| (7,6)  | 1:20:A:THR:CG2 | 1:14:A:VAL:CG2 | 1        | 2.3           |
| (7,10) | 1:20:E:THR:CG2 | 1:14:E:VAL:CG2 | 7        | 2.24          |
| (7,9)  | 1:20:D:THR:CG2 | 1:14:D:VAL:CG2 | 7        | 2.24          |
| (7,8)  | 1:20:C:THR:CG2 | 1:14:C:VAL:CG2 | 7        | 2.24          |
| (7,7)  | 1:20:B:THR:CG2 | 1:14:B:VAL:CG2 | 7        | 2.24          |
| (7,6)  | 1:20:A:THR:CG2 | 1:14:A:VAL:CG2 | 7        | 2.24          |
| (7,10) | 1:20:E:THR:CG2 | 1:26:E:THR:CG2 | 3        | 2.19          |
| (7,9)  | 1:20:D:THR:CG2 | 1:26:D:THR:CG2 | 3        | 2.19          |
| (7,8)  | 1:20:C:THR:CG2 | 1:26:C:THR:CG2 | 3        | 2.19          |
| (7,7)  | 1:20:B:THR:CG2 | 1:26:B:THR:CG2 | 3        | 2.19          |
| (7,6)  | 1:20:A:THR:CG2 | 1:26:A:THR:CG2 | 3        | 2.19          |
| (7,10) | 1:20:E:THR:CG2 | 1:26:E:THR:CG2 | 4        | 2.08          |
| (7,9)  | 1:20:D:THR:CG2 | 1:26:D:THR:CG2 | 4        | 2.08          |
| (7,8)  | 1:20:C:THR:CG2 | 1:26:C:THR:CG2 | 4        | 2.08          |
| (7,7)  | 1:20:B:THR:CG2 | 1:26:B:THR:CG2 | 4        | 2.08          |
| (7,6)  | 1:20:A:THR:CG2 | 1:26:A:THR:CG2 | 4        | 2.08          |
| (7,10) | 1:20:E:THR:CG2 | 1:26:E:THR:CG2 | 8        | 1.86          |
| (7,9)  | 1:20:D:THR:CG2 | 1:26:D:THR:CG2 | 8        | 1.86          |
| (7,8)  | 1:20:C:THR:CG2 | 1:26:C:THR:CG2 | 8        | 1.86          |
| (7,7)  | 1:20:B:THR:CG2 | 1:26:B:THR:CG2 | 8        | 1.86          |
| (7,6)  | 1:20:A:THR:CG2 | 1:26:A:THR:CG2 | 8        | 1.86          |
| (7,10) | 1:20:E:THR:CG2 | 1:14:E:VAL:CG2 | 2        | 1.79          |
| (7,9)  | 1:20:D:THR:CG2 | 1:14:D:VAL:CG2 | 2        | 1.79          |
| (7,8)  | 1:20:C:THR:CG2 | 1:14:C:VAL:CG2 | 2        | 1.79          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (7,7)   | 1:20:B:THR:CG2 | 1:14:B:VAL:CG2 | 2        | 1.79          |
| (7,6)   | 1:20:A:THR:CG2 | 1:14:A:VAL:CG2 | 2        | 1.79          |
| (7,10)  | 1:20:E:THR:CG2 | 1:26:E:THR:CG2 | 6        | 1.68          |
| (7,9)   | 1:20:D:THR:CG2 | 1:26:D:THR:CG2 | 6        | 1.68          |
| (7,8)   | 1:20:C:THR:CG2 | 1:26:C:THR:CG2 | 6        | 1.68          |
| (7,7)   | 1:20:B:THR:CG2 | 1:26:B:THR:CG2 | 6        | 1.68          |
| (7,6)   | 1:20:A:THR:CG2 | 1:26:A:THR:CG2 | 6        | 1.68          |
| (7,15)  | 1:37:E:THR:CG2 | 1:30:E:SER:CA  | 8        | 1.32          |
| (7,14)  | 1:37:D:THR:CG2 | 1:30:D:SER:CA  | 8        | 1.32          |
| (7,13)  | 1:37:C:THR:CG2 | 1:30:C:SER:CA  | 8        | 1.32          |
| (7,12)  | 1:37:B:THR:CG2 | 1:30:B:SER:CA  | 8        | 1.32          |
| (7,11)  | 1:37:A:THR:CG2 | 1:30:A:SER:CA  | 8        | 1.32          |
| (7,5)   | 1:37:E:THR:CA  | 1:32:E:ALA:CB  | 1        | 1.3           |
| (7,4)   | 1:37:D:THR:CA  | 1:32:D:ALA:CB  | 1        | 1.3           |
| (7,3)   | 1:37:C:THR:CA  | 1:32:C:ALA:CB  | 1        | 1.3           |
| (7,2)   | 1:37:B:THR:CA  | 1:32:B:ALA:CB  | 1        | 1.3           |
| (7,1)   | 1:37:A:THR:CA  | 1:32:A:ALA:CB  | 1        | 1.3           |
| (7,15)  | 1:37:E:THR:CG2 | 1:30:E:SER:CA  | 2        | 1.28          |
| (7,14)  | 1:37:D:THR:CG2 | 1:30:D:SER:CA  | 2        | 1.28          |
| (7,13)  | 1:37:C:THR:CG2 | 1:30:C:SER:CA  | 2        | 1.28          |
| (7,12)  | 1:37:B:THR:CG2 | 1:30:B:SER:CA  | 2        | 1.28          |
| (7,11)  | 1:37:A:THR:CG2 | 1:30:A:SER:CA  | 2        | 1.28          |
| (7,5)   | 1:37:E:THR:CA  | 1:32:E:ALA:CB  | 8        | 1.26          |
| (7,4)   | 1:37:D:THR:CA  | 1:32:D:ALA:CB  | 8        | 1.26          |
| (7,3)   | 1:37:C:THR:CA  | 1:32:C:ALA:CB  | 8        | 1.26          |
| (7,2)   | 1:37:B:THR:CA  | 1:32:B:ALA:CB  | 8        | 1.26          |
| (7,1)   | 1:37:A:THR:CA  | 1:32:A:ALA:CB  | 8        | 1.26          |
| (7,5)   | 1:37:E:THR:CA  | 1:32:E:ALA:CB  | 6        | 1.24          |
| (7,4)   | 1:37:D:THR:CA  | 1:32:D:ALA:CB  | 6        | 1.24          |
| (7,3)   | 1:37:C:THR:CA  | 1:32:C:ALA:CB  | 6        | 1.24          |
| (7,2)   | 1:37:B:THR:CA  | 1:32:B:ALA:CB  | 6        | 1.24          |
| (1,599) | 1:25:D:ILE:CG2 | 1:27:E:LEU:CG  | 7        | 1.24          |
| (1,598) | 1:25:C:ILE:CG2 | 1:27:D:LEU:CG  | 7        | 1.24          |
| (1,597) | 1:25:B:ILE:CG2 | 1:27:C:LEU:CG  | 7        | 1.24          |
| (1,596) | 1:25:A:ILE:CG2 | 1:27:B:LEU:CG  | 7        | 1.24          |
| (7,1)   | 1:37:A:THR:CA  | 1:32:A:ALA:CB  | 6        | 1.23          |
| (3,30)  | 1:33:E:PHE:CA  | 1:35:D:THR:N   | 6        | 1.23          |
| (3,29)  | 1:33:D:PHE:CA  | 1:35:C:THR:N   | 6        | 1.23          |
| (3,28)  | 1:33:C:PHE:CA  | 1:35:B:THR:N   | 6        | 1.23          |
| (3,27)  | 1:33:B:PHE:CA  | 1:35:A:THR:N   | 6        | 1.23          |
| (3,26)  | 1:33:A:PHE:CA  | 1:35:E:THR:N   | 6        | 1.23          |
| (1,600) | 1:25:E:ILE:CG2 | 1:27:A:LEU:CG  | 7        | 1.23          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (7,5)   | 1:37:E:THR:CA  | 1:32:E:ALA:CB  | 9        | 1.22          |
| (7,5)   | 1:37:E:THR:CA  | 1:32:E:ALA:CB  | 10       | 1.22          |
| (7,4)   | 1:37:D:THR:CA  | 1:32:D:ALA:CB  | 9        | 1.22          |
| (7,4)   | 1:37:D:THR:CA  | 1:32:D:ALA:CB  | 10       | 1.22          |
| (7,3)   | 1:37:C:THR:CA  | 1:32:C:ALA:CB  | 9        | 1.22          |
| (7,3)   | 1:37:C:THR:CA  | 1:32:C:ALA:CB  | 10       | 1.22          |
| (7,2)   | 1:37:B:THR:CA  | 1:32:B:ALA:CB  | 9        | 1.22          |
| (7,2)   | 1:37:B:THR:CA  | 1:32:B:ALA:CB  | 10       | 1.22          |
| (7,1)   | 1:37:A:THR:CA  | 1:32:A:ALA:CB  | 9        | 1.22          |
| (7,1)   | 1:37:A:THR:CA  | 1:32:A:ALA:CB  | 10       | 1.22          |
| (7,5)   | 1:37:E:THR:CA  | 1:32:E:ALA:CB  | 4        | 1.21          |
| (7,4)   | 1:37:D:THR:CA  | 1:32:D:ALA:CB  | 4        | 1.21          |
| (7,3)   | 1:37:C:THR:CA  | 1:32:C:ALA:CB  | 4        | 1.21          |
| (7,2)   | 1:37:B:THR:CA  | 1:32:B:ALA:CB  | 4        | 1.21          |
| (7,1)   | 1:37:A:THR:CA  | 1:32:A:ALA:CB  | 4        | 1.21          |
| (3,30)  | 1:33:E:PHE:CA  | 1:35:D:THR:N   | 2        | 1.21          |
| (3,29)  | 1:33:D:PHE:CA  | 1:35:C:THR:N   | 2        | 1.21          |
| (3,28)  | 1:33:C:PHE:CA  | 1:35:B:THR:N   | 2        | 1.21          |
| (3,27)  | 1:33:B:PHE:CA  | 1:35:A:THR:N   | 2        | 1.21          |
| (3,26)  | 1:33:A:PHE:CA  | 1:35:E:THR:N   | 2        | 1.21          |
| (1,600) | 1:25:E:ILE:CG2 | 1:27:E:LEU:CG  | 2        | 1.21          |
| (1,599) | 1:25:D:ILE:CG2 | 1:27:D:LEU:CG  | 2        | 1.21          |
| (1,598) | 1:25:C:ILE:CG2 | 1:27:C:LEU:CG  | 2        | 1.21          |
| (1,597) | 1:25:B:ILE:CG2 | 1:27:B:LEU:CG  | 2        | 1.21          |
| (1,596) | 1:25:A:ILE:CG2 | 1:27:A:LEU:CG  | 2        | 1.21          |
| (7,5)   | 1:37:E:THR:CA  | 1:32:E:ALA:CB  | 3        | 1.15          |
| (7,4)   | 1:37:D:THR:CA  | 1:32:D:ALA:CB  | 3        | 1.15          |
| (7,3)   | 1:37:C:THR:CA  | 1:32:C:ALA:CB  | 3        | 1.15          |
| (7,2)   | 1:37:B:THR:CA  | 1:32:B:ALA:CB  | 3        | 1.15          |
| (7,1)   | 1:37:A:THR:CA  | 1:32:A:ALA:CB  | 3        | 1.15          |
| (3,27)  | 1:33:B:PHE:CA  | 1:35:C:THR:N   | 3        | 1.14          |
| (1,585) | 1:25:E:ILE:CG1 | 1:27:E:LEU:CG  | 2        | 1.14          |
| (1,584) | 1:25:D:ILE:CG1 | 1:27:D:LEU:CG  | 2        | 1.14          |
| (1,583) | 1:25:C:ILE:CG1 | 1:27:C:LEU:CG  | 2        | 1.14          |
| (1,582) | 1:25:B:ILE:CG1 | 1:27:B:LEU:CG  | 2        | 1.14          |
| (1,581) | 1:25:A:ILE:CG1 | 1:27:A:LEU:CG  | 2        | 1.14          |
| (1,125) | 1:9:E:ILE:CG1  | 1:11:A:LEU:CD2 | 9        | 1.14          |
| (1,124) | 1:9:D:ILE:CG1  | 1:11:E:LEU:CD2 | 9        | 1.14          |
| (1,123) | 1:9:C:ILE:CG1  | 1:11:D:LEU:CD2 | 9        | 1.14          |
| (1,122) | 1:9:B:ILE:CG1  | 1:11:C:LEU:CD2 | 9        | 1.14          |
| (1,121) | 1:9:A:ILE:CG1  | 1:11:B:LEU:CD2 | 9        | 1.14          |
| (3,30)  | 1:33:E:PHE:CA  | 1:35:A:THR:N   | 3        | 1.13          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (3,29)  | 1:33:D:PHE:CA  | 1:35:E:THR:N   | 3        | 1.13          |
| (3,28)  | 1:33:C:PHE:CA  | 1:35:D:THR:N   | 3        | 1.13          |
| (3,26)  | 1:33:A:PHE:CA  | 1:35:B:THR:N   | 3        | 1.13          |
| (1,590) | 1:9:E:ILE:CG2  | 1:11:A:LEU:CG  | 10       | 1.12          |
| (1,589) | 1:9:D:ILE:CG2  | 1:11:E:LEU:CG  | 10       | 1.12          |
| (1,588) | 1:9:C:ILE:CG2  | 1:11:D:LEU:CG  | 10       | 1.12          |
| (1,587) | 1:9:B:ILE:CG2  | 1:11:C:LEU:CG  | 10       | 1.12          |
| (1,586) | 1:9:A:ILE:CG2  | 1:11:B:LEU:CG  | 10       | 1.12          |
| (7,15)  | 1:37:E:THR:CG2 | 1:30:E:SER:CA  | 6        | 1.11          |
| (7,14)  | 1:37:D:THR:CG2 | 1:30:D:SER:CA  | 6        | 1.11          |
| (7,13)  | 1:37:C:THR:CG2 | 1:30:C:SER:CA  | 6        | 1.11          |
| (7,12)  | 1:37:B:THR:CG2 | 1:30:B:SER:CA  | 6        | 1.11          |
| (7,11)  | 1:37:A:THR:CG2 | 1:30:A:SER:CA  | 6        | 1.11          |
| (2,54)  | 1:11:D:LEU:CG  | 1:13:D:ILE:CD1 | 7        | 1.11          |
| (2,53)  | 1:11:C:LEU:CG  | 1:13:C:ILE:CD1 | 7        | 1.11          |
| (2,52)  | 1:11:B:LEU:CG  | 1:13:B:ILE:CD1 | 7        | 1.11          |
| (2,51)  | 1:11:A:LEU:CG  | 1:13:A:ILE:CD1 | 7        | 1.11          |
| (1,839) | 1:11:D:LEU:CG  | 1:13:D:ILE:CD1 | 7        | 1.11          |
| (1,838) | 1:11:C:LEU:CG  | 1:13:C:ILE:CD1 | 7        | 1.11          |
| (1,837) | 1:11:B:LEU:CG  | 1:13:B:ILE:CD1 | 7        | 1.11          |
| (1,836) | 1:11:A:LEU:CG  | 1:13:A:ILE:CD1 | 7        | 1.11          |
| (7,5)   | 1:37:E:THR:CA  | 1:32:E:ALA:CB  | 5        | 1.1           |
| (7,4)   | 1:37:D:THR:CA  | 1:32:D:ALA:CB  | 5        | 1.1           |
| (7,3)   | 1:37:C:THR:CA  | 1:32:C:ALA:CB  | 5        | 1.1           |
| (7,2)   | 1:37:B:THR:CA  | 1:32:B:ALA:CB  | 5        | 1.1           |
| (7,1)   | 1:37:A:THR:CA  | 1:32:A:ALA:CB  | 5        | 1.1           |
| (2,55)  | 1:11:E:LEU:CG  | 1:13:E:ILE:CD1 | 7        | 1.1           |
| (1,840) | 1:11:E:LEU:CG  | 1:13:E:ILE:CD1 | 7        | 1.1           |
| (1,585) | 1:25:E:ILE:CG1 | 1:27:A:LEU:CG  | 7        | 1.1           |
| (1,584) | 1:25:D:ILE:CG1 | 1:27:E:LEU:CG  | 7        | 1.1           |
| (1,583) | 1:25:C:ILE:CG1 | 1:27:D:LEU:CG  | 7        | 1.1           |
| (1,582) | 1:25:B:ILE:CG1 | 1:27:C:LEU:CG  | 7        | 1.1           |
| (1,581) | 1:25:A:ILE:CG1 | 1:27:B:LEU:CG  | 7        | 1.1           |
| (3,30)  | 1:33:E:PHE:CA  | 1:35:D:THR:N   | 7        | 1.08          |
| (3,29)  | 1:33:D:PHE:CA  | 1:35:C:THR:N   | 7        | 1.08          |
| (3,28)  | 1:33:C:PHE:CA  | 1:35:B:THR:N   | 7        | 1.08          |
| (3,27)  | 1:33:B:PHE:CA  | 1:35:A:THR:N   | 7        | 1.08          |
| (3,26)  | 1:33:A:PHE:CA  | 1:35:E:THR:N   | 7        | 1.08          |
| (7,15)  | 1:37:E:THR:CG2 | 1:30:E:SER:CA  | 10       | 1.07          |
| (7,14)  | 1:37:D:THR:CG2 | 1:30:D:SER:CA  | 10       | 1.07          |
| (7,13)  | 1:37:C:THR:CG2 | 1:30:C:SER:CA  | 10       | 1.07          |
| (7,12)  | 1:37:B:THR:CG2 | 1:30:B:SER:CA  | 10       | 1.07          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (7,11)  | 1:37:A:THR:CG2 | 1:30:A:SER:CA  | 10       | 1.07          |
| (7,5)   | 1:37:E:THR:CA  | 1:32:E:ALA:CB  | 7        | 1.07          |
| (7,4)   | 1:37:D:THR:CA  | 1:32:D:ALA:CB  | 7        | 1.07          |
| (7,3)   | 1:37:C:THR:CA  | 1:32:C:ALA:CB  | 7        | 1.07          |
| (7,2)   | 1:37:B:THR:CA  | 1:32:B:ALA:CB  | 7        | 1.07          |
| (7,1)   | 1:37:A:THR:CA  | 1:32:A:ALA:CB  | 7        | 1.07          |
| (3,30)  | 1:33:E:PHE:CA  | 1:35:D:THR:N   | 4        | 1.03          |
| (3,29)  | 1:33:D:PHE:CA  | 1:35:C:THR:N   | 4        | 1.03          |
| (3,28)  | 1:33:C:PHE:CA  | 1:35:B:THR:N   | 4        | 1.03          |
| (3,27)  | 1:33:B:PHE:CA  | 1:35:A:THR:N   | 4        | 1.03          |
| (3,26)  | 1:33:A:PHE:CA  | 1:35:E:THR:N   | 4        | 1.03          |
| (1,585) | 1:25:E:ILE:CG1 | 1:27:A:LEU:CG  | 9        | 1.02          |
| (1,584) | 1:25:D:ILE:CG1 | 1:27:E:LEU:CG  | 9        | 1.01          |
| (1,583) | 1:25:C:ILE:CG1 | 1:27:D:LEU:CG  | 9        | 1.01          |
| (1,582) | 1:25:B:ILE:CG1 | 1:27:C:LEU:CG  | 9        | 1.01          |
| (1,581) | 1:25:A:ILE:CG1 | 1:27:B:LEU:CG  | 9        | 1.01          |
| (1,600) | 1:25:E:ILE:CG2 | 1:27:E:LEU:CG  | 5        | 1.0           |
| (1,599) | 1:25:D:ILE:CG2 | 1:27:D:LEU:CG  | 5        | 1.0           |
| (1,598) | 1:25:C:ILE:CG2 | 1:27:C:LEU:CG  | 5        | 1.0           |
| (1,597) | 1:25:B:ILE:CG2 | 1:27:B:LEU:CG  | 5        | 1.0           |
| (1,596) | 1:25:A:ILE:CG2 | 1:27:A:LEU:CG  | 5        | 1.0           |
| (1,123) | 1:9:C:ILE:CG1  | 1:11:C:LEU:CD2 | 4        | 1.0           |
| (1,121) | 1:9:A:ILE:CG1  | 1:11:A:LEU:CD2 | 4        | 1.0           |
| (1,600) | 1:25:E:ILE:CG2 | 1:27:A:LEU:CG  | 3        | 0.99          |
| (1,599) | 1:25:D:ILE:CG2 | 1:27:E:LEU:CG  | 3        | 0.99          |
| (1,598) | 1:25:C:ILE:CG2 | 1:27:D:LEU:CG  | 3        | 0.99          |
| (1,597) | 1:25:B:ILE:CG2 | 1:27:C:LEU:CG  | 3        | 0.99          |
| (1,596) | 1:25:A:ILE:CG2 | 1:27:B:LEU:CG  | 3        | 0.99          |
| (1,125) | 1:9:E:ILE:CG1  | 1:11:E:LEU:CD2 | 4        | 0.99          |
| (1,125) | 1:9:E:ILE:CG1  | 1:11:A:LEU:CD2 | 8        | 0.99          |
| (1,124) | 1:9:D:ILE:CG1  | 1:11:D:LEU:CD2 | 4        | 0.99          |
| (1,124) | 1:9:D:ILE:CG1  | 1:11:E:LEU:CD2 | 8        | 0.99          |
| (1,123) | 1:9:C:ILE:CG1  | 1:11:D:LEU:CD2 | 8        | 0.99          |
| (1,122) | 1:9:B:ILE:CG1  | 1:11:B:LEU:CD2 | 4        | 0.99          |
| (1,122) | 1:9:B:ILE:CG1  | 1:11:C:LEU:CD2 | 8        | 0.99          |
| (1,121) | 1:9:A:ILE:CG1  | 1:11:B:LEU:CD2 | 8        | 0.99          |
| (7,20)  | 1:37:E:THR:CG2 | 1:32:D:ALA:CB  | 8        | 0.98          |
| (7,19)  | 1:37:D:THR:CG2 | 1:32:C:ALA:CB  | 8        | 0.98          |
| (7,18)  | 1:37:C:THR:CG2 | 1:32:B:ALA:CB  | 8        | 0.98          |
| (7,17)  | 1:37:B:THR:CG2 | 1:32:A:ALA:CB  | 8        | 0.98          |
| (7,16)  | 1:37:A:THR:CG2 | 1:32:E:ALA:CB  | 8        | 0.98          |
| (7,15)  | 1:37:E:THR:CG2 | 1:30:E:SER:CA  | 5        | 0.97          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (7,14)  | 1:37:D:THR:CG2 | 1:30:D:SER:CA  | 5        | 0.97          |
| (7,13)  | 1:37:C:THR:CG2 | 1:30:C:SER:CA  | 5        | 0.97          |
| (7,12)  | 1:37:B:THR:CG2 | 1:30:B:SER:CA  | 5        | 0.97          |
| (7,11)  | 1:37:A:THR:CG2 | 1:30:A:SER:CA  | 5        | 0.97          |
| (1,870) | 1:32:E:ALA:CB  | 1:26:A:THR:CA  | 9        | 0.97          |
| (1,869) | 1:32:D:ALA:CB  | 1:26:E:THR:CA  | 9        | 0.97          |
| (1,868) | 1:32:C:ALA:CB  | 1:26:D:THR:CA  | 9        | 0.97          |
| (1,867) | 1:32:B:ALA:CB  | 1:26:C:THR:CA  | 9        | 0.97          |
| (1,866) | 1:32:A:ALA:CB  | 1:26:B:THR:CA  | 9        | 0.97          |
| (1,225) | 1:29:E:VAL:CA  | 1:25:E:ILE:CD1 | 4        | 0.97          |
| (1,224) | 1:29:D:VAL:CA  | 1:25:D:ILE:CD1 | 4        | 0.97          |
| (1,222) | 1:29:B:VAL:CA  | 1:25:B:ILE:CD1 | 4        | 0.97          |
| (1,221) | 1:29:A:VAL:CA  | 1:25:A:ILE:CD1 | 4        | 0.97          |
| (7,15)  | 1:37:E:THR:CG2 | 1:30:E:SER:CA  | 7        | 0.96          |
| (7,12)  | 1:37:B:THR:CG2 | 1:30:B:SER:CA  | 7        | 0.96          |
| (7,11)  | 1:37:A:THR:CG2 | 1:30:A:SER:CA  | 7        | 0.96          |
| (1,223) | 1:29:C:VAL:CA  | 1:25:C:ILE:CD1 | 4        | 0.96          |
| (7,14)  | 1:37:D:THR:CG2 | 1:30:D:SER:CA  | 7        | 0.95          |
| (7,13)  | 1:37:C:THR:CG2 | 1:30:C:SER:CA  | 7        | 0.95          |
| (1,835) | 1:11:E:LEU:CG  | 1:9:D:ILE:CG2  | 4        | 0.95          |
| (1,834) | 1:11:D:LEU:CG  | 1:9:C:ILE:CG2  | 4        | 0.95          |
| (1,833) | 1:11:C:LEU:CG  | 1:9:B:ILE:CG2  | 4        | 0.95          |
| (1,832) | 1:11:B:LEU:CG  | 1:9:A:ILE:CG2  | 4        | 0.95          |
| (1,831) | 1:11:A:LEU:CG  | 1:9:E:ILE:CG2  | 4        | 0.95          |
| (1,590) | 1:9:E:ILE:CG2  | 1:11:A:LEU:CG  | 4        | 0.95          |
| (1,590) | 1:9:E:ILE:CG2  | 1:11:E:LEU:CG  | 6        | 0.95          |
| (1,589) | 1:9:D:ILE:CG2  | 1:11:E:LEU:CG  | 4        | 0.95          |
| (1,589) | 1:9:D:ILE:CG2  | 1:11:D:LEU:CG  | 6        | 0.95          |
| (1,588) | 1:9:C:ILE:CG2  | 1:11:D:LEU:CG  | 4        | 0.95          |
| (1,588) | 1:9:C:ILE:CG2  | 1:11:C:LEU:CG  | 6        | 0.95          |
| (1,587) | 1:9:B:ILE:CG2  | 1:11:C:LEU:CG  | 4        | 0.95          |
| (1,587) | 1:9:B:ILE:CG2  | 1:11:B:LEU:CG  | 6        | 0.95          |
| (1,586) | 1:9:A:ILE:CG2  | 1:11:B:LEU:CG  | 4        | 0.95          |
| (1,586) | 1:9:A:ILE:CG2  | 1:11:A:LEU:CG  | 6        | 0.95          |
| (1,835) | 1:11:E:LEU:CG  | 1:13:E:ILE:CG2 | 10       | 0.94          |
| (1,834) | 1:11:D:LEU:CG  | 1:13:D:ILE:CG2 | 10       | 0.94          |
| (1,833) | 1:11:C:LEU:CG  | 1:9:C:ILE:CG2  | 7        | 0.94          |
| (1,833) | 1:11:C:LEU:CG  | 1:13:C:ILE:CG2 | 10       | 0.94          |
| (1,832) | 1:11:B:LEU:CG  | 1:13:B:ILE:CG2 | 10       | 0.94          |
| (1,831) | 1:11:A:LEU:CG  | 1:13:A:ILE:CG2 | 10       | 0.94          |
| (1,588) | 1:9:C:ILE:CG2  | 1:11:C:LEU:CG  | 7        | 0.94          |
| (1,835) | 1:11:E:LEU:CG  | 1:9:E:ILE:CG2  | 7        | 0.93          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,834)  | 1:11:D:LEU:CG  | 1:9:D:ILE:CG2  | 7        | 0.93          |
| (1,832)  | 1:11:B:LEU:CG  | 1:9:B:ILE:CG2  | 7        | 0.93          |
| (1,831)  | 1:11:A:LEU:CG  | 1:9:A:ILE:CG2  | 7        | 0.93          |
| (1,590)  | 1:9:E:ILE:CG2  | 1:11:E:LEU:CG  | 7        | 0.93          |
| (1,589)  | 1:9:D:ILE:CG2  | 1:11:D:LEU:CG  | 7        | 0.93          |
| (1,587)  | 1:9:B:ILE:CG2  | 1:11:B:LEU:CG  | 7        | 0.93          |
| (1,586)  | 1:9:A:ILE:CG2  | 1:11:A:LEU:CG  | 7        | 0.93          |
| (1,835)  | 1:11:E:LEU:CG  | 1:13:E:ILE:CG2 | 6        | 0.91          |
| (1,834)  | 1:11:D:LEU:CG  | 1:13:D:ILE:CG2 | 6        | 0.91          |
| (1,833)  | 1:11:C:LEU:CG  | 1:13:C:ILE:CG2 | 6        | 0.91          |
| (1,832)  | 1:11:B:LEU:CG  | 1:13:B:ILE:CG2 | 6        | 0.91          |
| (1,831)  | 1:11:A:LEU:CG  | 1:13:A:ILE:CG2 | 6        | 0.91          |
| (1,225)  | 1:29:E:VAL:CA  | 1:25:E:ILE:CD1 | 2        | 0.91          |
| (1,224)  | 1:29:D:VAL:CA  | 1:25:D:ILE:CD1 | 2        | 0.91          |
| (1,223)  | 1:29:C:VAL:CA  | 1:25:C:ILE:CD1 | 2        | 0.91          |
| (1,222)  | 1:29:B:VAL:CA  | 1:25:B:ILE:CD1 | 2        | 0.91          |
| (1,221)  | 1:29:A:VAL:CA  | 1:25:A:ILE:CD1 | 2        | 0.91          |
| (1,870)  | 1:32:E:ALA:CB  | 1:26:A:THR:CA  | 1        | 0.85          |
| (1,869)  | 1:32:D:ALA:CB  | 1:26:E:THR:CA  | 1        | 0.85          |
| (1,868)  | 1:32:C:ALA:CB  | 1:26:D:THR:CA  | 1        | 0.85          |
| (1,867)  | 1:32:B:ALA:CB  | 1:26:C:THR:CA  | 1        | 0.85          |
| (1,866)  | 1:32:A:ALA:CB  | 1:26:B:THR:CA  | 1        | 0.85          |
| (1,585)  | 1:25:E:ILE:CG1 | 1:27:E:LEU:CG  | 5        | 0.85          |
| (1,584)  | 1:25:D:ILE:CG1 | 1:27:D:LEU:CG  | 5        | 0.85          |
| (1,583)  | 1:25:C:ILE:CG1 | 1:27:C:LEU:CG  | 5        | 0.85          |
| (1,582)  | 1:25:B:ILE:CG1 | 1:27:B:LEU:CG  | 5        | 0.85          |
| (1,581)  | 1:25:A:ILE:CG1 | 1:27:A:LEU:CG  | 5        | 0.85          |
| (1,870)  | 1:32:E:ALA:CB  | 1:26:A:THR:CA  | 10       | 0.84          |
| (1,869)  | 1:32:D:ALA:CB  | 1:26:E:THR:CA  | 10       | 0.84          |
| (1,868)  | 1:32:C:ALA:CB  | 1:26:D:THR:CA  | 10       | 0.84          |
| (1,867)  | 1:32:B:ALA:CB  | 1:26:C:THR:CA  | 10       | 0.84          |
| (1,866)  | 1:32:A:ALA:CB  | 1:26:B:THR:CA  | 10       | 0.84          |
| (1,1010) | 1:27:E:LEU:CB  | 1:25:E:ILE:CD1 | 4        | 0.82          |
| (1,1009) | 1:27:D:LEU:CB  | 1:25:D:ILE:CD1 | 4        | 0.82          |
| (1,1008) | 1:27:C:LEU:CB  | 1:25:C:ILE:CD1 | 4        | 0.82          |
| (1,1007) | 1:27:B:LEU:CB  | 1:25:B:ILE:CD1 | 4        | 0.82          |
| (1,1006) | 1:27:A:LEU:CB  | 1:25:A:ILE:CD1 | 4        | 0.82          |
| (1,1010) | 1:27:E:LEU:CB  | 1:25:D:ILE:CD1 | 2        | 0.79          |
| (1,1009) | 1:27:D:LEU:CB  | 1:25:C:ILE:CD1 | 2        | 0.79          |
| (1,1008) | 1:27:C:LEU:CB  | 1:25:B:ILE:CD1 | 2        | 0.79          |
| (1,1007) | 1:27:B:LEU:CB  | 1:25:A:ILE:CD1 | 2        | 0.79          |
| (1,1006) | 1:27:A:LEU:CB  | 1:25:E:ILE:CD1 | 2        | 0.79          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (7,15)   | 1:37:E:THR:CG2 | 1:30:E:SER:CA  | 3        | 0.77          |
| (7,14)   | 1:37:D:THR:CG2 | 1:30:D:SER:CA  | 3        | 0.77          |
| (7,13)   | 1:37:C:THR:CG2 | 1:30:C:SER:CA  | 3        | 0.77          |
| (7,12)   | 1:37:B:THR:CG2 | 1:30:B:SER:CA  | 3        | 0.77          |
| (7,11)   | 1:37:A:THR:CG2 | 1:30:A:SER:CA  | 3        | 0.77          |
| (1,225)  | 1:29:E:VAL:CA  | 1:25:E:ILE:CD1 | 8        | 0.77          |
| (1,224)  | 1:29:D:VAL:CA  | 1:25:D:ILE:CD1 | 8        | 0.77          |
| (1,223)  | 1:29:C:VAL:CA  | 1:25:C:ILE:CD1 | 8        | 0.77          |
| (1,222)  | 1:29:B:VAL:CA  | 1:25:B:ILE:CD1 | 8        | 0.77          |
| (1,221)  | 1:29:A:VAL:CA  | 1:25:A:ILE:CD1 | 8        | 0.77          |
| (2,230)  | 1:29:E:VAL:CA  | 1:31:E:MET:CE  | 4        | 0.75          |
| (2,221)  | 1:29:D:VAL:CA  | 1:31:D:MET:CE  | 4        | 0.75          |
| (2,212)  | 1:29:C:VAL:CA  | 1:31:C:MET:CE  | 4        | 0.75          |
| (2,203)  | 1:29:B:VAL:CA  | 1:31:B:MET:CE  | 4        | 0.75          |
| (2,194)  | 1:29:A:VAL:CA  | 1:31:A:MET:CE  | 4        | 0.75          |
| (1,600)  | 1:25:E:ILE:CG2 | 1:27:A:LEU:CG  | 6        | 0.74          |
| (1,598)  | 1:25:C:ILE:CG2 | 1:27:D:LEU:CG  | 6        | 0.74          |
| (1,225)  | 1:29:E:VAL:CA  | 1:25:E:ILE:CD1 | 5        | 0.74          |
| (1,224)  | 1:29:D:VAL:CA  | 1:25:D:ILE:CD1 | 5        | 0.74          |
| (1,223)  | 1:29:C:VAL:CA  | 1:25:C:ILE:CD1 | 5        | 0.74          |
| (1,222)  | 1:29:B:VAL:CA  | 1:25:B:ILE:CD1 | 5        | 0.74          |
| (1,221)  | 1:29:A:VAL:CA  | 1:25:A:ILE:CD1 | 5        | 0.74          |
| (7,5)    | 1:37:E:THR:CA  | 1:32:E:ALA:CB  | 2        | 0.73          |
| (7,4)    | 1:37:D:THR:CA  | 1:32:D:ALA:CB  | 2        | 0.73          |
| (7,3)    | 1:37:C:THR:CA  | 1:32:C:ALA:CB  | 2        | 0.73          |
| (7,2)    | 1:37:B:THR:CA  | 1:32:B:ALA:CB  | 2        | 0.73          |
| (7,1)    | 1:37:A:THR:CA  | 1:32:A:ALA:CB  | 2        | 0.73          |
| (1,1115) | 1:20:E:THR:CG2 | 1:22:E:VAL:CG2 | 6        | 0.73          |
| (1,1114) | 1:20:D:THR:CG2 | 1:22:D:VAL:CG2 | 6        | 0.73          |
| (1,1113) | 1:20:C:THR:CG2 | 1:22:C:VAL:CG2 | 6        | 0.73          |
| (1,1112) | 1:20:B:THR:CG2 | 1:22:B:VAL:CG2 | 6        | 0.73          |
| (1,1111) | 1:20:A:THR:CG2 | 1:22:A:VAL:CG2 | 6        | 0.73          |
| (1,835)  | 1:11:E:LEU:CG  | 1:9:D:ILE:CG2  | 8        | 0.73          |
| (1,834)  | 1:11:D:LEU:CG  | 1:9:C:ILE:CG2  | 8        | 0.73          |
| (1,833)  | 1:11:C:LEU:CG  | 1:9:B:ILE:CG2  | 8        | 0.73          |
| (1,832)  | 1:11:B:LEU:CG  | 1:9:A:ILE:CG2  | 8        | 0.73          |
| (1,831)  | 1:11:A:LEU:CG  | 1:9:E:ILE:CG2  | 8        | 0.73          |
| (1,599)  | 1:25:D:ILE:CG2 | 1:27:E:LEU:CG  | 6        | 0.73          |
| (1,597)  | 1:25:B:ILE:CG2 | 1:27:C:LEU:CG  | 6        | 0.73          |
| (1,596)  | 1:25:A:ILE:CG2 | 1:27:B:LEU:CG  | 6        | 0.73          |
| (1,590)  | 1:9:E:ILE:CG2  | 1:11:A:LEU:CG  | 8        | 0.73          |
| (1,589)  | 1:9:D:ILE:CG2  | 1:11:E:LEU:CG  | 8        | 0.73          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,588)  | 1:9:C:ILE:CG2  | 1:11:D:LEU:CG  | 8        | 0.73          |
| (1,587)  | 1:9:B:ILE:CG2  | 1:11:C:LEU:CG  | 8        | 0.73          |
| (1,586)  | 1:9:A:ILE:CG2  | 1:11:B:LEU:CG  | 8        | 0.73          |
| (1,1008) | 1:27:C:LEU:CB  | 1:25:B:ILE:CD1 | 8        | 0.71          |
| (1,1010) | 1:27:E:LEU:CB  | 1:25:D:ILE:CD1 | 8        | 0.7           |
| (1,1009) | 1:27:D:LEU:CB  | 1:25:C:ILE:CD1 | 8        | 0.7           |
| (1,1007) | 1:27:B:LEU:CB  | 1:25:A:ILE:CD1 | 8        | 0.7           |
| (1,1006) | 1:27:A:LEU:CB  | 1:25:E:ILE:CD1 | 8        | 0.7           |
| (1,835)  | 1:11:E:LEU:CG  | 1:9:D:ILE:CG2  | 9        | 0.67          |
| (1,834)  | 1:11:D:LEU:CG  | 1:9:C:ILE:CG2  | 9        | 0.67          |
| (1,833)  | 1:11:C:LEU:CG  | 1:9:B:ILE:CG2  | 9        | 0.67          |
| (1,832)  | 1:11:B:LEU:CG  | 1:9:A:ILE:CG2  | 9        | 0.67          |
| (1,831)  | 1:11:A:LEU:CG  | 1:9:E:ILE:CG2  | 9        | 0.67          |
| (1,590)  | 1:9:E:ILE:CG2  | 1:11:A:LEU:CG  | 9        | 0.67          |
| (1,589)  | 1:9:D:ILE:CG2  | 1:11:E:LEU:CG  | 9        | 0.67          |
| (1,588)  | 1:9:C:ILE:CG2  | 1:11:D:LEU:CG  | 9        | 0.67          |
| (1,587)  | 1:9:B:ILE:CG2  | 1:11:C:LEU:CG  | 9        | 0.67          |
| (1,586)  | 1:9:A:ILE:CG2  | 1:11:B:LEU:CG  | 9        | 0.67          |
| (7,15)   | 1:37:E:THR:CG2 | 1:30:E:SER:CA  | 4        | 0.65          |
| (7,14)   | 1:37:D:THR:CG2 | 1:30:D:SER:CA  | 4        | 0.65          |
| (7,13)   | 1:37:C:THR:CG2 | 1:30:C:SER:CA  | 4        | 0.65          |
| (7,12)   | 1:37:B:THR:CG2 | 1:30:B:SER:CA  | 4        | 0.65          |
| (7,11)   | 1:37:A:THR:CG2 | 1:30:A:SER:CA  | 4        | 0.65          |
| (4,60)   | 1:27:E:LEU:CG  | 1:24:D:ALA:N   | 5        | 0.65          |
| (4,59)   | 1:27:D:LEU:CG  | 1:24:C:ALA:N   | 5        | 0.65          |
| (4,58)   | 1:27:C:LEU:CG  | 1:24:B:ALA:N   | 5        | 0.65          |
| (4,57)   | 1:27:B:LEU:CG  | 1:24:A:ALA:N   | 5        | 0.65          |
| (4,56)   | 1:27:A:LEU:CG  | 1:24:E:ALA:N   | 5        | 0.65          |
| (1,730)  | 1:9:A:ILE:CG2  | 1:11:A:LEU:CD1 | 7        | 0.64          |
| (1,729)  | 1:9:D:ILE:CG2  | 1:11:D:LEU:CD1 | 7        | 0.64          |
| (1,728)  | 1:9:B:ILE:CG2  | 1:11:B:LEU:CD1 | 7        | 0.64          |
| (1,727)  | 1:9:A:ILE:CG2  | 1:11:A:LEU:CD1 | 7        | 0.64          |
| (1,726)  | 1:9:A:ILE:CG2  | 1:11:A:LEU:CD1 | 7        | 0.64          |
| (2,55)   | 1:11:E:LEU:CG  | 1:13:E:ILE:CD1 | 8        | 0.63          |
| (2,55)   | 1:11:E:LEU:CG  | 1:13:E:ILE:CD1 | 9        | 0.63          |
| (2,54)   | 1:11:D:LEU:CG  | 1:13:D:ILE:CD1 | 8        | 0.63          |
| (2,54)   | 1:11:D:LEU:CG  | 1:13:D:ILE:CD1 | 9        | 0.63          |
| (2,53)   | 1:11:C:LEU:CG  | 1:13:C:ILE:CD1 | 8        | 0.63          |
| (2,53)   | 1:11:C:LEU:CG  | 1:13:C:ILE:CD1 | 9        | 0.63          |
| (2,52)   | 1:11:B:LEU:CG  | 1:13:B:ILE:CD1 | 8        | 0.63          |
| (2,52)   | 1:11:B:LEU:CG  | 1:13:B:ILE:CD1 | 9        | 0.63          |
| (2,51)   | 1:11:A:LEU:CG  | 1:13:A:ILE:CD1 | 8        | 0.63          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (2,51)   | 1:11:A:LEU:CG  | 1:13:A:ILE:CD1 | 9        | 0.63          |
| (1,840)  | 1:11:E:LEU:CG  | 1:13:E:ILE:CD1 | 8        | 0.63          |
| (1,840)  | 1:11:E:LEU:CG  | 1:13:E:ILE:CD1 | 9        | 0.63          |
| (1,839)  | 1:11:D:LEU:CG  | 1:13:D:ILE:CD1 | 8        | 0.63          |
| (1,839)  | 1:11:D:LEU:CG  | 1:13:D:ILE:CD1 | 9        | 0.63          |
| (1,838)  | 1:11:C:LEU:CG  | 1:13:C:ILE:CD1 | 8        | 0.63          |
| (1,838)  | 1:11:C:LEU:CG  | 1:13:C:ILE:CD1 | 9        | 0.63          |
| (1,837)  | 1:11:B:LEU:CG  | 1:13:B:ILE:CD1 | 8        | 0.63          |
| (1,837)  | 1:11:B:LEU:CG  | 1:13:B:ILE:CD1 | 9        | 0.63          |
| (1,836)  | 1:11:A:LEU:CG  | 1:13:A:ILE:CD1 | 8        | 0.63          |
| (1,836)  | 1:11:A:LEU:CG  | 1:13:A:ILE:CD1 | 9        | 0.63          |
| (1,1010) | 1:27:E:LEU:CB  | 1:25:D:ILE:CD1 | 5        | 0.62          |
| (1,1009) | 1:27:D:LEU:CB  | 1:25:C:ILE:CD1 | 5        | 0.62          |
| (1,1008) | 1:27:C:LEU:CB  | 1:25:B:ILE:CD1 | 5        | 0.62          |
| (1,1007) | 1:27:B:LEU:CB  | 1:25:A:ILE:CD1 | 5        | 0.62          |
| (1,1006) | 1:27:A:LEU:CB  | 1:25:E:ILE:CD1 | 5        | 0.62          |
| (1,125)  | 1:9:E:ILE:CG1  | 1:11:A:LEU:CD2 | 7        | 0.62          |
| (1,124)  | 1:9:D:ILE:CG1  | 1:11:E:LEU:CD2 | 7        | 0.62          |
| (1,123)  | 1:9:C:ILE:CG1  | 1:11:D:LEU:CD2 | 7        | 0.62          |
| (1,122)  | 1:9:B:ILE:CG1  | 1:11:C:LEU:CD2 | 7        | 0.62          |
| (1,121)  | 1:9:A:ILE:CG1  | 1:11:B:LEU:CD2 | 7        | 0.62          |
| (1,1010) | 1:27:E:LEU:CB  | 1:25:E:ILE:CD1 | 1        | 0.6           |
| (1,1009) | 1:27:D:LEU:CB  | 1:25:D:ILE:CD1 | 1        | 0.6           |
| (1,1008) | 1:27:C:LEU:CB  | 1:25:C:ILE:CD1 | 1        | 0.6           |
| (1,1007) | 1:27:B:LEU:CB  | 1:25:B:ILE:CD1 | 1        | 0.6           |
| (1,1006) | 1:27:A:LEU:CB  | 1:25:A:ILE:CD1 | 1        | 0.6           |
| (1,320)  | 1:9:E:ILE:CB   | 1:11:E:LEU:CD2 | 5        | 0.6           |
| (1,319)  | 1:9:D:ILE:CB   | 1:11:D:LEU:CD2 | 5        | 0.6           |
| (1,318)  | 1:9:C:ILE:CB   | 1:11:C:LEU:CD2 | 5        | 0.6           |
| (1,317)  | 1:9:B:ILE:CB   | 1:11:B:LEU:CD2 | 5        | 0.6           |
| (1,316)  | 1:9:A:ILE:CB   | 1:11:A:LEU:CD2 | 5        | 0.6           |
| (1,225)  | 1:29:E:VAL:CA  | 1:25:E:ILE:CD1 | 7        | 0.6           |
| (1,224)  | 1:29:D:VAL:CA  | 1:25:D:ILE:CD1 | 7        | 0.6           |
| (1,223)  | 1:29:C:VAL:CA  | 1:25:C:ILE:CD1 | 7        | 0.6           |
| (1,222)  | 1:29:B:VAL:CA  | 1:25:B:ILE:CD1 | 7        | 0.6           |
| (1,221)  | 1:29:A:VAL:CA  | 1:25:A:ILE:CD1 | 7        | 0.6           |
| (7,20)   | 1:37:E:THR:CG2 | 1:32:E:ALA:CB  | 10       | 0.59          |
| (7,19)   | 1:37:D:THR:CG2 | 1:32:D:ALA:CB  | 10       | 0.59          |
| (7,18)   | 1:37:C:THR:CG2 | 1:32:C:ALA:CB  | 10       | 0.59          |
| (7,17)   | 1:37:B:THR:CG2 | 1:32:B:ALA:CB  | 10       | 0.59          |
| (7,16)   | 1:37:A:THR:CG2 | 1:32:A:ALA:CB  | 10       | 0.59          |
| (1,600)  | 1:25:E:ILE:CG2 | 1:27:E:LEU:CG  | 9        | 0.59          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,599) | 1:25:D:ILE:CG2 | 1:27:D:LEU:CG  | 9        | 0.59          |
| (1,598) | 1:25:C:ILE:CG2 | 1:27:C:LEU:CG  | 9        | 0.59          |
| (1,597) | 1:25:B:ILE:CG2 | 1:27:B:LEU:CG  | 9        | 0.59          |
| (1,596) | 1:25:A:ILE:CG2 | 1:27:A:LEU:CG  | 9        | 0.59          |
| (3,120) | 1:18:E:ILE:CA  | 1:16:A:PHE:N   | 4        | 0.58          |
| (3,119) | 1:18:D:ILE:CA  | 1:16:E:PHE:N   | 4        | 0.58          |
| (3,118) | 1:18:C:ILE:CA  | 1:16:D:PHE:N   | 4        | 0.58          |
| (3,117) | 1:18:B:ILE:CA  | 1:16:C:PHE:N   | 4        | 0.58          |
| (3,116) | 1:18:A:ILE:CA  | 1:16:B:PHE:N   | 4        | 0.58          |
| (2,15)  | 1:13:E:ILE:CD1 | 1:14:E:VAL:CG1 | 5        | 0.56          |
| (2,14)  | 1:13:D:ILE:CD1 | 1:14:D:VAL:CG1 | 5        | 0.56          |
| (2,13)  | 1:13:C:ILE:CD1 | 1:14:C:VAL:CG1 | 5        | 0.56          |
| (2,12)  | 1:13:B:ILE:CD1 | 1:14:B:VAL:CG1 | 5        | 0.56          |
| (2,11)  | 1:13:A:ILE:CD1 | 1:14:A:VAL:CG1 | 5        | 0.56          |
| (7,20)  | 1:37:E:THR:CG2 | 1:32:E:ALA:CB  | 5        | 0.54          |
| (7,19)  | 1:37:D:THR:CG2 | 1:32:D:ALA:CB  | 5        | 0.54          |
| (7,18)  | 1:37:C:THR:CG2 | 1:32:C:ALA:CB  | 5        | 0.54          |
| (7,17)  | 1:37:B:THR:CG2 | 1:32:B:ALA:CB  | 5        | 0.54          |
| (7,16)  | 1:37:A:THR:CG2 | 1:32:A:ALA:CB  | 5        | 0.54          |
| (1,780) | 1:27:D:LEU:CA  | 1:25:D:ILE:CD1 | 4        | 0.54          |
| (1,779) | 1:27:D:LEU:CA  | 1:25:D:ILE:CD1 | 4        | 0.54          |
| (1,778) | 1:27:D:LEU:CA  | 1:25:D:ILE:CD1 | 4        | 0.54          |
| (1,777) | 1:27:C:LEU:CA  | 1:25:C:ILE:CD1 | 4        | 0.54          |
| (1,776) | 1:27:A:LEU:CA  | 1:25:A:ILE:CD1 | 4        | 0.54          |
| (1,325) | 1:25:E:ILE:CB  | 1:27:E:LEU:CG  | 9        | 0.54          |
| (1,324) | 1:25:D:ILE:CB  | 1:27:D:LEU:CG  | 9        | 0.54          |
| (1,323) | 1:25:C:ILE:CB  | 1:27:C:LEU:CG  | 9        | 0.54          |
| (1,322) | 1:25:B:ILE:CB  | 1:27:B:LEU:CG  | 9        | 0.54          |
| (1,321) | 1:25:A:ILE:CB  | 1:27:A:LEU:CG  | 9        | 0.54          |
| (2,40)  | 1:14:E:VAL:CG2 | 1:13:E:ILE:CD1 | 1        | 0.53          |
| (2,39)  | 1:14:D:VAL:CG2 | 1:13:D:ILE:CD1 | 1        | 0.53          |
| (2,38)  | 1:14:C:VAL:CG2 | 1:13:C:ILE:CD1 | 1        | 0.53          |
| (2,37)  | 1:14:B:VAL:CG2 | 1:13:B:ILE:CD1 | 1        | 0.53          |
| (2,36)  | 1:14:A:VAL:CG2 | 1:13:A:ILE:CD1 | 1        | 0.53          |
| (1,995) | 1:27:E:LEU:CG  | 1:29:E:VAL:CG2 | 7        | 0.53          |
| (1,994) | 1:27:D:LEU:CG  | 1:29:D:VAL:CG2 | 7        | 0.53          |
| (1,993) | 1:27:C:LEU:CG  | 1:29:C:VAL:CG2 | 7        | 0.53          |
| (1,992) | 1:27:B:LEU:CG  | 1:29:B:VAL:CG2 | 7        | 0.53          |
| (1,991) | 1:27:A:LEU:CG  | 1:29:A:VAL:CG2 | 7        | 0.53          |
| (1,435) | 1:29:E:VAL:CG2 | 1:27:E:LEU:CG  | 7        | 0.53          |
| (1,434) | 1:29:D:VAL:CG2 | 1:27:D:LEU:CG  | 7        | 0.53          |
| (1,433) | 1:29:C:VAL:CG2 | 1:27:C:LEU:CG  | 7        | 0.53          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,432)  | 1:29:B:VAL:CG2 | 1:27:B:LEU:CG  | 7        | 0.53          |
| (1,431)  | 1:29:A:VAL:CG2 | 1:27:A:LEU:CG  | 7        | 0.53          |
| (2,40)   | 1:14:E:VAL:CG2 | 1:13:E:ILE:CD1 | 2        | 0.52          |
| (2,39)   | 1:14:D:VAL:CG2 | 1:13:D:ILE:CD1 | 2        | 0.52          |
| (2,38)   | 1:14:C:VAL:CG2 | 1:13:C:ILE:CD1 | 2        | 0.52          |
| (2,37)   | 1:14:B:VAL:CG2 | 1:13:B:ILE:CD1 | 2        | 0.52          |
| (2,36)   | 1:14:A:VAL:CG2 | 1:13:A:ILE:CD1 | 2        | 0.52          |
| (1,515)  | 1:15:E:ASN:CA  | 1:11:E:LEU:CD1 | 5        | 0.52          |
| (1,514)  | 1:15:D:ASN:CA  | 1:11:D:LEU:CD1 | 5        | 0.52          |
| (1,513)  | 1:15:C:ASN:CA  | 1:11:C:LEU:CD1 | 5        | 0.52          |
| (1,512)  | 1:15:B:ASN:CA  | 1:11:B:LEU:CD1 | 5        | 0.52          |
| (1,511)  | 1:15:A:ASN:CA  | 1:11:A:LEU:CD1 | 5        | 0.52          |
| (1,225)  | 1:29:E:VAL:CA  | 1:25:E:ILE:CD1 | 3        | 0.52          |
| (1,224)  | 1:29:D:VAL:CA  | 1:25:D:ILE:CD1 | 3        | 0.52          |
| (1,223)  | 1:29:C:VAL:CA  | 1:25:C:ILE:CD1 | 3        | 0.52          |
| (1,222)  | 1:29:B:VAL:CA  | 1:25:B:ILE:CD1 | 3        | 0.52          |
| (1,221)  | 1:29:A:VAL:CA  | 1:25:A:ILE:CD1 | 3        | 0.52          |
| (4,60)   | 1:27:E:LEU:CG  | 1:24:D:ALA:N   | 3        | 0.51          |
| (4,59)   | 1:27:D:LEU:CG  | 1:24:C:ALA:N   | 3        | 0.51          |
| (4,58)   | 1:27:C:LEU:CG  | 1:24:B:ALA:N   | 3        | 0.51          |
| (4,57)   | 1:27:B:LEU:CG  | 1:24:A:ALA:N   | 3        | 0.51          |
| (4,56)   | 1:27:A:LEU:CG  | 1:24:E:ALA:N   | 3        | 0.51          |
| (1,1000) | 1:11:E:LEU:CB  | 1:13:D:ILE:CG2 | 4        | 0.5           |
| (1,999)  | 1:11:D:LEU:CB  | 1:13:C:ILE:CG2 | 4        | 0.5           |
| (1,998)  | 1:11:C:LEU:CB  | 1:13:B:ILE:CG2 | 4        | 0.5           |
| (1,997)  | 1:11:B:LEU:CB  | 1:13:A:ILE:CG2 | 4        | 0.5           |
| (1,996)  | 1:11:A:LEU:CB  | 1:13:E:ILE:CG2 | 4        | 0.5           |
| (1,870)  | 1:32:E:ALA:CB  | 1:26:A:THR:CA  | 3        | 0.5           |
| (1,869)  | 1:32:D:ALA:CB  | 1:26:E:THR:CA  | 3        | 0.5           |
| (1,868)  | 1:32:C:ALA:CB  | 1:26:D:THR:CA  | 3        | 0.5           |
| (1,867)  | 1:32:B:ALA:CB  | 1:26:C:THR:CA  | 3        | 0.5           |
| (1,866)  | 1:32:A:ALA:CB  | 1:26:B:THR:CA  | 3        | 0.5           |
| (1,585)  | 1:25:E:ILE:CG1 | 1:27:E:LEU:CG  | 3        | 0.5           |
| (1,585)  | 1:25:E:ILE:CG1 | 1:27:E:LEU:CG  | 6        | 0.5           |
| (1,584)  | 1:25:D:ILE:CG1 | 1:27:D:LEU:CG  | 3        | 0.5           |
| (1,584)  | 1:25:D:ILE:CG1 | 1:27:D:LEU:CG  | 6        | 0.5           |
| (1,583)  | 1:25:C:ILE:CG1 | 1:27:C:LEU:CG  | 3        | 0.5           |
| (1,583)  | 1:25:C:ILE:CG1 | 1:27:C:LEU:CG  | 6        | 0.5           |
| (1,582)  | 1:25:B:ILE:CG1 | 1:27:B:LEU:CG  | 3        | 0.5           |
| (1,582)  | 1:25:B:ILE:CG1 | 1:27:B:LEU:CG  | 6        | 0.5           |
| (1,581)  | 1:25:A:ILE:CG1 | 1:27:A:LEU:CG  | 3        | 0.5           |
| (1,581)  | 1:25:A:ILE:CG1 | 1:27:A:LEU:CG  | 6        | 0.5           |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,285) | 1:11:E:LEU:CB  | 1:13:D:ILE:CG2 | 4        | 0.5           |
| (1,284) | 1:11:D:LEU:CB  | 1:13:C:ILE:CG2 | 4        | 0.5           |
| (1,283) | 1:11:C:LEU:CB  | 1:13:B:ILE:CG2 | 4        | 0.5           |
| (1,282) | 1:11:B:LEU:CB  | 1:13:A:ILE:CG2 | 4        | 0.5           |
| (1,281) | 1:11:A:LEU:CB  | 1:13:E:ILE:CG2 | 4        | 0.5           |
| (7,20)  | 1:37:E:THR:CG2 | 1:32:D:ALA:CB  | 6        | 0.49          |
| (7,19)  | 1:37:D:THR:CG2 | 1:32:C:ALA:CB  | 6        | 0.49          |
| (7,18)  | 1:37:C:THR:CG2 | 1:32:B:ALA:CB  | 6        | 0.49          |
| (7,17)  | 1:37:B:THR:CG2 | 1:32:A:ALA:CB  | 6        | 0.49          |
| (7,16)  | 1:37:A:THR:CG2 | 1:32:E:ALA:CB  | 6        | 0.49          |
| (1,515) | 1:15:E:ASN:CA  | 1:11:E:LEU:CD1 | 7        | 0.49          |
| (1,514) | 1:15:D:ASN:CA  | 1:11:D:LEU:CD1 | 7        | 0.49          |
| (1,513) | 1:15:C:ASN:CA  | 1:11:C:LEU:CD1 | 7        | 0.49          |
| (1,512) | 1:15:B:ASN:CA  | 1:11:B:LEU:CD1 | 7        | 0.49          |
| (1,511) | 1:15:A:ASN:CA  | 1:11:A:LEU:CD1 | 7        | 0.49          |
| (2,55)  | 1:11:E:LEU:CG  | 1:9:D:ILE:CD1  | 10       | 0.48          |
| (2,54)  | 1:11:D:LEU:CG  | 1:9:C:ILE:CD1  | 10       | 0.48          |
| (2,53)  | 1:11:C:LEU:CG  | 1:9:B:ILE:CD1  | 10       | 0.48          |
| (2,52)  | 1:11:B:LEU:CG  | 1:9:A:ILE:CD1  | 10       | 0.48          |
| (2,51)  | 1:11:A:LEU:CG  | 1:9:E:ILE:CD1  | 10       | 0.48          |
| (1,840) | 1:11:E:LEU:CG  | 1:9:D:ILE:CD1  | 10       | 0.48          |
| (1,839) | 1:11:D:LEU:CG  | 1:9:C:ILE:CD1  | 10       | 0.48          |
| (1,838) | 1:11:C:LEU:CG  | 1:9:B:ILE:CD1  | 10       | 0.48          |
| (1,837) | 1:11:B:LEU:CG  | 1:9:A:ILE:CD1  | 10       | 0.48          |
| (1,836) | 1:11:A:LEU:CG  | 1:9:E:ILE:CD1  | 10       | 0.48          |
| (2,230) | 1:29:E:VAL:CA  | 1:31:E:MET:CE  | 10       | 0.47          |
| (2,221) | 1:29:D:VAL:CA  | 1:31:D:MET:CE  | 10       | 0.47          |
| (2,212) | 1:29:C:VAL:CA  | 1:31:C:MET:CE  | 10       | 0.47          |
| (2,203) | 1:29:B:VAL:CA  | 1:31:B:MET:CE  | 10       | 0.47          |
| (2,194) | 1:29:A:VAL:CA  | 1:31:A:MET:CE  | 10       | 0.47          |
| (6,10)  | 1:10:E:GLY:CA  | 1:7:D:GLU:CG   | 1        | 0.46          |
| (6,9)   | 1:10:D:GLY:CA  | 1:7:C:GLU:CG   | 1        | 0.46          |
| (6,8)   | 1:10:C:GLY:CA  | 1:7:B:GLU:CG   | 1        | 0.46          |
| (6,7)   | 1:10:B:GLY:CA  | 1:7:A:GLU:CG   | 1        | 0.46          |
| (6,6)   | 1:10:A:GLY:CA  | 1:7:E:GLU:CG   | 1        | 0.46          |
| (2,180) | 1:34:E:LEU:CA  | 1:34:E:LEU:CB  | 1        | 0.46          |
| (2,180) | 1:34:E:LEU:CA  | 1:34:E:LEU:CB  | 2        | 0.46          |
| (2,180) | 1:34:E:LEU:CA  | 1:34:E:LEU:CB  | 4        | 0.46          |
| (2,180) | 1:34:E:LEU:CA  | 1:34:E:LEU:CB  | 5        | 0.46          |
| (2,180) | 1:34:E:LEU:CA  | 1:34:E:LEU:CB  | 7        | 0.46          |
| (2,180) | 1:34:E:LEU:CA  | 1:34:E:LEU:CB  | 9        | 0.46          |
| (2,180) | 1:34:E:LEU:CA  | 1:34:E:LEU:CB  | 10       | 0.46          |

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| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (2,179) | 1:34:D:LEU:CA | 1:34:D:LEU:CB | 1        | 0.46          |
| (2,179) | 1:34:D:LEU:CA | 1:34:D:LEU:CB | 2        | 0.46          |
| (2,179) | 1:34:D:LEU:CA | 1:34:D:LEU:CB | 4        | 0.46          |
| (2,179) | 1:34:D:LEU:CA | 1:34:D:LEU:CB | 5        | 0.46          |
| (2,179) | 1:34:D:LEU:CA | 1:34:D:LEU:CB | 6        | 0.46          |
| (2,179) | 1:34:D:LEU:CA | 1:34:D:LEU:CB | 7        | 0.46          |
| (2,179) | 1:34:D:LEU:CA | 1:34:D:LEU:CB | 9        | 0.46          |
| (2,179) | 1:34:D:LEU:CA | 1:34:D:LEU:CB | 10       | 0.46          |
| (2,178) | 1:34:C:LEU:CA | 1:34:C:LEU:CB | 1        | 0.46          |
| (2,178) | 1:34:C:LEU:CA | 1:34:C:LEU:CB | 2        | 0.46          |
| (2,178) | 1:34:C:LEU:CA | 1:34:C:LEU:CB | 4        | 0.46          |
| (2,178) | 1:34:C:LEU:CA | 1:34:C:LEU:CB | 5        | 0.46          |
| (2,178) | 1:34:C:LEU:CA | 1:34:C:LEU:CB | 7        | 0.46          |
| (2,178) | 1:34:C:LEU:CA | 1:34:C:LEU:CB | 9        | 0.46          |
| (2,178) | 1:34:C:LEU:CA | 1:34:C:LEU:CB | 10       | 0.46          |
| (2,177) | 1:34:B:LEU:CA | 1:34:B:LEU:CB | 1        | 0.46          |
| (2,177) | 1:34:B:LEU:CA | 1:34:B:LEU:CB | 2        | 0.46          |
| (2,177) | 1:34:B:LEU:CA | 1:34:B:LEU:CB | 4        | 0.46          |
| (2,177) | 1:34:B:LEU:CA | 1:34:B:LEU:CB | 5        | 0.46          |
| (2,177) | 1:34:B:LEU:CA | 1:34:B:LEU:CB | 7        | 0.46          |
| (2,177) | 1:34:B:LEU:CA | 1:34:B:LEU:CB | 8        | 0.46          |
| (2,177) | 1:34:B:LEU:CA | 1:34:B:LEU:CB | 9        | 0.46          |
| (2,177) | 1:34:B:LEU:CA | 1:34:B:LEU:CB | 10       | 0.46          |
| (2,176) | 1:34:A:LEU:CA | 1:34:A:LEU:CB | 1        | 0.46          |
| (2,176) | 1:34:A:LEU:CA | 1:34:A:LEU:CB | 2        | 0.46          |
| (2,176) | 1:34:A:LEU:CA | 1:34:A:LEU:CB | 4        | 0.46          |
| (2,176) | 1:34:A:LEU:CA | 1:34:A:LEU:CB | 5        | 0.46          |
| (2,176) | 1:34:A:LEU:CA | 1:34:A:LEU:CB | 6        | 0.46          |
| (2,176) | 1:34:A:LEU:CA | 1:34:A:LEU:CB | 9        | 0.46          |
| (2,176) | 1:34:A:LEU:CA | 1:34:A:LEU:CB | 10       | 0.46          |
| (1,495) | 1:7:E:GLU:CB  | 1:3:E:PRO:CA  | 3        | 0.46          |
| (1,494) | 1:7:D:GLU:CB  | 1:3:D:PRO:CA  | 3        | 0.46          |
| (1,493) | 1:7:C:GLU:CB  | 1:3:C:PRO:CA  | 3        | 0.46          |
| (1,492) | 1:7:B:GLU:CB  | 1:3:B:PRO:CA  | 3        | 0.46          |
| (1,491) | 1:7:A:GLU:CB  | 1:3:A:PRO:CA  | 3        | 0.46          |
| (3,70)  | 1:27:E:LEU:CB | 1:25:D:ILE:N  | 1        | 0.45          |
| (3,69)  | 1:27:D:LEU:CB | 1:25:C:ILE:N  | 1        | 0.45          |
| (3,68)  | 1:27:C:LEU:CB | 1:25:B:ILE:N  | 1        | 0.45          |
| (3,67)  | 1:27:B:LEU:CB | 1:25:A:ILE:N  | 1        | 0.45          |
| (3,66)  | 1:27:A:LEU:CB | 1:25:E:ILE:N  | 1        | 0.45          |
| (2,180) | 1:34:E:LEU:CA | 1:34:E:LEU:CB | 3        | 0.45          |
| (2,180) | 1:34:E:LEU:CA | 1:34:E:LEU:CB | 6        | 0.45          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (2,180)  | 1:34:E:LEU:CA  | 1:34:E:LEU:CB  | 8        | 0.45          |
| (2,179)  | 1:34:D:LEU:CA  | 1:34:D:LEU:CB  | 3        | 0.45          |
| (2,179)  | 1:34:D:LEU:CA  | 1:34:D:LEU:CB  | 8        | 0.45          |
| (2,178)  | 1:34:C:LEU:CA  | 1:34:C:LEU:CB  | 3        | 0.45          |
| (2,178)  | 1:34:C:LEU:CA  | 1:34:C:LEU:CB  | 6        | 0.45          |
| (2,178)  | 1:34:C:LEU:CA  | 1:34:C:LEU:CB  | 8        | 0.45          |
| (2,177)  | 1:34:B:LEU:CA  | 1:34:B:LEU:CB  | 3        | 0.45          |
| (2,177)  | 1:34:B:LEU:CA  | 1:34:B:LEU:CB  | 6        | 0.45          |
| (2,176)  | 1:34:A:LEU:CA  | 1:34:A:LEU:CB  | 3        | 0.45          |
| (2,176)  | 1:34:A:LEU:CA  | 1:34:A:LEU:CB  | 7        | 0.45          |
| (2,176)  | 1:34:A:LEU:CA  | 1:34:A:LEU:CB  | 8        | 0.45          |
| (1,1010) | 1:27:E:LEU:CB  | 1:25:E:ILE:CD1 | 3        | 0.45          |
| (1,1009) | 1:27:D:LEU:CB  | 1:25:D:ILE:CD1 | 3        | 0.45          |
| (1,1008) | 1:27:C:LEU:CB  | 1:25:C:ILE:CD1 | 3        | 0.45          |
| (1,1007) | 1:27:B:LEU:CB  | 1:25:B:ILE:CD1 | 3        | 0.45          |
| (1,1006) | 1:27:A:LEU:CB  | 1:25:A:ILE:CD1 | 3        | 0.45          |
| (1,325)  | 1:25:E:ILE:CB  | 1:27:E:LEU:CG  | 6        | 0.45          |
| (1,324)  | 1:25:D:ILE:CB  | 1:27:D:LEU:CG  | 6        | 0.45          |
| (1,323)  | 1:25:C:ILE:CB  | 1:27:C:LEU:CG  | 6        | 0.45          |
| (1,322)  | 1:25:B:ILE:CB  | 1:27:B:LEU:CG  | 6        | 0.45          |
| (1,321)  | 1:25:A:ILE:CB  | 1:27:A:LEU:CG  | 6        | 0.45          |
| (3,70)   | 1:27:E:LEU:CB  | 1:25:D:ILE:N   | 8        | 0.44          |
| (3,69)   | 1:27:D:LEU:CB  | 1:25:C:ILE:N   | 8        | 0.44          |
| (3,68)   | 1:27:C:LEU:CB  | 1:25:B:ILE:N   | 8        | 0.44          |
| (3,67)   | 1:27:B:LEU:CB  | 1:25:A:ILE:N   | 8        | 0.44          |
| (3,66)   | 1:27:A:LEU:CB  | 1:25:E:ILE:N   | 8        | 0.44          |
| (1,780)  | 1:27:E:LEU:CA  | 1:25:D:ILE:CD1 | 8        | 0.44          |
| (1,779)  | 1:27:E:LEU:CA  | 1:25:D:ILE:CD1 | 8        | 0.44          |
| (1,778)  | 1:27:E:LEU:CA  | 1:25:D:ILE:CD1 | 8        | 0.44          |
| (1,777)  | 1:27:D:LEU:CA  | 1:25:C:ILE:CD1 | 8        | 0.44          |
| (1,776)  | 1:27:C:LEU:CA  | 1:25:B:ILE:CD1 | 8        | 0.44          |
| (7,20)   | 1:37:E:THR:CG2 | 1:32:E:ALA:CB  | 7        | 0.43          |
| (7,19)   | 1:37:D:THR:CG2 | 1:32:D:ALA:CB  | 7        | 0.43          |
| (7,18)   | 1:37:C:THR:CG2 | 1:32:C:ALA:CB  | 7        | 0.43          |
| (7,16)   | 1:37:A:THR:CG2 | 1:32:A:ALA:CB  | 7        | 0.43          |
| (3,120)  | 1:18:E:ILE:CA  | 1:16:A:PHE:N   | 3        | 0.43          |
| (3,119)  | 1:18:D:ILE:CA  | 1:16:E:PHE:N   | 3        | 0.43          |
| (3,118)  | 1:18:C:ILE:CA  | 1:16:D:PHE:N   | 3        | 0.43          |
| (3,117)  | 1:18:B:ILE:CA  | 1:16:C:PHE:N   | 3        | 0.43          |
| (3,116)  | 1:18:A:ILE:CA  | 1:16:B:PHE:N   | 3        | 0.43          |
| (1,870)  | 1:32:E:ALA:CB  | 1:26:A:THR:CA  | 5        | 0.43          |
| (1,869)  | 1:32:D:ALA:CB  | 1:26:E:THR:CA  | 5        | 0.43          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,868)  | 1:32:C:ALA:CB  | 1:26:D:THR:CA  | 5        | 0.43          |
| (1,867)  | 1:32:B:ALA:CB  | 1:26:C:THR:CA  | 5        | 0.43          |
| (1,866)  | 1:32:A:ALA:CB  | 1:26:B:THR:CA  | 5        | 0.43          |
| (7,17)   | 1:37:B:THR:CG2 | 1:32:B:ALA:CB  | 7        | 0.42          |
| (1,485)  | 1:7:E:GLU:CA   | 1:3:E:PRO:CA   | 3        | 0.42          |
| (1,484)  | 1:7:D:GLU:CA   | 1:3:D:PRO:CA   | 3        | 0.42          |
| (1,483)  | 1:7:C:GLU:CA   | 1:3:C:PRO:CA   | 3        | 0.42          |
| (1,482)  | 1:7:B:GLU:CA   | 1:3:B:PRO:CA   | 3        | 0.42          |
| (1,481)  | 1:7:A:GLU:CA   | 1:3:A:PRO:CA   | 3        | 0.42          |
| (3,120)  | 1:18:E:ILE:CA  | 1:16:A:PHE:N   | 6        | 0.41          |
| (3,120)  | 1:18:E:ILE:CA  | 1:16:A:PHE:N   | 9        | 0.41          |
| (3,119)  | 1:18:D:ILE:CA  | 1:16:E:PHE:N   | 6        | 0.41          |
| (3,119)  | 1:18:D:ILE:CA  | 1:16:E:PHE:N   | 9        | 0.41          |
| (3,118)  | 1:18:C:ILE:CA  | 1:16:D:PHE:N   | 6        | 0.41          |
| (3,118)  | 1:18:C:ILE:CA  | 1:16:D:PHE:N   | 9        | 0.41          |
| (3,117)  | 1:18:B:ILE:CA  | 1:16:C:PHE:N   | 6        | 0.41          |
| (3,117)  | 1:18:B:ILE:CA  | 1:16:C:PHE:N   | 9        | 0.41          |
| (3,116)  | 1:18:A:ILE:CA  | 1:16:B:PHE:N   | 6        | 0.41          |
| (3,116)  | 1:18:A:ILE:CA  | 1:16:B:PHE:N   | 9        | 0.41          |
| (3,70)   | 1:27:E:LEU:CB  | 1:25:D:ILE:N   | 4        | 0.41          |
| (3,69)   | 1:27:D:LEU:CB  | 1:25:C:ILE:N   | 4        | 0.41          |
| (3,68)   | 1:27:C:LEU:CB  | 1:25:B:ILE:N   | 4        | 0.41          |
| (3,67)   | 1:27:B:LEU:CB  | 1:25:A:ILE:N   | 4        | 0.41          |
| (1,325)  | 1:25:E:ILE:CB  | 1:27:E:LEU:CG  | 3        | 0.41          |
| (1,324)  | 1:25:D:ILE:CB  | 1:27:D:LEU:CG  | 3        | 0.41          |
| (1,323)  | 1:25:C:ILE:CB  | 1:27:C:LEU:CG  | 3        | 0.41          |
| (1,322)  | 1:25:B:ILE:CB  | 1:27:B:LEU:CG  | 3        | 0.41          |
| (1,321)  | 1:25:A:ILE:CB  | 1:27:A:LEU:CG  | 3        | 0.41          |
| (3,66)   | 1:27:A:LEU:CB  | 1:25:E:ILE:N   | 4        | 0.4           |
| (1,1010) | 1:27:E:LEU:CB  | 1:25:D:ILE:CD1 | 10       | 0.4           |
| (1,1008) | 1:27:C:LEU:CB  | 1:25:B:ILE:CD1 | 10       | 0.4           |
| (1,780)  | 1:27:A:LEU:CA  | 1:25:E:ILE:CD1 | 2        | 0.4           |
| (1,779)  | 1:27:A:LEU:CA  | 1:25:E:ILE:CD1 | 2        | 0.4           |
| (1,778)  | 1:27:C:LEU:CA  | 1:25:B:ILE:CD1 | 2        | 0.4           |
| (1,777)  | 1:27:C:LEU:CA  | 1:25:B:ILE:CD1 | 2        | 0.4           |
| (1,776)  | 1:27:C:LEU:CA  | 1:25:B:ILE:CD1 | 2        | 0.4           |
| (3,120)  | 1:18:E:ILE:CA  | 1:16:A:PHE:N   | 7        | 0.39          |
| (3,119)  | 1:18:D:ILE:CA  | 1:16:E:PHE:N   | 7        | 0.39          |
| (3,118)  | 1:18:C:ILE:CA  | 1:16:D:PHE:N   | 7        | 0.39          |
| (3,117)  | 1:18:B:ILE:CA  | 1:16:C:PHE:N   | 7        | 0.39          |
| (3,116)  | 1:18:A:ILE:CA  | 1:16:B:PHE:N   | 7        | 0.39          |
| (3,70)   | 1:27:E:LEU:CB  | 1:25:D:ILE:N   | 5        | 0.39          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (3,69)   | 1:27:D:LEU:CB  | 1:25:C:ILE:N   | 5        | 0.39          |
| (3,68)   | 1:27:C:LEU:CB  | 1:25:B:ILE:N   | 5        | 0.39          |
| (3,67)   | 1:27:B:LEU:CB  | 1:25:A:ILE:N   | 5        | 0.39          |
| (3,66)   | 1:27:A:LEU:CB  | 1:25:E:ILE:N   | 5        | 0.39          |
| (1,1009) | 1:27:D:LEU:CB  | 1:25:C:ILE:CD1 | 10       | 0.39          |
| (1,1007) | 1:27:B:LEU:CB  | 1:25:A:ILE:CD1 | 10       | 0.39          |
| (1,1006) | 1:27:A:LEU:CB  | 1:25:E:ILE:CD1 | 10       | 0.39          |
| (7,20)   | 1:37:E:THR:CG2 | 1:32:D:ALA:CB  | 2        | 0.38          |
| (7,19)   | 1:37:D:THR:CG2 | 1:32:C:ALA:CB  | 2        | 0.38          |
| (7,18)   | 1:37:C:THR:CG2 | 1:32:B:ALA:CB  | 2        | 0.38          |
| (7,17)   | 1:37:B:THR:CG2 | 1:32:A:ALA:CB  | 2        | 0.38          |
| (7,16)   | 1:37:A:THR:CG2 | 1:32:E:ALA:CB  | 2        | 0.38          |
| (1,515)  | 1:15:E:ASN:CA  | 1:11:E:LEU:CD1 | 6        | 0.38          |
| (1,514)  | 1:15:D:ASN:CA  | 1:11:D:LEU:CD1 | 6        | 0.38          |
| (1,513)  | 1:15:C:ASN:CA  | 1:11:C:LEU:CD1 | 6        | 0.38          |
| (1,512)  | 1:15:B:ASN:CA  | 1:11:B:LEU:CD1 | 6        | 0.38          |
| (1,511)  | 1:15:A:ASN:CA  | 1:11:A:LEU:CD1 | 6        | 0.38          |
| (1,325)  | 1:25:E:ILE:CB  | 1:27:E:LEU:CG  | 7        | 0.38          |
| (1,324)  | 1:25:D:ILE:CB  | 1:27:D:LEU:CG  | 7        | 0.38          |
| (1,323)  | 1:25:C:ILE:CB  | 1:27:C:LEU:CG  | 7        | 0.38          |
| (1,322)  | 1:25:B:ILE:CB  | 1:27:B:LEU:CG  | 7        | 0.38          |
| (1,321)  | 1:25:A:ILE:CB  | 1:27:A:LEU:CG  | 7        | 0.38          |
| (3,70)   | 1:27:E:LEU:CB  | 1:25:D:ILE:N   | 2        | 0.37          |
| (3,70)   | 1:27:E:LEU:CB  | 1:25:D:ILE:N   | 7        | 0.37          |
| (3,69)   | 1:27:D:LEU:CB  | 1:25:C:ILE:N   | 2        | 0.37          |
| (3,69)   | 1:27:D:LEU:CB  | 1:25:C:ILE:N   | 7        | 0.37          |
| (3,68)   | 1:27:C:LEU:CB  | 1:25:B:ILE:N   | 2        | 0.37          |
| (3,68)   | 1:27:C:LEU:CB  | 1:25:B:ILE:N   | 7        | 0.37          |
| (3,67)   | 1:27:B:LEU:CB  | 1:25:A:ILE:N   | 2        | 0.37          |
| (3,67)   | 1:27:B:LEU:CB  | 1:25:A:ILE:N   | 7        | 0.37          |
| (3,66)   | 1:27:A:LEU:CB  | 1:25:E:ILE:N   | 2        | 0.37          |
| (3,66)   | 1:27:A:LEU:CB  | 1:25:E:ILE:N   | 7        | 0.37          |
| (2,210)  | 1:29:C:VAL:CA  | 1:27:D:LEU:CA  | 5        | 0.37          |
| (1,870)  | 1:32:E:ALA:CB  | 1:26:A:THR:CA  | 2        | 0.37          |
| (1,870)  | 1:32:E:ALA:CB  | 1:26:A:THR:CA  | 4        | 0.37          |
| (1,869)  | 1:32:D:ALA:CB  | 1:26:E:THR:CA  | 2        | 0.37          |
| (1,869)  | 1:32:D:ALA:CB  | 1:26:E:THR:CA  | 4        | 0.37          |
| (1,868)  | 1:32:C:ALA:CB  | 1:26:D:THR:CA  | 2        | 0.37          |
| (1,868)  | 1:32:C:ALA:CB  | 1:26:D:THR:CA  | 4        | 0.37          |
| (1,867)  | 1:32:B:ALA:CB  | 1:26:C:THR:CA  | 2        | 0.37          |
| (1,867)  | 1:32:B:ALA:CB  | 1:26:C:THR:CA  | 4        | 0.37          |
| (1,866)  | 1:32:A:ALA:CB  | 1:26:B:THR:CA  | 2        | 0.37          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,866) | 1:32:A:ALA:CB  | 1:26:B:THR:CA  | 4        | 0.37          |
| (3,70)  | 1:27:E:LEU:CB  | 1:25:D:ILE:N   | 3        | 0.36          |
| (3,69)  | 1:27:D:LEU:CB  | 1:25:C:ILE:N   | 3        | 0.36          |
| (3,68)  | 1:27:C:LEU:CB  | 1:25:B:ILE:N   | 3        | 0.36          |
| (3,67)  | 1:27:B:LEU:CB  | 1:25:A:ILE:N   | 3        | 0.36          |
| (3,66)  | 1:27:A:LEU:CB  | 1:25:E:ILE:N   | 3        | 0.36          |
| (2,228) | 1:29:E:VAL:CA  | 1:27:A:LEU:CA  | 5        | 0.36          |
| (2,219) | 1:29:D:VAL:CA  | 1:27:E:LEU:CA  | 5        | 0.36          |
| (2,201) | 1:29:B:VAL:CA  | 1:27:C:LEU:CA  | 5        | 0.36          |
| (2,192) | 1:29:A:VAL:CA  | 1:27:B:LEU:CA  | 5        | 0.36          |
| (1,995) | 1:27:E:LEU:CG  | 1:29:D:VAL:CG2 | 6        | 0.35          |
| (1,994) | 1:27:D:LEU:CG  | 1:29:C:VAL:CG2 | 6        | 0.35          |
| (1,993) | 1:27:C:LEU:CG  | 1:29:B:VAL:CG2 | 6        | 0.35          |
| (1,992) | 1:27:B:LEU:CG  | 1:29:A:VAL:CG2 | 6        | 0.35          |
| (1,991) | 1:27:A:LEU:CG  | 1:29:E:VAL:CG2 | 6        | 0.35          |
| (1,435) | 1:29:E:VAL:CG2 | 1:27:A:LEU:CG  | 6        | 0.35          |
| (1,434) | 1:29:D:VAL:CG2 | 1:27:E:LEU:CG  | 6        | 0.35          |
| (1,433) | 1:29:C:VAL:CG2 | 1:27:D:LEU:CG  | 6        | 0.35          |
| (1,432) | 1:29:B:VAL:CG2 | 1:27:C:LEU:CG  | 6        | 0.35          |
| (1,431) | 1:29:A:VAL:CG2 | 1:27:B:LEU:CG  | 6        | 0.35          |
| (3,70)  | 1:27:E:LEU:CB  | 1:25:D:ILE:N   | 9        | 0.34          |
| (3,69)  | 1:27:D:LEU:CB  | 1:25:C:ILE:N   | 9        | 0.34          |
| (3,68)  | 1:27:C:LEU:CB  | 1:25:B:ILE:N   | 9        | 0.34          |
| (3,67)  | 1:27:B:LEU:CB  | 1:25:A:ILE:N   | 9        | 0.34          |
| (3,66)  | 1:27:A:LEU:CB  | 1:25:E:ILE:N   | 9        | 0.34          |
| (1,835) | 1:11:E:LEU:CG  | 1:9:E:ILE:CG2  | 5        | 0.34          |
| (1,834) | 1:11:D:LEU:CG  | 1:9:D:ILE:CG2  | 5        | 0.34          |
| (1,833) | 1:11:C:LEU:CG  | 1:9:C:ILE:CG2  | 5        | 0.34          |
| (1,832) | 1:11:B:LEU:CG  | 1:9:B:ILE:CG2  | 5        | 0.34          |
| (1,831) | 1:11:A:LEU:CG  | 1:9:A:ILE:CG2  | 5        | 0.34          |
| (1,590) | 1:9:E:ILE:CG2  | 1:11:E:LEU:CG  | 5        | 0.34          |
| (1,589) | 1:9:D:ILE:CG2  | 1:11:D:LEU:CG  | 5        | 0.34          |
| (1,588) | 1:9:C:ILE:CG2  | 1:11:C:LEU:CG  | 5        | 0.34          |
| (1,587) | 1:9:B:ILE:CG2  | 1:11:B:LEU:CG  | 5        | 0.34          |
| (1,586) | 1:9:A:ILE:CG2  | 1:11:A:LEU:CG  | 5        | 0.34          |
| (1,350) | 1:13:A:ILE:CD1 | 1:11:B:LEU:CG  | 5        | 0.34          |
| (1,349) | 1:13:A:ILE:CD1 | 1:11:B:LEU:CG  | 5        | 0.34          |
| (1,348) | 1:13:A:ILE:CD1 | 1:11:B:LEU:CG  | 5        | 0.34          |
| (1,347) | 1:13:A:ILE:CD1 | 1:11:B:LEU:CG  | 5        | 0.34          |
| (1,346) | 1:13:A:ILE:CD1 | 1:11:B:LEU:CG  | 5        | 0.34          |
| (3,120) | 1:18:E:ILE:CA  | 1:16:A:PHE:N   | 10       | 0.33          |
| (3,119) | 1:18:D:ILE:CA  | 1:16:E:PHE:N   | 10       | 0.33          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (3,118)  | 1:18:C:ILE:CA  | 1:16:D:PHE:N   | 10       | 0.33          |
| (3,117)  | 1:18:B:ILE:CA  | 1:16:C:PHE:N   | 10       | 0.33          |
| (3,116)  | 1:18:A:ILE:CA  | 1:16:B:PHE:N   | 10       | 0.33          |
| (3,70)   | 1:27:E:LEU:CB  | 1:25:D:ILE:N   | 6        | 0.33          |
| (3,69)   | 1:27:D:LEU:CB  | 1:25:C:ILE:N   | 6        | 0.33          |
| (3,68)   | 1:27:C:LEU:CB  | 1:25:B:ILE:N   | 6        | 0.33          |
| (3,67)   | 1:27:B:LEU:CB  | 1:25:A:ILE:N   | 6        | 0.33          |
| (3,66)   | 1:27:A:LEU:CB  | 1:25:E:ILE:N   | 6        | 0.33          |
| (1,870)  | 1:32:E:ALA:CB  | 1:26:A:THR:CA  | 7        | 0.33          |
| (1,869)  | 1:32:D:ALA:CB  | 1:26:E:THR:CA  | 7        | 0.33          |
| (1,868)  | 1:32:C:ALA:CB  | 1:26:D:THR:CA  | 7        | 0.33          |
| (1,867)  | 1:32:B:ALA:CB  | 1:26:C:THR:CA  | 7        | 0.33          |
| (1,866)  | 1:32:A:ALA:CB  | 1:26:B:THR:CA  | 7        | 0.33          |
| (3,45)   | 1:22:E:VAL:CB  | 1:26:D:THR:N   | 7        | 0.32          |
| (3,44)   | 1:22:D:VAL:CB  | 1:26:C:THR:N   | 7        | 0.32          |
| (3,43)   | 1:22:C:VAL:CB  | 1:26:B:THR:N   | 7        | 0.32          |
| (3,42)   | 1:22:B:VAL:CB  | 1:26:A:THR:N   | 7        | 0.32          |
| (3,41)   | 1:22:A:VAL:CB  | 1:26:E:THR:N   | 7        | 0.32          |
| (2,25)   | 1:35:E:THR:CG2 | 1:33:E:PHE:CB  | 10       | 0.32          |
| (2,24)   | 1:35:D:THR:CG2 | 1:33:D:PHE:CB  | 10       | 0.32          |
| (2,23)   | 1:35:C:THR:CG2 | 1:33:C:PHE:CB  | 10       | 0.32          |
| (2,22)   | 1:35:B:THR:CG2 | 1:33:B:PHE:CB  | 10       | 0.32          |
| (2,21)   | 1:35:A:THR:CG2 | 1:33:A:PHE:CB  | 10       | 0.32          |
| (1,780)  | 1:27:E:LEU:CA  | 1:25:D:ILE:CD1 | 5        | 0.32          |
| (1,779)  | 1:27:D:LEU:CA  | 1:25:C:ILE:CD1 | 5        | 0.32          |
| (1,778)  | 1:27:C:LEU:CA  | 1:25:B:ILE:CD1 | 5        | 0.32          |
| (1,777)  | 1:27:C:LEU:CA  | 1:25:B:ILE:CD1 | 5        | 0.32          |
| (1,776)  | 1:27:C:LEU:CA  | 1:25:B:ILE:CD1 | 5        | 0.32          |
| (2,230)  | 1:29:E:VAL:CA  | 1:31:E:MET:CE  | 1        | 0.3           |
| (2,221)  | 1:29:D:VAL:CA  | 1:31:D:MET:CE  | 1        | 0.3           |
| (2,212)  | 1:29:C:VAL:CA  | 1:31:C:MET:CE  | 1        | 0.3           |
| (2,203)  | 1:29:B:VAL:CA  | 1:31:B:MET:CE  | 1        | 0.3           |
| (2,194)  | 1:29:A:VAL:CA  | 1:31:A:MET:CE  | 1        | 0.3           |
| (1,1060) | 1:9:E:ILE:CB   | 1:11:A:LEU:CG  | 9        | 0.3           |
| (1,1059) | 1:9:D:ILE:CB   | 1:11:E:LEU:CG  | 9        | 0.3           |
| (1,1058) | 1:9:C:ILE:CB   | 1:11:D:LEU:CG  | 9        | 0.3           |
| (1,1057) | 1:9:B:ILE:CB   | 1:11:C:LEU:CG  | 9        | 0.3           |
| (1,1056) | 1:9:A:ILE:CB   | 1:11:B:LEU:CG  | 9        | 0.3           |
| (1,845)  | 1:11:E:LEU:CG  | 1:9:D:ILE:CB   | 9        | 0.3           |
| (1,844)  | 1:11:D:LEU:CG  | 1:9:C:ILE:CB   | 9        | 0.3           |
| (1,843)  | 1:11:C:LEU:CG  | 1:9:B:ILE:CB   | 9        | 0.3           |
| (1,842)  | 1:11:B:LEU:CG  | 1:9:A:ILE:CB   | 9        | 0.3           |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,841)  | 1:11:A:LEU:CG  | 1:9:E:ILE:CB   | 9        | 0.3           |
| (1,125)  | 1:9:E:ILE:CG1  | 1:11:A:LEU:CD2 | 6        | 0.3           |
| (1,124)  | 1:9:D:ILE:CG1  | 1:11:E:LEU:CD2 | 6        | 0.3           |
| (1,123)  | 1:9:C:ILE:CG1  | 1:11:D:LEU:CD2 | 6        | 0.3           |
| (1,122)  | 1:9:B:ILE:CG1  | 1:11:C:LEU:CD2 | 6        | 0.3           |
| (1,121)  | 1:9:A:ILE:CG1  | 1:11:B:LEU:CD2 | 6        | 0.3           |
| (3,70)   | 1:27:E:LEU:CB  | 1:25:D:ILE:N   | 10       | 0.29          |
| (3,69)   | 1:27:D:LEU:CB  | 1:25:C:ILE:N   | 10       | 0.29          |
| (3,68)   | 1:27:C:LEU:CB  | 1:25:B:ILE:N   | 10       | 0.29          |
| (3,67)   | 1:27:B:LEU:CB  | 1:25:A:ILE:N   | 10       | 0.29          |
| (3,66)   | 1:27:A:LEU:CB  | 1:25:E:ILE:N   | 10       | 0.29          |
| (2,228)  | 1:29:E:VAL:CA  | 1:27:A:LEU:CA  | 9        | 0.29          |
| (2,219)  | 1:29:D:VAL:CA  | 1:27:E:LEU:CA  | 9        | 0.29          |
| (2,210)  | 1:29:C:VAL:CA  | 1:27:D:LEU:CA  | 9        | 0.29          |
| (2,201)  | 1:29:B:VAL:CA  | 1:27:C:LEU:CA  | 9        | 0.29          |
| (2,192)  | 1:29:A:VAL:CA  | 1:27:B:LEU:CA  | 9        | 0.29          |
| (1,1115) | 1:20:E:THR:CG2 | 1:22:E:VAL:CG2 | 9        | 0.29          |
| (1,1114) | 1:20:D:THR:CG2 | 1:22:D:VAL:CG2 | 9        | 0.29          |
| (1,1113) | 1:20:C:THR:CG2 | 1:22:C:VAL:CG2 | 9        | 0.29          |
| (1,1112) | 1:20:B:THR:CG2 | 1:22:B:VAL:CG2 | 9        | 0.29          |
| (1,1111) | 1:20:A:THR:CG2 | 1:22:A:VAL:CG2 | 9        | 0.29          |
| (1,600)  | 1:25:E:ILE:CG2 | 1:27:A:LEU:CG  | 4        | 0.29          |
| (1,599)  | 1:25:D:ILE:CG2 | 1:27:E:LEU:CG  | 4        | 0.29          |
| (1,598)  | 1:25:C:ILE:CG2 | 1:27:D:LEU:CG  | 4        | 0.29          |
| (1,597)  | 1:25:B:ILE:CG2 | 1:27:C:LEU:CG  | 4        | 0.29          |
| (1,596)  | 1:25:A:ILE:CG2 | 1:27:B:LEU:CG  | 4        | 0.29          |
| (1,125)  | 1:9:E:ILE:CG1  | 1:11:E:LEU:CD2 | 5        | 0.29          |
| (1,124)  | 1:9:D:ILE:CG1  | 1:11:D:LEU:CD2 | 5        | 0.29          |
| (1,123)  | 1:9:C:ILE:CG1  | 1:11:C:LEU:CD2 | 5        | 0.29          |
| (1,122)  | 1:9:B:ILE:CG1  | 1:11:B:LEU:CD2 | 5        | 0.29          |
| (1,121)  | 1:9:A:ILE:CG1  | 1:11:A:LEU:CD2 | 5        | 0.29          |
| (1,870)  | 1:32:E:ALA:CB  | 1:26:A:THR:CA  | 6        | 0.28          |
| (1,869)  | 1:32:D:ALA:CB  | 1:26:E:THR:CA  | 6        | 0.28          |
| (1,868)  | 1:32:C:ALA:CB  | 1:26:D:THR:CA  | 6        | 0.28          |
| (1,867)  | 1:32:B:ALA:CB  | 1:26:C:THR:CA  | 6        | 0.28          |
| (1,866)  | 1:32:A:ALA:CB  | 1:26:B:THR:CA  | 6        | 0.28          |
| (1,325)  | 1:25:E:ILE:CB  | 1:27:E:LEU:CG  | 2        | 0.28          |
| (1,324)  | 1:25:D:ILE:CB  | 1:27:D:LEU:CG  | 2        | 0.28          |
| (1,323)  | 1:25:C:ILE:CB  | 1:27:C:LEU:CG  | 2        | 0.28          |
| (1,322)  | 1:25:B:ILE:CB  | 1:27:B:LEU:CG  | 2        | 0.28          |
| (1,321)  | 1:25:A:ILE:CB  | 1:27:A:LEU:CG  | 2        | 0.28          |
| (3,30)   | 1:33:E:PHE:CA  | 1:35:A:THR:N   | 8        | 0.27          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (3,29)   | 1:33:D:PHE:CA  | 1:35:E:THR:N   | 8        | 0.27          |
| (3,28)   | 1:33:C:PHE:CA  | 1:35:D:THR:N   | 8        | 0.27          |
| (3,27)   | 1:33:B:PHE:CA  | 1:35:C:THR:N   | 8        | 0.27          |
| (3,26)   | 1:33:A:PHE:CA  | 1:35:B:THR:N   | 8        | 0.27          |
| (3,20)   | 1:34:E:LEU:CB  | 1:35:D:THR:N   | 3        | 0.27          |
| (3,20)   | 1:34:E:LEU:CB  | 1:35:D:THR:N   | 6        | 0.27          |
| (3,19)   | 1:34:D:LEU:CB  | 1:35:C:THR:N   | 3        | 0.27          |
| (3,19)   | 1:34:D:LEU:CB  | 1:35:C:THR:N   | 6        | 0.27          |
| (3,18)   | 1:34:C:LEU:CB  | 1:35:B:THR:N   | 3        | 0.27          |
| (3,18)   | 1:34:C:LEU:CB  | 1:35:B:THR:N   | 6        | 0.27          |
| (3,17)   | 1:34:B:LEU:CB  | 1:35:A:THR:N   | 3        | 0.27          |
| (3,17)   | 1:34:B:LEU:CB  | 1:35:A:THR:N   | 6        | 0.27          |
| (3,16)   | 1:34:A:LEU:CB  | 1:35:E:THR:N   | 3        | 0.27          |
| (3,16)   | 1:34:A:LEU:CB  | 1:35:E:THR:N   | 6        | 0.27          |
| (1,1115) | 1:20:E:THR:CG2 | 1:22:E:VAL:CG2 | 1        | 0.27          |
| (1,1114) | 1:20:D:THR:CG2 | 1:22:D:VAL:CG2 | 1        | 0.27          |
| (1,1113) | 1:20:C:THR:CG2 | 1:22:C:VAL:CG2 | 1        | 0.27          |
| (1,1112) | 1:20:B:THR:CG2 | 1:22:B:VAL:CG2 | 1        | 0.27          |
| (1,1111) | 1:20:A:THR:CG2 | 1:22:A:VAL:CG2 | 1        | 0.27          |
| (1,550)  | 1:7:E:GLU:CB   | 1:9:E:ILE:CG2  | 3        | 0.27          |
| (1,549)  | 1:7:D:GLU:CB   | 1:9:D:ILE:CG2  | 3        | 0.27          |
| (1,548)  | 1:7:C:GLU:CB   | 1:9:C:ILE:CG2  | 3        | 0.27          |
| (1,547)  | 1:7:B:GLU:CB   | 1:9:B:ILE:CG2  | 3        | 0.27          |
| (1,546)  | 1:7:A:GLU:CB   | 1:9:A:ILE:CG2  | 3        | 0.27          |
| (1,225)  | 1:29:E:VAL:CA  | 1:25:E:ILE:CD1 | 1        | 0.27          |
| (1,224)  | 1:29:D:VAL:CA  | 1:25:D:ILE:CD1 | 1        | 0.27          |
| (1,223)  | 1:29:C:VAL:CA  | 1:25:C:ILE:CD1 | 1        | 0.27          |
| (1,222)  | 1:29:B:VAL:CA  | 1:25:B:ILE:CD1 | 1        | 0.27          |
| (1,221)  | 1:29:A:VAL:CA  | 1:25:A:ILE:CD1 | 1        | 0.27          |
| (3,20)   | 1:34:E:LEU:CB  | 1:35:D:THR:N   | 7        | 0.26          |
| (3,19)   | 1:34:D:LEU:CB  | 1:35:C:THR:N   | 7        | 0.26          |
| (3,18)   | 1:34:C:LEU:CB  | 1:35:B:THR:N   | 7        | 0.26          |
| (3,17)   | 1:34:B:LEU:CB  | 1:35:A:THR:N   | 7        | 0.26          |
| (3,16)   | 1:34:A:LEU:CB  | 1:35:E:THR:N   | 7        | 0.26          |
| (2,25)   | 1:35:E:THR:CG2 | 1:33:E:PHE:CB  | 9        | 0.26          |
| (2,24)   | 1:35:D:THR:CG2 | 1:33:D:PHE:CB  | 9        | 0.26          |
| (2,23)   | 1:35:C:THR:CG2 | 1:33:C:PHE:CB  | 9        | 0.26          |
| (2,22)   | 1:35:B:THR:CG2 | 1:33:B:PHE:CB  | 9        | 0.26          |
| (2,21)   | 1:35:A:THR:CG2 | 1:33:A:PHE:CB  | 9        | 0.26          |
| (1,726)  | 1:13:A:ILE:CG2 | 1:11:B:LEU:CD1 | 6        | 0.26          |
| (4,60)   | 1:27:E:LEU:CG  | 1:24:D:ALA:N   | 6        | 0.25          |
| (4,59)   | 1:27:D:LEU:CG  | 1:24:C:ALA:N   | 6        | 0.25          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (4,58)   | 1:27:C:LEU:CG  | 1:24:B:ALA:N   | 6        | 0.25          |
| (4,57)   | 1:27:B:LEU:CG  | 1:24:A:ALA:N   | 6        | 0.25          |
| (4,56)   | 1:27:A:LEU:CG  | 1:24:E:ALA:N   | 6        | 0.25          |
| (3,150)  | 1:13:E:ILE:CA  | 1:16:A:PHE:N   | 1        | 0.25          |
| (3,149)  | 1:13:D:ILE:CA  | 1:16:E:PHE:N   | 1        | 0.25          |
| (3,148)  | 1:13:C:ILE:CA  | 1:16:D:PHE:N   | 1        | 0.25          |
| (3,147)  | 1:13:B:ILE:CA  | 1:16:C:PHE:N   | 1        | 0.25          |
| (3,146)  | 1:13:A:ILE:CA  | 1:16:B:PHE:N   | 1        | 0.25          |
| (3,45)   | 1:22:E:VAL:CB  | 1:26:D:THR:N   | 8        | 0.25          |
| (3,44)   | 1:22:D:VAL:CB  | 1:26:C:THR:N   | 8        | 0.25          |
| (3,43)   | 1:22:C:VAL:CB  | 1:26:B:THR:N   | 8        | 0.25          |
| (3,42)   | 1:22:B:VAL:CB  | 1:26:A:THR:N   | 8        | 0.25          |
| (3,41)   | 1:22:A:VAL:CB  | 1:26:E:THR:N   | 8        | 0.25          |
| (3,20)   | 1:34:E:LEU:CB  | 1:35:D:THR:N   | 2        | 0.25          |
| (3,20)   | 1:34:E:LEU:CB  | 1:35:D:THR:N   | 10       | 0.25          |
| (3,19)   | 1:34:D:LEU:CB  | 1:35:C:THR:N   | 2        | 0.25          |
| (3,19)   | 1:34:D:LEU:CB  | 1:35:C:THR:N   | 10       | 0.25          |
| (3,18)   | 1:34:C:LEU:CB  | 1:35:B:THR:N   | 2        | 0.25          |
| (3,18)   | 1:34:C:LEU:CB  | 1:35:B:THR:N   | 10       | 0.25          |
| (3,17)   | 1:34:B:LEU:CB  | 1:35:A:THR:N   | 2        | 0.25          |
| (3,17)   | 1:34:B:LEU:CB  | 1:35:A:THR:N   | 10       | 0.25          |
| (3,16)   | 1:34:A:LEU:CB  | 1:35:E:THR:N   | 2        | 0.25          |
| (3,16)   | 1:34:A:LEU:CB  | 1:35:E:THR:N   | 10       | 0.25          |
| (2,228)  | 1:29:E:VAL:CA  | 1:27:A:LEU:CA  | 8        | 0.25          |
| (2,219)  | 1:29:D:VAL:CA  | 1:27:E:LEU:CA  | 8        | 0.25          |
| (2,210)  | 1:29:C:VAL:CA  | 1:27:D:LEU:CA  | 8        | 0.25          |
| (2,201)  | 1:29:B:VAL:CA  | 1:27:C:LEU:CA  | 8        | 0.25          |
| (2,192)  | 1:29:A:VAL:CA  | 1:27:B:LEU:CA  | 8        | 0.25          |
| (1,1060) | 1:9:E:ILE:CB   | 1:11:A:LEU:CG  | 8        | 0.25          |
| (1,1059) | 1:9:D:ILE:CB   | 1:11:E:LEU:CG  | 8        | 0.25          |
| (1,1058) | 1:9:C:ILE:CB   | 1:11:D:LEU:CG  | 8        | 0.25          |
| (1,1057) | 1:9:B:ILE:CB   | 1:11:C:LEU:CG  | 8        | 0.25          |
| (1,1056) | 1:9:A:ILE:CB   | 1:11:B:LEU:CG  | 8        | 0.25          |
| (1,845)  | 1:11:E:LEU:CG  | 1:9:D:ILE:CB   | 8        | 0.25          |
| (1,844)  | 1:11:D:LEU:CG  | 1:9:C:ILE:CB   | 8        | 0.25          |
| (1,843)  | 1:11:C:LEU:CG  | 1:9:B:ILE:CB   | 8        | 0.25          |
| (1,842)  | 1:11:B:LEU:CG  | 1:9:A:ILE:CB   | 8        | 0.25          |
| (1,841)  | 1:11:A:LEU:CG  | 1:9:E:ILE:CB   | 8        | 0.25          |
| (1,730)  | 1:13:E:ILE:CG2 | 1:11:A:LEU:CD1 | 6        | 0.25          |
| (1,729)  | 1:13:D:ILE:CG2 | 1:11:E:LEU:CD1 | 6        | 0.25          |
| (1,728)  | 1:13:C:ILE:CG2 | 1:11:D:LEU:CD1 | 6        | 0.25          |
| (1,727)  | 1:13:B:ILE:CG2 | 1:11:C:LEU:CD1 | 6        | 0.25          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (3,150)  | 1:13:E:ILE:CA  | 1:16:A:PHE:N   | 3        | 0.24          |
| (3,149)  | 1:13:D:ILE:CA  | 1:16:E:PHE:N   | 3        | 0.24          |
| (3,148)  | 1:13:C:ILE:CA  | 1:16:D:PHE:N   | 3        | 0.24          |
| (3,147)  | 1:13:B:ILE:CA  | 1:16:C:PHE:N   | 3        | 0.24          |
| (3,146)  | 1:13:A:ILE:CA  | 1:16:B:PHE:N   | 3        | 0.24          |
| (3,20)   | 1:34:E:LEU:CB  | 1:35:D:THR:N   | 1        | 0.24          |
| (3,20)   | 1:34:E:LEU:CB  | 1:35:D:THR:N   | 4        | 0.24          |
| (3,19)   | 1:34:D:LEU:CB  | 1:35:C:THR:N   | 1        | 0.24          |
| (3,19)   | 1:34:D:LEU:CB  | 1:35:C:THR:N   | 4        | 0.24          |
| (3,18)   | 1:34:C:LEU:CB  | 1:35:B:THR:N   | 1        | 0.24          |
| (3,18)   | 1:34:C:LEU:CB  | 1:35:B:THR:N   | 4        | 0.24          |
| (3,17)   | 1:34:B:LEU:CB  | 1:35:A:THR:N   | 1        | 0.24          |
| (3,17)   | 1:34:B:LEU:CB  | 1:35:A:THR:N   | 4        | 0.24          |
| (3,16)   | 1:34:A:LEU:CB  | 1:35:E:THR:N   | 1        | 0.24          |
| (3,16)   | 1:34:A:LEU:CB  | 1:35:E:THR:N   | 4        | 0.24          |
| (1,1125) | 1:20:E:THR:CG2 | 1:24:E:ALA:CA  | 5        | 0.24          |
| (1,1124) | 1:20:D:THR:CG2 | 1:24:D:ALA:CA  | 5        | 0.24          |
| (1,1123) | 1:20:C:THR:CG2 | 1:24:C:ALA:CA  | 5        | 0.24          |
| (1,1122) | 1:20:B:THR:CG2 | 1:24:B:ALA:CA  | 5        | 0.24          |
| (1,1121) | 1:20:A:THR:CG2 | 1:24:A:ALA:CA  | 5        | 0.24          |
| (1,1000) | 1:11:E:LEU:CB  | 1:13:E:ILE:CG2 | 1        | 0.22          |
| (1,999)  | 1:11:D:LEU:CB  | 1:13:D:ILE:CG2 | 1        | 0.22          |
| (1,998)  | 1:11:C:LEU:CB  | 1:13:C:ILE:CG2 | 1        | 0.22          |
| (1,997)  | 1:11:B:LEU:CB  | 1:13:B:ILE:CG2 | 1        | 0.22          |
| (1,996)  | 1:11:A:LEU:CB  | 1:13:A:ILE:CG2 | 1        | 0.22          |
| (1,640)  | 1:13:E:ILE:CG2 | 1:11:E:LEU:CB  | 1        | 0.22          |
| (1,639)  | 1:13:D:ILE:CG2 | 1:11:D:LEU:CB  | 1        | 0.22          |
| (1,638)  | 1:13:C:ILE:CG2 | 1:11:C:LEU:CB  | 1        | 0.22          |
| (1,637)  | 1:13:B:ILE:CG2 | 1:11:B:LEU:CB  | 1        | 0.22          |
| (1,636)  | 1:13:A:ILE:CG2 | 1:11:A:LEU:CB  | 1        | 0.22          |
| (1,285)  | 1:11:E:LEU:CB  | 1:13:E:ILE:CG2 | 1        | 0.22          |
| (1,284)  | 1:11:D:LEU:CB  | 1:13:D:ILE:CG2 | 1        | 0.22          |
| (1,283)  | 1:11:C:LEU:CB  | 1:13:C:ILE:CG2 | 1        | 0.22          |
| (1,282)  | 1:11:B:LEU:CB  | 1:13:B:ILE:CG2 | 1        | 0.22          |
| (1,281)  | 1:11:A:LEU:CB  | 1:13:A:ILE:CG2 | 1        | 0.22          |
| (3,150)  | 1:13:E:ILE:CA  | 1:16:A:PHE:N   | 5        | 0.21          |
| (3,149)  | 1:13:D:ILE:CA  | 1:16:E:PHE:N   | 5        | 0.21          |
| (3,148)  | 1:13:C:ILE:CA  | 1:16:D:PHE:N   | 5        | 0.21          |
| (3,147)  | 1:13:B:ILE:CA  | 1:16:C:PHE:N   | 5        | 0.21          |
| (3,146)  | 1:13:A:ILE:CA  | 1:16:B:PHE:N   | 5        | 0.21          |
| (3,17)   | 1:34:B:LEU:CB  | 1:35:A:THR:N   | 9        | 0.21          |
| (2,25)   | 1:35:E:THR:CG2 | 1:33:E:PHE:CB  | 1        | 0.21          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (2,24)   | 1:35:D:THR:CG2 | 1:33:D:PHE:CB  | 1        | 0.21          |
| (2,23)   | 1:35:C:THR:CG2 | 1:33:C:PHE:CB  | 1        | 0.21          |
| (2,22)   | 1:35:B:THR:CG2 | 1:33:B:PHE:CB  | 1        | 0.21          |
| (2,21)   | 1:35:A:THR:CG2 | 1:33:A:PHE:CB  | 1        | 0.21          |
| (1,1080) | 1:23:E:SER:CB  | 1:25:D:ILE:CG2 | 4        | 0.21          |
| (1,1079) | 1:23:D:SER:CB  | 1:25:C:ILE:CG2 | 4        | 0.21          |
| (1,1078) | 1:23:C:SER:CB  | 1:25:B:ILE:CG2 | 4        | 0.21          |
| (1,1077) | 1:23:B:SER:CB  | 1:25:A:ILE:CG2 | 4        | 0.21          |
| (1,1076) | 1:23:A:SER:CB  | 1:25:E:ILE:CG2 | 4        | 0.21          |
| (1,625)  | 1:25:E:ILE:CG2 | 1:23:A:SER:CB  | 4        | 0.21          |
| (1,624)  | 1:25:D:ILE:CG2 | 1:23:E:SER:CB  | 4        | 0.21          |
| (1,623)  | 1:25:C:ILE:CG2 | 1:23:D:SER:CB  | 4        | 0.21          |
| (1,622)  | 1:25:B:ILE:CG2 | 1:23:C:SER:CB  | 4        | 0.21          |
| (1,621)  | 1:25:A:ILE:CG2 | 1:23:B:SER:CB  | 4        | 0.21          |
| (3,150)  | 1:13:E:ILE:CA  | 1:16:A:PHE:N   | 6        | 0.2           |
| (3,150)  | 1:13:E:ILE:CA  | 1:16:A:PHE:N   | 9        | 0.2           |
| (3,150)  | 1:13:E:ILE:CA  | 1:16:A:PHE:N   | 10       | 0.2           |
| (3,149)  | 1:13:D:ILE:CA  | 1:16:E:PHE:N   | 6        | 0.2           |
| (3,149)  | 1:13:D:ILE:CA  | 1:16:E:PHE:N   | 9        | 0.2           |
| (3,149)  | 1:13:D:ILE:CA  | 1:16:E:PHE:N   | 10       | 0.2           |
| (3,148)  | 1:13:C:ILE:CA  | 1:16:D:PHE:N   | 6        | 0.2           |
| (3,148)  | 1:13:C:ILE:CA  | 1:16:D:PHE:N   | 9        | 0.2           |
| (3,148)  | 1:13:C:ILE:CA  | 1:16:D:PHE:N   | 10       | 0.2           |
| (3,147)  | 1:13:B:ILE:CA  | 1:16:C:PHE:N   | 6        | 0.2           |
| (3,147)  | 1:13:B:ILE:CA  | 1:16:C:PHE:N   | 9        | 0.2           |
| (3,147)  | 1:13:B:ILE:CA  | 1:16:C:PHE:N   | 10       | 0.2           |
| (3,146)  | 1:13:A:ILE:CA  | 1:16:B:PHE:N   | 6        | 0.2           |
| (3,146)  | 1:13:A:ILE:CA  | 1:16:B:PHE:N   | 9        | 0.2           |
| (3,146)  | 1:13:A:ILE:CA  | 1:16:B:PHE:N   | 10       | 0.2           |
| (3,120)  | 1:18:E:ILE:CA  | 1:16:A:PHE:N   | 5        | 0.2           |
| (3,119)  | 1:18:D:ILE:CA  | 1:16:E:PHE:N   | 5        | 0.2           |
| (3,118)  | 1:18:C:ILE:CA  | 1:16:D:PHE:N   | 5        | 0.2           |
| (3,117)  | 1:18:B:ILE:CA  | 1:16:C:PHE:N   | 5        | 0.2           |
| (3,116)  | 1:18:A:ILE:CA  | 1:16:B:PHE:N   | 5        | 0.2           |
| (3,20)   | 1:34:E:LEU:CB  | 1:35:D:THR:N   | 9        | 0.2           |
| (3,19)   | 1:34:D:LEU:CB  | 1:35:C:THR:N   | 9        | 0.2           |
| (3,18)   | 1:34:C:LEU:CB  | 1:35:B:THR:N   | 9        | 0.2           |
| (3,16)   | 1:34:A:LEU:CB  | 1:35:E:THR:N   | 9        | 0.2           |
| (1,1060) | 1:9:E:ILE:CB   | 1:11:E:LEU:CG  | 4        | 0.2           |
| (1,1059) | 1:9:D:ILE:CB   | 1:11:D:LEU:CG  | 4        | 0.2           |
| (1,1058) | 1:9:C:ILE:CB   | 1:11:C:LEU:CG  | 4        | 0.2           |
| (1,1057) | 1:9:B:ILE:CB   | 1:11:B:LEU:CG  | 4        | 0.2           |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1056) | 1:9:A:ILE:CB   | 1:11:A:LEU:CG  | 4        | 0.2           |
| (1,845)  | 1:11:E:LEU:CG  | 1:9:E:ILE:CB   | 4        | 0.2           |
| (1,844)  | 1:11:D:LEU:CG  | 1:9:D:ILE:CB   | 4        | 0.2           |
| (1,843)  | 1:11:C:LEU:CG  | 1:9:C:ILE:CB   | 4        | 0.2           |
| (1,842)  | 1:11:B:LEU:CG  | 1:9:B:ILE:CB   | 4        | 0.2           |
| (1,841)  | 1:11:A:LEU:CG  | 1:9:A:ILE:CB   | 4        | 0.2           |
| (1,140)  | 1:18:E:ILE:CA  | 1:14:E:VAL:CG2 | 4        | 0.2           |
| (1,139)  | 1:18:D:ILE:CA  | 1:14:D:VAL:CG2 | 4        | 0.2           |
| (1,138)  | 1:18:C:ILE:CA  | 1:14:C:VAL:CG2 | 4        | 0.2           |
| (1,137)  | 1:18:B:ILE:CA  | 1:14:B:VAL:CG2 | 4        | 0.2           |
| (1,136)  | 1:18:A:ILE:CA  | 1:14:A:VAL:CG2 | 4        | 0.2           |
| (3,20)   | 1:34:E:LEU:CB  | 1:35:D:THR:N   | 5        | 0.19          |
| (3,19)   | 1:34:D:LEU:CB  | 1:35:C:THR:N   | 5        | 0.19          |
| (3,19)   | 1:34:D:LEU:CB  | 1:35:C:THR:N   | 8        | 0.19          |
| (3,18)   | 1:34:C:LEU:CB  | 1:35:B:THR:N   | 5        | 0.19          |
| (3,17)   | 1:34:B:LEU:CB  | 1:35:A:THR:N   | 5        | 0.19          |
| (3,17)   | 1:34:B:LEU:CB  | 1:35:A:THR:N   | 8        | 0.19          |
| (3,16)   | 1:34:A:LEU:CB  | 1:35:E:THR:N   | 5        | 0.19          |
| (1,870)  | 1:32:E:ALA:CB  | 1:26:A:THR:CA  | 8        | 0.19          |
| (1,869)  | 1:32:D:ALA:CB  | 1:26:E:THR:CA  | 8        | 0.19          |
| (1,868)  | 1:32:C:ALA:CB  | 1:26:D:THR:CA  | 8        | 0.19          |
| (1,867)  | 1:32:B:ALA:CB  | 1:26:C:THR:CA  | 8        | 0.19          |
| (1,866)  | 1:32:A:ALA:CB  | 1:26:B:THR:CA  | 8        | 0.19          |
| (7,20)   | 1:37:E:THR:CG2 | 1:32:D:ALA:CB  | 4        | 0.18          |
| (7,19)   | 1:37:D:THR:CG2 | 1:32:C:ALA:CB  | 4        | 0.18          |
| (7,18)   | 1:37:C:THR:CG2 | 1:32:B:ALA:CB  | 4        | 0.18          |
| (7,17)   | 1:37:B:THR:CG2 | 1:32:A:ALA:CB  | 4        | 0.18          |
| (7,16)   | 1:37:A:THR:CG2 | 1:32:E:ALA:CB  | 4        | 0.18          |
| (4,60)   | 1:27:E:LEU:CG  | 1:24:D:ALA:N   | 7        | 0.18          |
| (4,59)   | 1:27:D:LEU:CG  | 1:24:C:ALA:N   | 7        | 0.18          |
| (4,58)   | 1:27:C:LEU:CG  | 1:24:B:ALA:N   | 7        | 0.18          |
| (4,57)   | 1:27:B:LEU:CG  | 1:24:A:ALA:N   | 7        | 0.18          |
| (4,56)   | 1:27:A:LEU:CG  | 1:24:E:ALA:N   | 7        | 0.18          |
| (3,150)  | 1:13:E:ILE:CA  | 1:16:A:PHE:N   | 8        | 0.18          |
| (3,149)  | 1:13:D:ILE:CA  | 1:16:E:PHE:N   | 8        | 0.18          |
| (3,148)  | 1:13:C:ILE:CA  | 1:16:D:PHE:N   | 8        | 0.18          |
| (3,147)  | 1:13:B:ILE:CA  | 1:16:C:PHE:N   | 8        | 0.18          |
| (3,146)  | 1:13:A:ILE:CA  | 1:16:B:PHE:N   | 8        | 0.18          |
| (3,45)   | 1:22:E:VAL:CB  | 1:26:D:THR:N   | 5        | 0.18          |
| (3,44)   | 1:22:D:VAL:CB  | 1:26:C:THR:N   | 5        | 0.18          |
| (3,43)   | 1:22:C:VAL:CB  | 1:26:B:THR:N   | 5        | 0.18          |
| (3,42)   | 1:22:B:VAL:CB  | 1:26:A:THR:N   | 5        | 0.18          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (3,41)  | 1:22:A:VAL:CB  | 1:26:E:THR:N   | 5        | 0.18          |
| (3,30)  | 1:33:E:PHE:CA  | 1:35:A:THR:N   | 1        | 0.18          |
| (3,29)  | 1:33:D:PHE:CA  | 1:35:E:THR:N   | 1        | 0.18          |
| (3,28)  | 1:33:C:PHE:CA  | 1:35:D:THR:N   | 1        | 0.18          |
| (3,27)  | 1:33:B:PHE:CA  | 1:35:C:THR:N   | 1        | 0.18          |
| (3,26)  | 1:33:A:PHE:CA  | 1:35:B:THR:N   | 1        | 0.18          |
| (3,20)  | 1:34:E:LEU:CB  | 1:35:D:THR:N   | 8        | 0.18          |
| (3,18)  | 1:34:C:LEU:CB  | 1:35:B:THR:N   | 8        | 0.18          |
| (3,16)  | 1:34:A:LEU:CB  | 1:35:E:THR:N   | 8        | 0.18          |
| (7,20)  | 1:37:E:THR:CG2 | 1:32:D:ALA:CB  | 3        | 0.17          |
| (7,19)  | 1:37:D:THR:CG2 | 1:32:C:ALA:CB  | 3        | 0.17          |
| (7,18)  | 1:37:C:THR:CG2 | 1:32:B:ALA:CB  | 3        | 0.17          |
| (7,17)  | 1:37:B:THR:CG2 | 1:32:A:ALA:CB  | 3        | 0.17          |
| (7,16)  | 1:37:A:THR:CG2 | 1:32:E:ALA:CB  | 3        | 0.17          |
| (3,150) | 1:13:E:ILE:CA  | 1:16:A:PHE:N   | 2        | 0.17          |
| (3,149) | 1:13:D:ILE:CA  | 1:16:E:PHE:N   | 2        | 0.17          |
| (3,148) | 1:13:C:ILE:CA  | 1:16:D:PHE:N   | 2        | 0.17          |
| (3,147) | 1:13:B:ILE:CA  | 1:16:C:PHE:N   | 2        | 0.17          |
| (3,146) | 1:13:A:ILE:CA  | 1:16:B:PHE:N   | 2        | 0.17          |
| (1,350) | 1:25:E:ILE:CD1 | 1:28:E:LEU:CG  | 7        | 0.17          |
| (1,349) | 1:25:D:ILE:CD1 | 1:28:D:LEU:CG  | 7        | 0.17          |
| (1,348) | 1:25:C:ILE:CD1 | 1:28:C:LEU:CG  | 7        | 0.17          |
| (1,347) | 1:25:B:ILE:CD1 | 1:28:B:LEU:CG  | 7        | 0.17          |
| (1,346) | 1:25:A:ILE:CD1 | 1:28:A:LEU:CG  | 7        | 0.17          |
| (3,55)  | 1:34:E:LEU:CB  | 1:37:D:THR:N   | 4        | 0.16          |
| (3,55)  | 1:34:E:LEU:CB  | 1:37:D:THR:N   | 6        | 0.16          |
| (3,54)  | 1:34:D:LEU:CB  | 1:37:C:THR:N   | 4        | 0.16          |
| (3,54)  | 1:34:D:LEU:CB  | 1:37:C:THR:N   | 6        | 0.16          |
| (3,53)  | 1:34:C:LEU:CB  | 1:37:B:THR:N   | 4        | 0.16          |
| (3,53)  | 1:34:C:LEU:CB  | 1:37:B:THR:N   | 6        | 0.16          |
| (3,52)  | 1:34:B:LEU:CB  | 1:37:A:THR:N   | 4        | 0.16          |
| (3,52)  | 1:34:B:LEU:CB  | 1:37:A:THR:N   | 6        | 0.16          |
| (3,51)  | 1:34:A:LEU:CB  | 1:37:E:THR:N   | 4        | 0.16          |
| (3,51)  | 1:34:A:LEU:CB  | 1:37:E:THR:N   | 6        | 0.16          |
| (3,45)  | 1:22:E:VAL:CB  | 1:26:D:THR:N   | 10       | 0.16          |
| (3,44)  | 1:22:D:VAL:CB  | 1:26:C:THR:N   | 10       | 0.16          |
| (3,43)  | 1:22:C:VAL:CB  | 1:26:B:THR:N   | 10       | 0.16          |
| (3,42)  | 1:22:B:VAL:CB  | 1:26:A:THR:N   | 10       | 0.16          |
| (3,41)  | 1:22:A:VAL:CB  | 1:26:E:THR:N   | 10       | 0.16          |
| (2,140) | 1:13:E:ILE:CA  | 1:11:A:LEU:CD2 | 1        | 0.16          |
| (2,139) | 1:13:D:ILE:CA  | 1:11:E:LEU:CD2 | 1        | 0.16          |
| (2,138) | 1:13:C:ILE:CA  | 1:11:D:LEU:CD2 | 1        | 0.16          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (2,137)  | 1:13:B:ILE:CA  | 1:11:C:LEU:CD2 | 1        | 0.16          |
| (2,136)  | 1:13:A:ILE:CA  | 1:11:B:LEU:CD2 | 1        | 0.16          |
| (2,55)   | 1:11:E:LEU:CG  | 1:9:D:ILE:CD1  | 5        | 0.16          |
| (2,54)   | 1:11:D:LEU:CG  | 1:9:C:ILE:CD1  | 5        | 0.16          |
| (2,53)   | 1:11:C:LEU:CG  | 1:9:B:ILE:CD1  | 5        | 0.16          |
| (2,52)   | 1:11:B:LEU:CG  | 1:9:A:ILE:CD1  | 5        | 0.16          |
| (2,51)   | 1:11:A:LEU:CG  | 1:9:E:ILE:CD1  | 5        | 0.16          |
| (1,1125) | 1:20:E:THR:CG2 | 1:24:E:ALA:CA  | 9        | 0.16          |
| (1,1124) | 1:20:D:THR:CG2 | 1:24:D:ALA:CA  | 9        | 0.16          |
| (1,1122) | 1:20:B:THR:CG2 | 1:24:B:ALA:CA  | 9        | 0.16          |
| (1,840)  | 1:11:E:LEU:CG  | 1:9:D:ILE:CD1  | 5        | 0.16          |
| (1,839)  | 1:11:D:LEU:CG  | 1:9:C:ILE:CD1  | 5        | 0.16          |
| (1,838)  | 1:11:C:LEU:CG  | 1:9:B:ILE:CD1  | 5        | 0.16          |
| (1,837)  | 1:11:B:LEU:CG  | 1:9:A:ILE:CD1  | 5        | 0.16          |
| (1,836)  | 1:11:A:LEU:CG  | 1:9:E:ILE:CD1  | 5        | 0.16          |
| (4,60)   | 1:27:E:LEU:CG  | 1:24:D:ALA:N   | 2        | 0.15          |
| (4,59)   | 1:27:D:LEU:CG  | 1:24:C:ALA:N   | 2        | 0.15          |
| (4,58)   | 1:27:C:LEU:CG  | 1:24:B:ALA:N   | 2        | 0.15          |
| (4,57)   | 1:27:B:LEU:CG  | 1:24:A:ALA:N   | 2        | 0.15          |
| (4,56)   | 1:27:A:LEU:CG  | 1:24:E:ALA:N   | 2        | 0.15          |
| (2,54)   | 1:11:D:LEU:CG  | 1:13:D:ILE:CD1 | 6        | 0.15          |
| (2,53)   | 1:11:C:LEU:CG  | 1:13:C:ILE:CD1 | 6        | 0.15          |
| (2,52)   | 1:11:B:LEU:CG  | 1:13:B:ILE:CD1 | 6        | 0.15          |
| (2,51)   | 1:11:A:LEU:CG  | 1:13:A:ILE:CD1 | 6        | 0.15          |
| (2,25)   | 1:35:E:THR:CG2 | 1:33:E:PHE:CB  | 8        | 0.15          |
| (2,24)   | 1:35:D:THR:CG2 | 1:33:D:PHE:CB  | 8        | 0.15          |
| (2,23)   | 1:35:C:THR:CG2 | 1:33:C:PHE:CB  | 8        | 0.15          |
| (2,22)   | 1:35:B:THR:CG2 | 1:33:B:PHE:CB  | 8        | 0.15          |
| (2,21)   | 1:35:A:THR:CG2 | 1:33:A:PHE:CB  | 8        | 0.15          |
| (1,1123) | 1:20:C:THR:CG2 | 1:24:C:ALA:CA  | 9        | 0.15          |
| (1,1121) | 1:20:A:THR:CG2 | 1:24:A:ALA:CA  | 9        | 0.15          |
| (1,839)  | 1:11:D:LEU:CG  | 1:13:D:ILE:CD1 | 6        | 0.15          |
| (1,838)  | 1:11:C:LEU:CG  | 1:13:C:ILE:CD1 | 6        | 0.15          |
| (1,837)  | 1:11:B:LEU:CG  | 1:13:B:ILE:CD1 | 6        | 0.15          |
| (1,836)  | 1:11:A:LEU:CG  | 1:13:A:ILE:CD1 | 6        | 0.15          |
| (1,325)  | 1:25:E:ILE:CB  | 1:27:E:LEU:CG  | 1        | 0.15          |
| (1,324)  | 1:25:D:ILE:CB  | 1:27:D:LEU:CG  | 1        | 0.15          |
| (1,323)  | 1:25:C:ILE:CB  | 1:27:C:LEU:CG  | 1        | 0.15          |
| (1,322)  | 1:25:B:ILE:CB  | 1:27:B:LEU:CG  | 1        | 0.15          |
| (1,321)  | 1:25:A:ILE:CB  | 1:27:A:LEU:CG  | 1        | 0.15          |
| (3,150)  | 1:13:E:ILE:CA  | 1:16:A:PHE:N   | 4        | 0.14          |
| (3,150)  | 1:13:E:ILE:CA  | 1:16:A:PHE:N   | 7        | 0.14          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (3,149)  | 1:13:D:ILE:CA  | 1:16:E:PHE:N   | 4        | 0.14          |
| (3,149)  | 1:13:D:ILE:CA  | 1:16:E:PHE:N   | 7        | 0.14          |
| (3,148)  | 1:13:C:ILE:CA  | 1:16:D:PHE:N   | 4        | 0.14          |
| (3,148)  | 1:13:C:ILE:CA  | 1:16:D:PHE:N   | 7        | 0.14          |
| (3,147)  | 1:13:B:ILE:CA  | 1:16:C:PHE:N   | 4        | 0.14          |
| (3,147)  | 1:13:B:ILE:CA  | 1:16:C:PHE:N   | 7        | 0.14          |
| (3,146)  | 1:13:A:ILE:CA  | 1:16:B:PHE:N   | 4        | 0.14          |
| (3,146)  | 1:13:A:ILE:CA  | 1:16:B:PHE:N   | 7        | 0.14          |
| (2,170)  | 1:13:E:ILE:CB  | 1:11:A:LEU:CD1 | 7        | 0.14          |
| (2,169)  | 1:13:D:ILE:CB  | 1:11:E:LEU:CD1 | 7        | 0.14          |
| (2,168)  | 1:13:C:ILE:CB  | 1:11:D:LEU:CD1 | 7        | 0.14          |
| (2,167)  | 1:13:B:ILE:CB  | 1:11:C:LEU:CD1 | 7        | 0.14          |
| (2,166)  | 1:13:A:ILE:CB  | 1:11:B:LEU:CD1 | 7        | 0.14          |
| (2,55)   | 1:11:E:LEU:CG  | 1:13:E:ILE:CD1 | 6        | 0.14          |
| (1,840)  | 1:11:E:LEU:CG  | 1:13:E:ILE:CD1 | 6        | 0.14          |
| (7,20)   | 1:37:E:THR:CG2 | 1:32:D:ALA:CB  | 9        | 0.13          |
| (7,19)   | 1:37:D:THR:CG2 | 1:32:C:ALA:CB  | 9        | 0.13          |
| (7,18)   | 1:37:C:THR:CG2 | 1:32:B:ALA:CB  | 9        | 0.13          |
| (7,17)   | 1:37:B:THR:CG2 | 1:32:A:ALA:CB  | 9        | 0.13          |
| (7,16)   | 1:37:A:THR:CG2 | 1:32:E:ALA:CB  | 9        | 0.13          |
| (4,60)   | 1:27:E:LEU:CG  | 1:24:D:ALA:N   | 9        | 0.12          |
| (4,59)   | 1:27:D:LEU:CG  | 1:24:C:ALA:N   | 9        | 0.12          |
| (4,58)   | 1:27:C:LEU:CG  | 1:24:B:ALA:N   | 9        | 0.12          |
| (4,57)   | 1:27:B:LEU:CG  | 1:24:A:ALA:N   | 9        | 0.12          |
| (4,56)   | 1:27:A:LEU:CG  | 1:24:E:ALA:N   | 9        | 0.12          |
| (2,140)  | 1:13:E:ILE:CA  | 1:11:A:LEU:CD2 | 3        | 0.12          |
| (2,139)  | 1:13:D:ILE:CA  | 1:11:E:LEU:CD2 | 3        | 0.12          |
| (2,138)  | 1:13:C:ILE:CA  | 1:11:D:LEU:CD2 | 3        | 0.12          |
| (2,137)  | 1:13:B:ILE:CA  | 1:11:C:LEU:CD2 | 3        | 0.12          |
| (2,136)  | 1:13:A:ILE:CA  | 1:11:B:LEU:CD2 | 3        | 0.12          |
| (2,105)  | 1:31:E:MET:CA  | 1:33:A:PHE:CE2 | 6        | 0.12          |
| (2,104)  | 1:31:D:MET:CA  | 1:33:E:PHE:CE2 | 6        | 0.12          |
| (2,103)  | 1:31:C:MET:CA  | 1:33:D:PHE:CE2 | 6        | 0.12          |
| (2,102)  | 1:31:B:MET:CA  | 1:33:C:PHE:CE2 | 6        | 0.12          |
| (2,101)  | 1:31:A:MET:CA  | 1:33:B:PHE:CE2 | 6        | 0.12          |
| (1,1125) | 1:20:E:THR:CG2 | 1:24:E:ALA:CA  | 1        | 0.12          |
| (1,1124) | 1:20:D:THR:CG2 | 1:24:D:ALA:CA  | 1        | 0.12          |
| (1,1123) | 1:20:C:THR:CG2 | 1:24:C:ALA:CA  | 1        | 0.12          |
| (1,1122) | 1:20:B:THR:CG2 | 1:24:B:ALA:CA  | 1        | 0.12          |
| (1,1121) | 1:20:A:THR:CG2 | 1:24:A:ALA:CA  | 1        | 0.12          |
| (2,219)  | 1:29:D:VAL:CA  | 1:27:E:LEU:CA  | 4        | 0.11          |
| (2,192)  | 1:29:A:VAL:CA  | 1:27:B:LEU:CA  | 4        | 0.11          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (2,55)   | 1:11:E:LEU:CG  | 1:13:E:ILE:CD1 | 3        | 0.11          |
| (2,54)   | 1:11:D:LEU:CG  | 1:13:D:ILE:CD1 | 3        | 0.11          |
| (2,53)   | 1:11:C:LEU:CG  | 1:13:C:ILE:CD1 | 3        | 0.11          |
| (2,52)   | 1:11:B:LEU:CG  | 1:13:B:ILE:CD1 | 3        | 0.11          |
| (2,51)   | 1:11:A:LEU:CG  | 1:13:A:ILE:CD1 | 3        | 0.11          |
| (1,1124) | 1:20:D:THR:CG2 | 1:24:D:ALA:CA  | 7        | 0.11          |
| (1,1123) | 1:20:C:THR:CG2 | 1:24:C:ALA:CA  | 7        | 0.11          |
| (1,1121) | 1:20:A:THR:CG2 | 1:24:A:ALA:CA  | 7        | 0.11          |
| (1,1057) | 1:9:B:ILE:CB   | 1:11:B:LEU:CG  | 6        | 0.11          |
| (1,1056) | 1:9:A:ILE:CB   | 1:11:A:LEU:CG  | 6        | 0.11          |
| (1,842)  | 1:11:B:LEU:CG  | 1:9:B:ILE:CB   | 6        | 0.11          |
| (1,841)  | 1:11:A:LEU:CG  | 1:9:A:ILE:CB   | 6        | 0.11          |
| (1,840)  | 1:11:E:LEU:CG  | 1:13:E:ILE:CD1 | 3        | 0.11          |
| (1,839)  | 1:11:D:LEU:CG  | 1:13:D:ILE:CD1 | 3        | 0.11          |
| (1,838)  | 1:11:C:LEU:CG  | 1:13:C:ILE:CD1 | 3        | 0.11          |
| (1,837)  | 1:11:B:LEU:CG  | 1:13:B:ILE:CD1 | 3        | 0.11          |
| (1,836)  | 1:11:A:LEU:CG  | 1:13:A:ILE:CD1 | 3        | 0.11          |
| (2,228)  | 1:29:E:VAL:CA  | 1:27:A:LEU:CA  | 4        | 0.1           |
| (2,210)  | 1:29:C:VAL:CA  | 1:27:D:LEU:CA  | 4        | 0.1           |
| (2,201)  | 1:29:B:VAL:CA  | 1:27:C:LEU:CA  | 4        | 0.1           |
| (1,1125) | 1:20:E:THR:CG2 | 1:24:E:ALA:CA  | 7        | 0.1           |
| (1,1122) | 1:20:B:THR:CG2 | 1:24:B:ALA:CA  | 7        | 0.1           |
| (1,1085) | 1:23:E:SER:CB  | 1:25:D:ILE:CD1 | 10       | 0.1           |
| (1,1084) | 1:23:D:SER:CB  | 1:25:C:ILE:CD1 | 10       | 0.1           |
| (1,1083) | 1:23:C:SER:CB  | 1:25:B:ILE:CD1 | 10       | 0.1           |
| (1,1082) | 1:23:B:SER:CB  | 1:25:A:ILE:CD1 | 10       | 0.1           |
| (1,1081) | 1:23:A:SER:CB  | 1:25:E:ILE:CD1 | 10       | 0.1           |
| (1,1060) | 1:9:E:ILE:CB   | 1:11:E:LEU:CG  | 6        | 0.1           |
| (1,1059) | 1:9:D:ILE:CB   | 1:11:D:LEU:CG  | 6        | 0.1           |
| (1,1058) | 1:9:C:ILE:CB   | 1:11:C:LEU:CG  | 6        | 0.1           |
| (1,845)  | 1:11:E:LEU:CG  | 1:9:E:ILE:CB   | 6        | 0.1           |
| (1,844)  | 1:11:D:LEU:CG  | 1:9:D:ILE:CB   | 6        | 0.1           |
| (1,843)  | 1:11:C:LEU:CG  | 1:9:C:ILE:CB   | 6        | 0.1           |
| (1,630)  | 1:25:E:ILE:CG2 | 1:28:E:LEU:CG  | 10       | 0.1           |
| (1,629)  | 1:25:D:ILE:CG2 | 1:28:D:LEU:CG  | 10       | 0.1           |
| (1,628)  | 1:25:C:ILE:CG2 | 1:28:C:LEU:CG  | 10       | 0.1           |
| (1,627)  | 1:25:B:ILE:CG2 | 1:28:B:LEU:CG  | 10       | 0.1           |
| (1,626)  | 1:25:A:ILE:CG2 | 1:28:A:LEU:CG  | 10       | 0.1           |



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

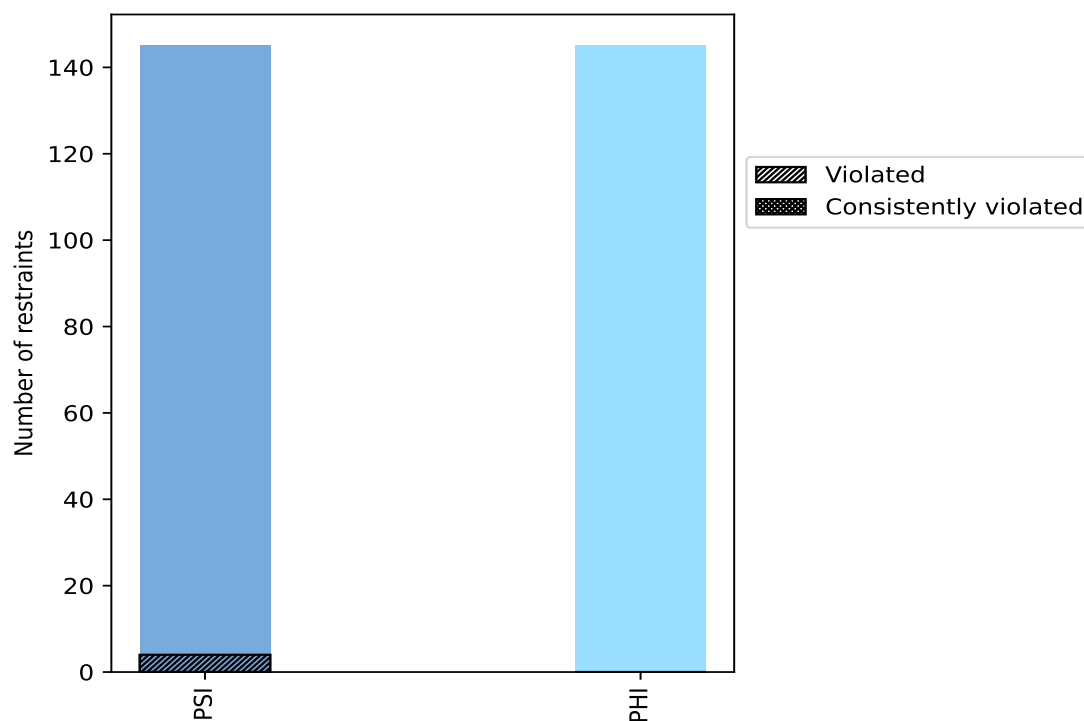
### 10.1 Summary of dihedral-angle violations [i](#)

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

| Angle type | Count | % <sup>1</sup> | Violated <sup>3</sup> |                |                | Consistently Violated <sup>4</sup> |                |                |
|------------|-------|----------------|-----------------------|----------------|----------------|------------------------------------|----------------|----------------|
|            |       |                | Count                 | % <sup>2</sup> | % <sup>1</sup> | Count                              | % <sup>2</sup> | % <sup>1</sup> |
| PSI        | 145   | 50.0           | 4                     | 2.8            | 1.4            | 0                                  | 0.0            | 0.0            |
| PHI        | 145   | 50.0           | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Total      | 290   | 100.0          | 4                     | 1.4            | 1.4            | 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

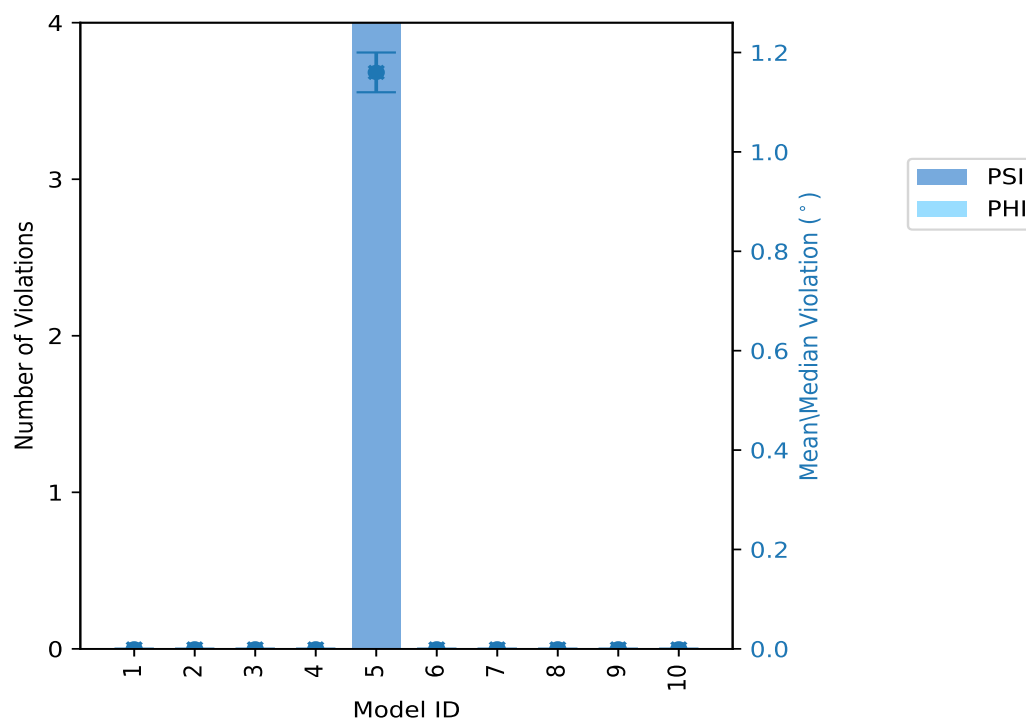


## 10.2 Dihedral-angle violation statistics for each model [i](#)

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

| Model ID | Number of violations |     |       | Mean (°) | Max (°) | SD (°) | Median (°) |
|----------|----------------------|-----|-------|----------|---------|--------|------------|
|          | PSI                  | PHI | Total |          |         |        |            |
| 1        | 0                    | 0   | 0     | 0.0      | 0.0     | 0.0    | 0.0        |
| 2        | 0                    | 0   | 0     | 0.0      | 0.0     | 0.0    | 0.0        |
| 3        | 0                    | 0   | 0     | 0.0      | 0.0     | 0.0    | 0.0        |
| 4        | 0                    | 0   | 0     | 0.0      | 0.0     | 0.0    | 0.0        |
| 5        | 4                    | 0   | 4     | 1.16     | 1.22    | 0.04   | 1.16       |
| 6        | 0                    | 0   | 0     | 0.0      | 0.0     | 0.0    | 0.0        |
| 7        | 0                    | 0   | 0     | 0.0      | 0.0     | 0.0    | 0.0        |
| 8        | 0                    | 0   | 0     | 0.0      | 0.0     | 0.0    | 0.0        |
| 9        | 0                    | 0   | 0     | 0.0      | 0.0     | 0.0    | 0.0        |
| 10       | 0                    | 0   | 0     | 0.0      | 0.0     | 0.0    | 0.0        |

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



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

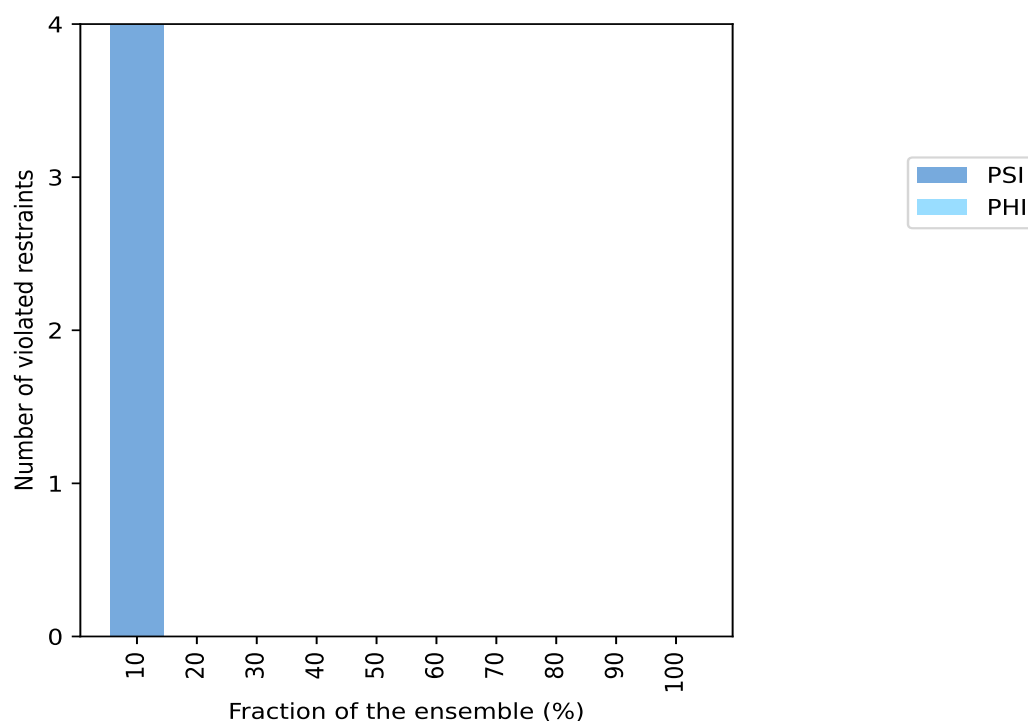
### 10.3 Dihedral-angle violation statistics for the ensemble [i](#)

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

| Number of violated restraints |     |       | Fraction of the ensemble |       |
|-------------------------------|-----|-------|--------------------------|-------|
| PSI                           | PHI | Total | Count <sup>1</sup>       | %     |
| 4                             | 0   | 4     | 1                        | 10.0  |
| 0                             | 0   | 0     | 2                        | 20.0  |
| 0                             | 0   | 0     | 3                        | 30.0  |
| 0                             | 0   | 0     | 4                        | 40.0  |
| 0                             | 0   | 0     | 5                        | 50.0  |
| 0                             | 0   | 0     | 6                        | 60.0  |
| 0                             | 0   | 0     | 7                        | 70.0  |
| 0                             | 0   | 0     | 8                        | 80.0  |
| 0                             | 0   | 0     | 9                        | 90.0  |
| 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](#)

No violations found

## 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.

Data insufficient to plot histogram

### 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 (°) |
|---------|--------------|---------------|--------------|--------------|----------|---------------|
| (1,92)  | 1:25:B:ILE:N | 1:25:B:ILE:CA | 1:25:B:ILE:C | 1:26:B:THR:N | 5        | 1.22          |
| (1,150) | 1:25:C:ILE:N | 1:25:C:ILE:CA | 1:25:C:ILE:C | 1:26:C:THR:N | 5        | 1.19          |
| (1,34)  | 1:25:A:ILE:N | 1:25:A:ILE:CA | 1:25:A:ILE:C | 1:26:A:THR:N | 5        | 1.13          |
| (1,266) | 1:25:E:ILE:N | 1:25:E:ILE:CA | 1:25:E:ILE:C | 1:26:E:THR:N | 5        | 1.12          |