



# Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2026 – 08:44 PM UTC

PDB ID : 2MK9 / pdb\_00002mk9  
BMRB ID : 19764  
Title : Spatial structure of the dimeric transmembrane domain of Toll-like receptor 3  
Authors : Mineev, K.S.; Goncharuk, S.A.; Arseniev, A.S.  
Deposited on : 2014-02-04

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

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

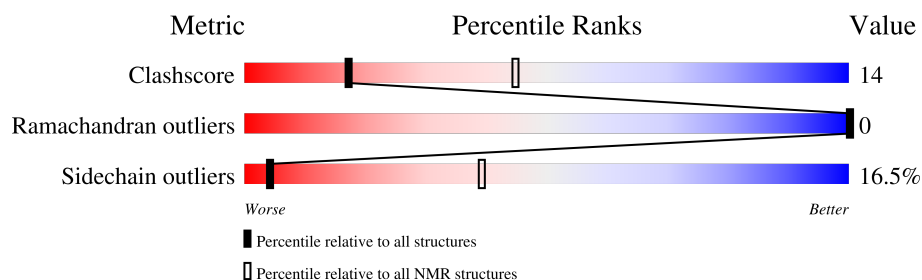
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 49%.

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



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

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 34     |                  |
| 1   | B     | 34     |                  |

## 2 Ensemble composition and analysis

This entry contains 10 models. Model 3 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *fewest violations*.

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:8-A:32, B:110-B:132 (48) | 0.57              | 3            |

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

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

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

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

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1172 atoms, of which 594 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Toll-like receptor 3.

| Mol | Chain | Residues | Atoms |     |     |    |    |   |  | Trace |
|-----|-------|----------|-------|-----|-----|----|----|---|--|-------|
| 1   | A     | 34       | Total | C   | H   | N  | O  | S |  | 0     |
|     |       |          | 586   | 202 | 297 | 41 | 44 | 2 |  |       |
| 1   | B     | 34       | Total | C   | H   | N  | O  | S |  | 0     |
|     |       |          | 586   | 202 | 297 | 41 | 44 | 2 |  |       |

There are 2 discrepancies between the modelled and reference sequences:

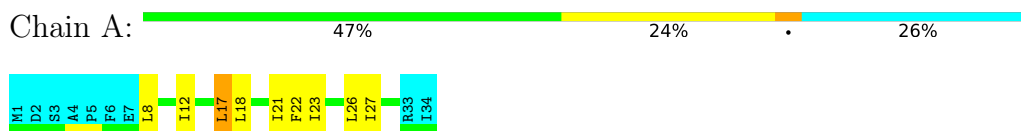
| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| A     | 1       | MET      | -      | initiating methionine | UNP O15455 |
| B     | 101     | MET      | -      | initiating methionine | UNP O15455 |

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

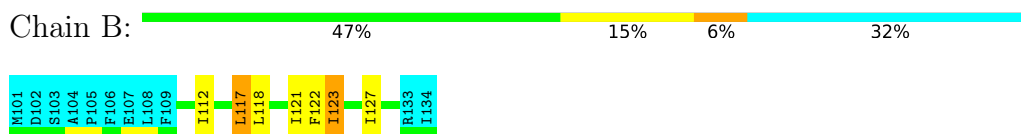
### 4.1 Average score per residue in the NMR ensemble

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: Toll-like receptor 3



- Molecule 1: Toll-like receptor 3



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

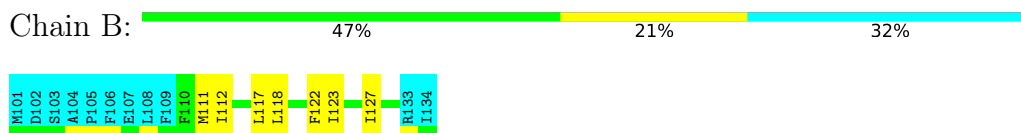
Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1

- Molecule 1: Toll-like receptor 3

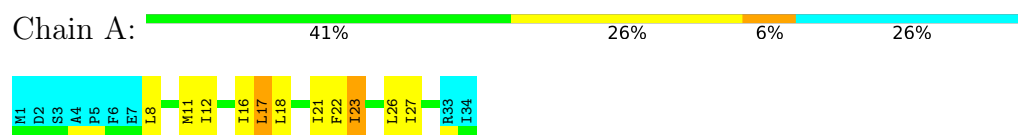


- Molecule 1: Toll-like receptor 3

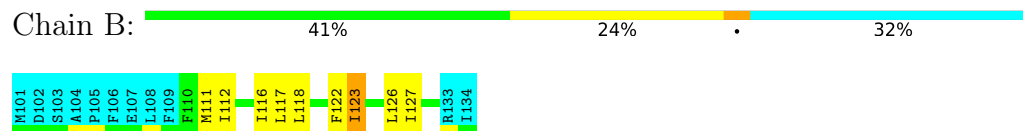


### 4.2.2 Score per residue for model 2

- Molecule 1: Toll-like receptor 3

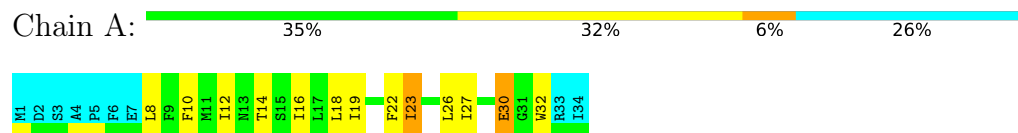


- Molecule 1: Toll-like receptor 3

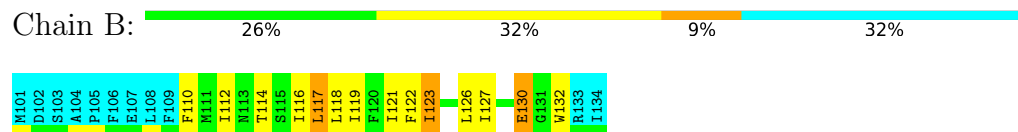


### 4.2.3 Score per residue for model 3 (medoid)

- Molecule 1: Toll-like receptor 3

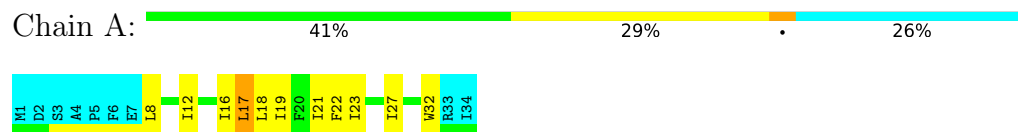


- Molecule 1: Toll-like receptor 3

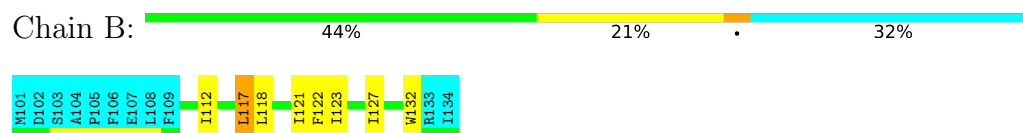


### 4.2.4 Score per residue for model 4

- Molecule 1: Toll-like receptor 3

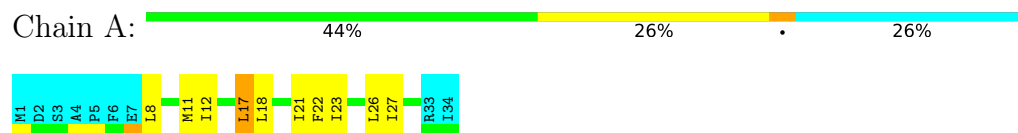


- Molecule 1: Toll-like receptor 3

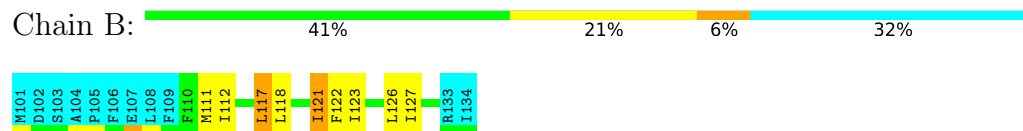


### 4.2.5 Score per residue for model 5

- Molecule 1: Toll-like receptor 3

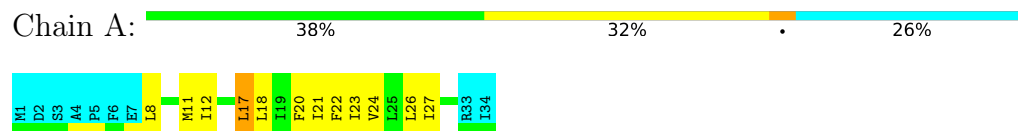


- Molecule 1: Toll-like receptor 3

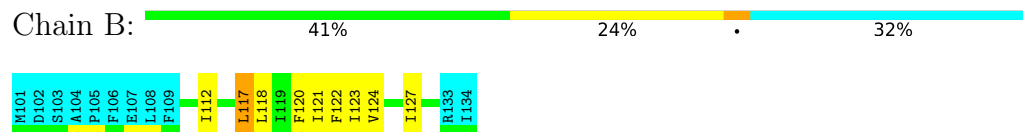


### 4.2.6 Score per residue for model 6

- Molecule 1: Toll-like receptor 3

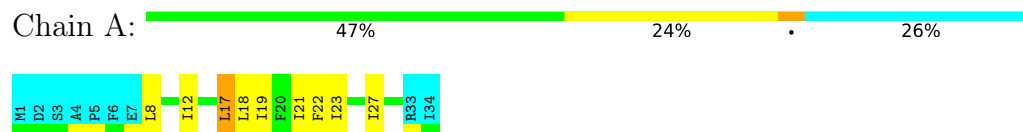


- Molecule 1: Toll-like receptor 3

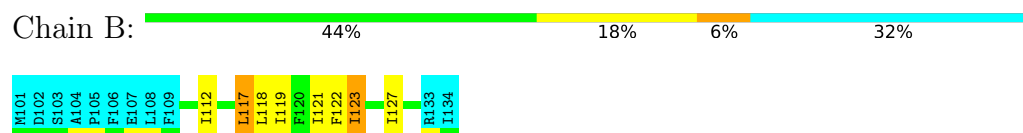


### 4.2.7 Score per residue for model 7

- Molecule 1: Toll-like receptor 3

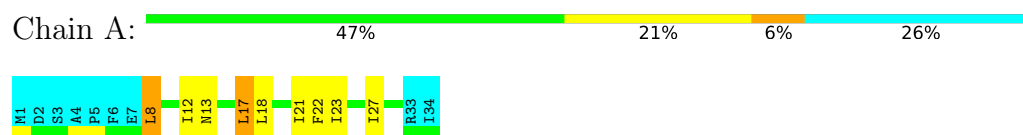


- Molecule 1: Toll-like receptor 3

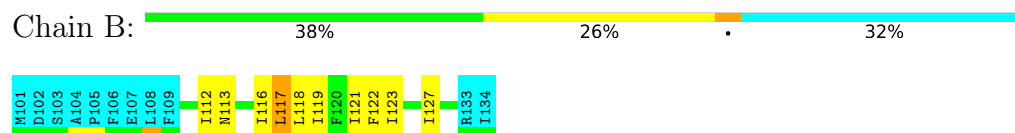


### 4.2.8 Score per residue for model 8

- Molecule 1: Toll-like receptor 3

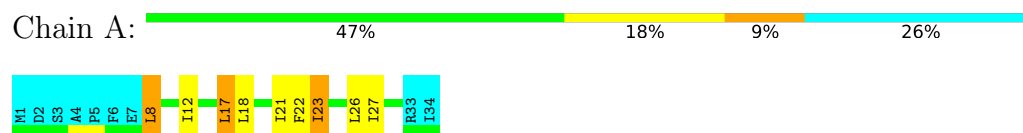


- Molecule 1: Toll-like receptor 3

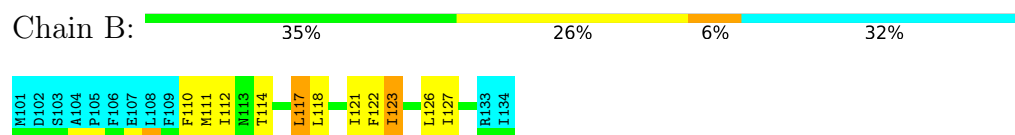


### 4.2.9 Score per residue for model 9

- Molecule 1: Toll-like receptor 3

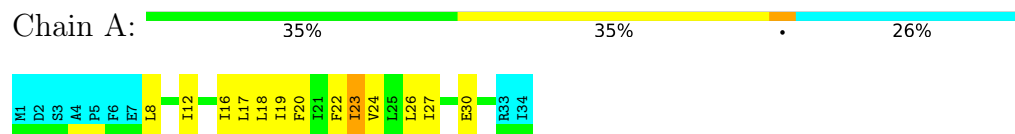


- Molecule 1: Toll-like receptor 3

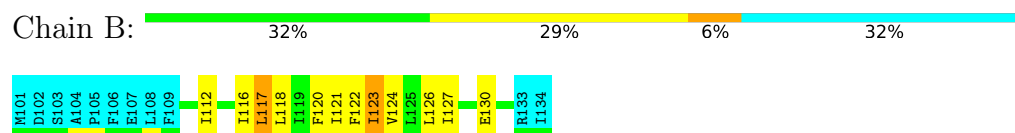


### 4.2.10 Score per residue for model 10

- Molecule 1: Toll-like receptor 3



- Molecule 1: Toll-like receptor 3



## 5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 10 were deposited, based on the following criterion: *structures with the least restraint violations*.

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

| Software name | Classification     | Version |
|---------------|--------------------|---------|
| CYANA         | structure solution | 3.0     |
| CYANA         | refinement         |         |

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

| Chemical shift file(s)                       | working_cs.cif |
|----------------------------------------------|----------------|
| Number of chemical shift lists               | 1              |
| Total number of shifts                       | 486            |
| Number of shifts mapped to atoms             | 486            |
| Number of unparsed shifts                    | 0              |
| Number of shifts with mapping errors         | 0              |
| Number of shifts with mapping warnings       | 0              |
| Assignment completeness (well-defined parts) | 49%            |

## 6 Model quality [i](#)

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

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes |
|-----|-------|-------|----------|----------|---------|
| 1   | A     | 216   | 228      | 228      | 8±2     |
| 1   | B     | 197   | 208      | 208      | 7±2     |
| All | All   | 4130  | 4360     | 4360     | 116     |

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 14.

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

| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:18:LEU:HD12  | 1:B:118:LEU:HD12 | 0.82     | 1.49        | 3      | 10    |
| 1:A:18:LEU:HD22  | 1:A:22:PHE:CZ    | 0.65     | 2.27        | 4      | 9     |
| 1:A:8:LEU:O      | 1:A:12:ILE:HD12  | 0.65     | 1.92        | 7      | 10    |
| 1:B:118:LEU:HD22 | 1:B:122:PHE:CZ   | 0.62     | 2.29        | 2      | 9     |
| 1:A:12:ILE:O     | 1:A:16:ILE:HD12  | 0.59     | 1.97        | 2      | 2     |
| 1:B:122:PHE:O    | 1:B:126:LEU:HD13 | 0.59     | 1.98        | 5      | 1     |
| 1:A:18:LEU:CD1   | 1:B:118:LEU:HD12 | 0.59     | 2.27        | 3      | 9     |
| 1:B:112:ILE:O    | 1:B:116:ILE:HD12 | 0.58     | 1.99        | 2      | 2     |
| 1:A:22:PHE:O     | 1:A:26:LEU:HD13  | 0.58     | 1.98        | 5      | 2     |
| 1:A:18:LEU:HD12  | 1:B:118:LEU:CD1  | 0.57     | 2.29        | 2      | 9     |
| 1:A:26:LEU:HD21  | 1:B:123:ILE:HG13 | 0.54     | 1.80        | 10     | 1     |
| 1:A:23:ILE:CG1   | 1:B:126:LEU:HD21 | 0.53     | 2.34        | 2      | 3     |
| 1:A:23:ILE:HG13  | 1:B:126:LEU:HD21 | 0.52     | 1.82        | 10     | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:26:LEU:HD21  | 1:B:123:ILE:CG1  | 0.51     | 2.35        | 2      | 4     |
| 1:B:117:LEU:HD22 | 1:B:121:ILE:HD11 | 0.50     | 1.84        | 7      | 8     |
| 1:B:110:PHE:O    | 1:B:114:THR:HG22 | 0.49     | 2.07        | 9      | 2     |
| 1:A:17:LEU:HD22  | 1:A:21:ILE:CD1   | 0.48     | 2.39        | 9      | 3     |
| 1:A:20:PHE:O     | 1:A:24:VAL:HG23  | 0.48     | 2.08        | 10     | 2     |
| 1:A:17:LEU:HD22  | 1:A:21:ILE:HD11  | 0.47     | 1.85        | 7      | 7     |
| 1:B:118:LEU:HD22 | 1:B:122:PHE:CE2  | 0.47     | 2.45        | 7      | 1     |
| 1:B:117:LEU:HD22 | 1:B:121:ILE:CD1  | 0.47     | 2.40        | 3      | 5     |
| 1:A:18:LEU:HD22  | 1:A:22:PHE:CE2   | 0.45     | 2.47        | 7      | 1     |
| 1:B:116:ILE:HA   | 1:B:119:ILE:HD12 | 0.45     | 1.89        | 3      | 2     |
| 1:A:16:ILE:HA    | 1:A:19:ILE:HD12  | 0.44     | 1.88        | 4      | 2     |
| 1:A:22:PHE:O     | 1:A:26:LEU:HD23  | 0.44     | 2.12        | 10     | 1     |
| 1:B:120:PHE:O    | 1:B:124:VAL:HG23 | 0.44     | 2.13        | 10     | 2     |
| 1:A:19:ILE:O     | 1:A:23:ILE:HD13  | 0.43     | 2.13        | 10     | 2     |
| 1:B:119:ILE:O    | 1:B:123:ILE:HD13 | 0.43     | 2.13        | 7      | 1     |
| 1:A:26:LEU:HD21  | 1:B:123:ILE:HD11 | 0.42     | 1.90        | 9      | 1     |
| 1:B:122:PHE:O    | 1:B:126:LEU:HD23 | 0.41     | 2.14        | 10     | 1     |
| 1:A:26:LEU:O     | 1:A:30:GLU:N     | 0.41     | 2.53        | 3      | 1     |
| 1:A:10:PHE:O     | 1:A:14:THR:HG22  | 0.41     | 2.16        | 3      | 1     |
| 1:B:126:LEU:O    | 1:B:130:GLU:N    | 0.40     | 2.53        | 3      | 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     | 25/34 (74%)   | 22±1 (86±3%) | 4±1 (14±3%) | 0±0 (0±0%) | 100         | 100 |
| 1   | B     | 23/34 (68%)   | 20±1 (85±3%) | 4±1 (15±3%) | 0±0 (0±0%) | 100         | 100 |
| All | All   | 480/680 (71%) | 410 (85%)    | 70 (15%)    | 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     | 24/32 (75%)   | 20±1 (84±3%) | 4±1 (16±3%) | 4           | 40 |
| 1   | B     | 22/32 (69%)   | 18±1 (83±3%) | 4±1 (17±3%) | 4           | 38 |
| All | All   | 460/640 (72%) | 384 (83%)    | 76 (17%)    | 4           | 39 |

All 16 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  | ILE  | 10             |
| 1   | B     | 117 | LEU  | 10             |
| 1   | B     | 123 | ILE  | 10             |
| 1   | B     | 127 | ILE  | 10             |
| 1   | A     | 17  | LEU  | 9              |
| 1   | A     | 23  | ILE  | 9              |
| 1   | A     | 30  | GLU  | 3              |
| 1   | B     | 111 | MET  | 2              |
| 1   | A     | 11  | MET  | 2              |
| 1   | A     | 32  | TRP  | 2              |
| 1   | B     | 130 | GLU  | 2              |
| 1   | B     | 132 | TRP  | 2              |
| 1   | A     | 8   | LEU  | 2              |
| 1   | B     | 121 | ILE  | 1              |
| 1   | A     | 13  | ASN  | 1              |
| 1   | B     | 113 | ASN  | 1              |

### 6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 6.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 6.7 Other polymers [i](#)

There are no such molecules in this entry.

## 6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 49% for the well-defined parts and 46% for the entire structure.

### 7.1 Chemical shift list 1

File name: working\_cs.cif

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

#### 7.1.1 Bookkeeping

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

|                                         |     |
|-----------------------------------------|-----|
| Total number of shifts                  | 486 |
| Number of shifts mapped to atoms        | 486 |
| Number of unparsed shifts               | 0   |
| Number of shifts with mapping errors    | 0   |
| Number of shifts with mapping warnings  | 0   |
| Number of shift outliers (ShiftChecker) | 1   |

#### 7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

| Nucleus                | # values | Correction $\pm$ precision, ppm | Suggested action           |
|------------------------|----------|---------------------------------|----------------------------|
| $^{13}\text{C}_\alpha$ | 34       | $-0.66 \pm 0.15$                | Should be checked          |
| $^{13}\text{C}_\beta$  | 33       | $0.72 \pm 0.05$                 | Should be checked          |
| $^{13}\text{C}'$       | 31       | $0.28 \pm 0.10$                 | None needed ( $< 0.5$ ppm) |
| $^{15}\text{N}$        | 33       | $0.88 \pm 0.27$                 | Should be applied          |

#### 7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 49%, i.e. 377 atoms were assigned a chemical shift out of a possible 768. 0 out of 11 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total         | $^1\text{H}$  | $^{13}\text{C}$ | $^{15}\text{N}$ |
|-----------|---------------|---------------|-----------------|-----------------|
| Backbone  | 125/242 (52%) | 51/98 (52%)   | 49/96 (51%)     | 25/48 (52%)     |
| Sidechain | 203/398 (51%) | 140/271 (52%) | 63/125 (50%)    | 0/2 (0%)        |

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|          | Total         | <sup>1</sup> H | <sup>13</sup> C | <sup>15</sup> N |
|----------|---------------|----------------|-----------------|-----------------|
| Aromatic | 49/128 (38%)  | 29/65 (45%)    | 20/59 (34%)     | 0/4 (0%)        |
| Overall  | 377/768 (49%) | 220/434 (51%)  | 132/280 (47%)   | 25/54 (46%)     |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 46%, i.e. 484 atoms were assigned a chemical shift out of a possible 1052. 0 out of 12 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total          | <sup>1</sup> H | <sup>13</sup> C | <sup>15</sup> N |
|-----------|----------------|----------------|-----------------|-----------------|
| Backbone  | 165/338 (49%)  | 67/136 (49%)   | 65/136 (48%)    | 33/66 (50%)     |
| Sidechain | 267/556 (48%)  | 184/374 (49%)  | 82/174 (47%)    | 1/8 (12%)       |
| Aromatic  | 52/158 (33%)   | 31/80 (39%)    | 21/74 (28%)     | 0/4 (0%)        |
| Overall   | 484/1052 (46%) | 282/590 (48%)  | 168/384 (44%)   | 34/78 (44%)     |

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

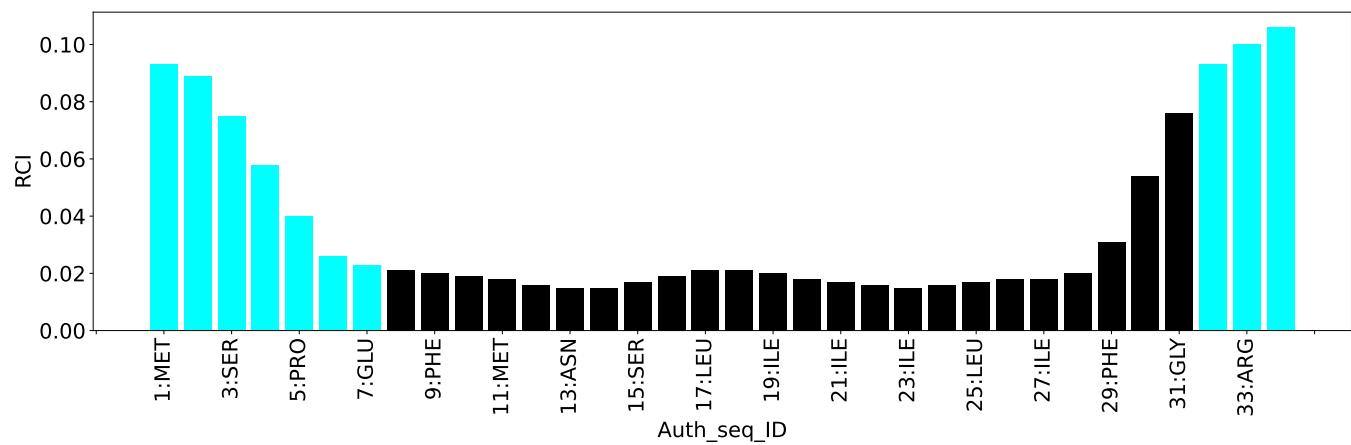
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

| List Id | Chain | Res | Type | Atom | Shift, ppm | Expected range, ppm | Z-score |
|---------|-------|-----|------|------|------------|---------------------|---------|
| 1       | A     | 14  | THR  | HG1  | 4.58       | 0.08 – 2.19         | 16.3    |

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

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

Random coil index (RCI) for chain A:



## 8 NMR restraints analysis

### 8.1 Conformationally restricting restraints

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

| Description                                              | Value |
|----------------------------------------------------------|-------|
| Total distance restraints                                | 913   |
| Intra-residue ( $ i-j =0$ )                              | 264   |
| Sequential ( $ i-j =1$ )                                 | 270   |
| Medium range ( $ i-j >1$ and $ i-j <5$ )                 | 325   |
| Long range ( $ i-j \geq 5$ )                             | 12    |
| Inter-chain                                              | 42    |
| Hydrogen bond restraints                                 | 0     |
| Disulfide bond restraints                                | 0     |
| Total dihedral-angle restraints                          | 136   |
| Number of unmapped restraints                            | 0     |
| Number of restraints per residue                         | 15.4  |
| Number of long range restraints per residue <sup>1</sup> | 0.2   |

<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)  | 23.7                                   | 0.2     |
| 0.2-0.5 (Medium) | 8.2                                    | 0.5     |
| >0.5 (Large)     | 39.4                                   | 20.02   |

### 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)   | 10.0                                   | 9.63    |
| 10.0-20.0 (Medium) | 0.2                                    | 10.65   |
| >20.0 (Large)      | None                                   | None    |

## 9 Distance violation analysis ⓘ

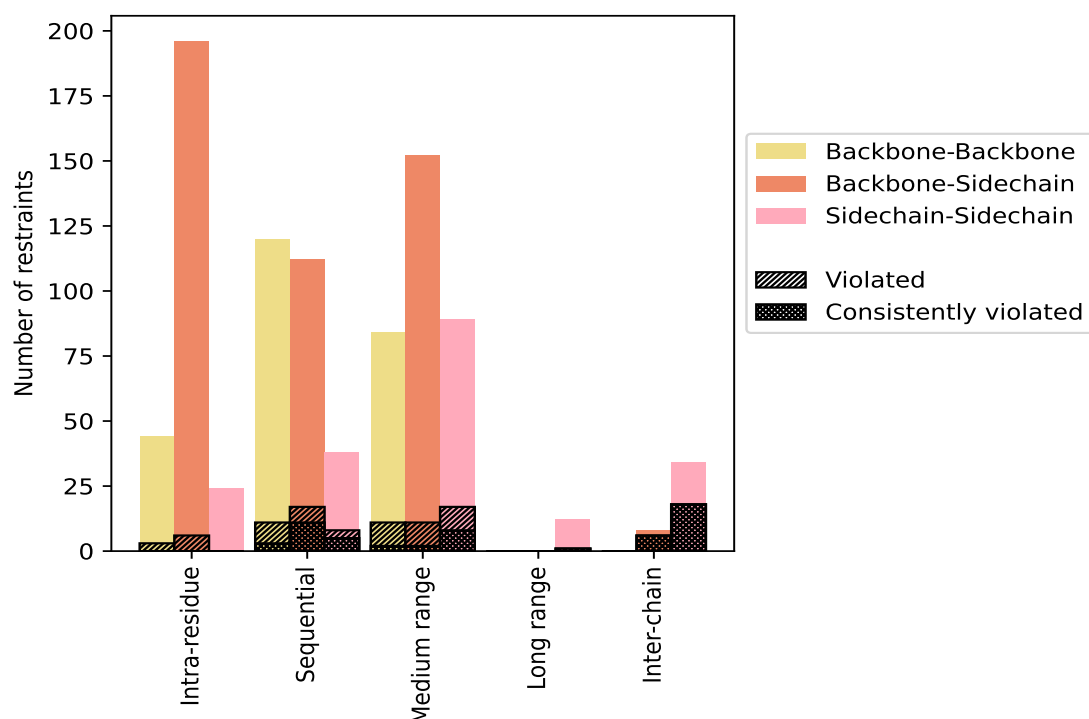
### 9.1 Summary of distance violations ⓘ

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.

| Restraints 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>264</b> | <b>28.9</b>    | <b>9</b>              | <b>3.4</b>     | <b>1.0</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| Backbone-Backbone                                                           | 44         | 4.8            | 3                     | 6.8            | 0.3            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 196        | 21.5           | 6                     | 3.1            | 0.7            | 0                                  | 0.0            | 0.0            |
| Sidechain-Sidechain                                                         | 24         | 2.6            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| <b>Sequential (<math> i-j =1</math>)</b>                                    | <b>270</b> | <b>29.6</b>    | <b>36</b>             | <b>13.3</b>    | <b>3.9</b>     | <b>19</b>                          | <b>7.0</b>     | <b>2.1</b>     |
| Backbone-Backbone                                                           | 120        | 13.1           | 11                    | 9.2            | 1.2            | 3                                  | 2.5            | 0.3            |
| Backbone-Sidechain                                                          | 112        | 12.3           | 17                    | 15.2           | 1.9            | 11                                 | 9.8            | 1.2            |
| Sidechain-Sidechain                                                         | 38         | 4.2            | 8                     | 21.1           | 0.9            | 5                                  | 13.2           | 0.5            |
| <b>Medium range (<math> i-j &gt;1</math> &amp; <math> i-j &lt;5</math>)</b> | <b>325</b> | <b>35.6</b>    | <b>39</b>             | <b>12.0</b>    | <b>4.3</b>     | <b>12</b>                          | <b>3.7</b>     | <b>1.3</b>     |
| Backbone-Backbone                                                           | 84         | 9.2            | 11                    | 13.1           | 1.2            | 2                                  | 2.4            | 0.2            |
| Backbone-Sidechain                                                          | 152        | 16.6           | 11                    | 7.2            | 1.2            | 2                                  | 1.3            | 0.2            |
| Sidechain-Sidechain                                                         | 89         | 9.7            | 17                    | 19.1           | 1.9            | 8                                  | 9.0            | 0.9            |
| <b>Long range (<math> i-j \geq 5</math>)</b>                                | <b>12</b>  | <b>1.3</b>     | <b>1</b>              | <b>8.3</b>     | <b>0.1</b>     | <b>1</b>                           | <b>8.3</b>     | <b>0.1</b>     |
| Backbone-Backbone                                                           | 0          | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 0          | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Sidechain-Sidechain                                                         | 12         | 1.3            | 1                     | 8.3            | 0.1            | 1                                  | 8.3            | 0.1            |
| <b>Inter-chain</b>                                                          | <b>42</b>  | <b>4.6</b>     | <b>24</b>             | <b>57.1</b>    | <b>2.6</b>     | <b>24</b>                          | <b>57.1</b>    | <b>2.6</b>     |
| Backbone-Backbone                                                           | 0          | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 8          | 0.9            | 6                     | 75.0           | 0.7            | 6                                  | 75.0           | 0.7            |
| Sidechain-Sidechain                                                         | 34         | 3.7            | 18                    | 52.9           | 2.0            | 18                                 | 52.9           | 2.0            |
| <b>Hydrogen bond</b>                                                        | <b>0</b>   | <b>0.0</b>     | <b>0</b>              | <b>0.0</b>     | <b>0.0</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| <b>Disulfide bond</b>                                                       | <b>0</b>   | <b>0.0</b>     | <b>0</b>              | <b>0.0</b>     | <b>0.0</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| <b>Total</b>                                                                | <b>913</b> | <b>100.0</b>   | <b>109</b>            | <b>11.9</b>    | <b>11.9</b>    | <b>56</b>                          | <b>6.1</b>     | <b>6.1</b>     |
| Backbone-Backbone                                                           | 248        | 27.2           | 25                    | 10.1           | 2.7            | 5                                  | 2.0            | 0.5            |
| Backbone-Sidechain                                                          | 468        | 51.3           | 40                    | 8.5            | 4.4            | 19                                 | 4.1            | 2.1            |
| Sidechain-Sidechain                                                         | 197        | 21.6           | 44                    | 22.3           | 4.8            | 32                                 | 16.2           | 3.5            |

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

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



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

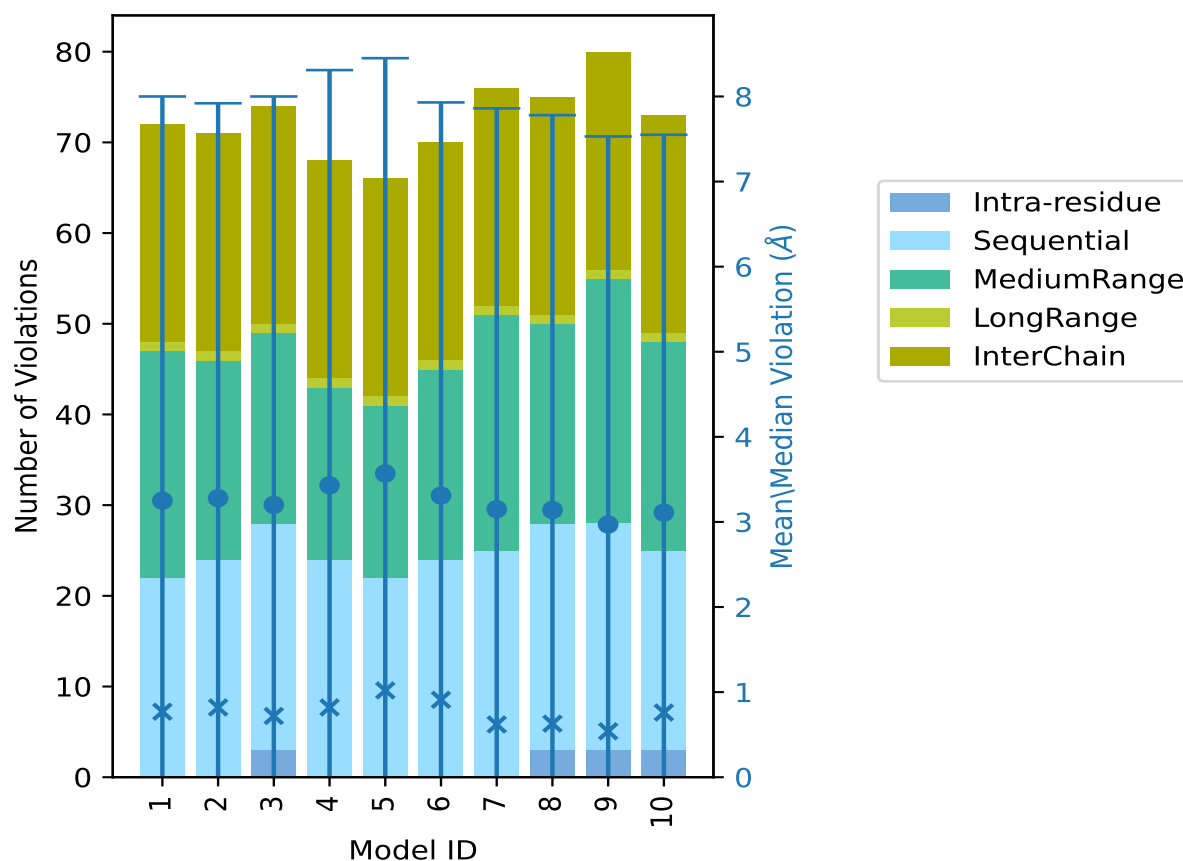
## 9.2 Distance violation statistics for each model [i](#)

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

| Model ID | Number of violations |                 |                 |                 |                 |       | Mean (Å) | Max (Å) | SD <sup>6</sup> (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
|          | IR <sup>1</sup>      | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total |          |         |                     |            |
| 1        | 0                    | 22              | 25              | 1               | 24              | 72    | 3.25     | 19.04   | 4.75                | 0.77       |
| 2        | 0                    | 24              | 22              | 1               | 24              | 71    | 3.28     | 17.65   | 4.64                | 0.82       |
| 3        | 3                    | 25              | 21              | 1               | 24              | 74    | 3.2      | 20.02   | 4.8                 | 0.72       |
| 4        | 0                    | 24              | 19              | 1               | 24              | 68    | 3.43     | 19.44   | 4.88                | 0.82       |
| 5        | 0                    | 22              | 19              | 1               | 24              | 66    | 3.57     | 19.56   | 4.88                | 1.02       |
| 6        | 0                    | 24              | 21              | 1               | 24              | 70    | 3.31     | 17.65   | 4.62                | 0.91       |
| 7        | 0                    | 25              | 26              | 1               | 24              | 76    | 3.15     | 19.02   | 4.71                | 0.62       |
| 8        | 3                    | 25              | 22              | 1               | 24              | 75    | 3.14     | 18.96   | 4.64                | 0.63       |
| 9        | 3                    | 25              | 27              | 1               | 24              | 80    | 2.97     | 19.33   | 4.56                | 0.54       |
| 10       | 3                    | 22              | 23              | 1               | 24              | 73    | 3.11     | 16.15   | 4.44                | 0.76       |

<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, 804(IR:255, SQ:234, MR:286, LR:11, IC:18) 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>       | %    |
| 6                             | 9               | 9               | 0               | 0               | 24    | 1                        | 10.0 |
| 3                             | 2               | 6               | 0               | 0               | 11    | 2                        | 20.0 |
| 0                             | 0               | 2               | 0               | 0               | 2     | 3                        | 30.0 |

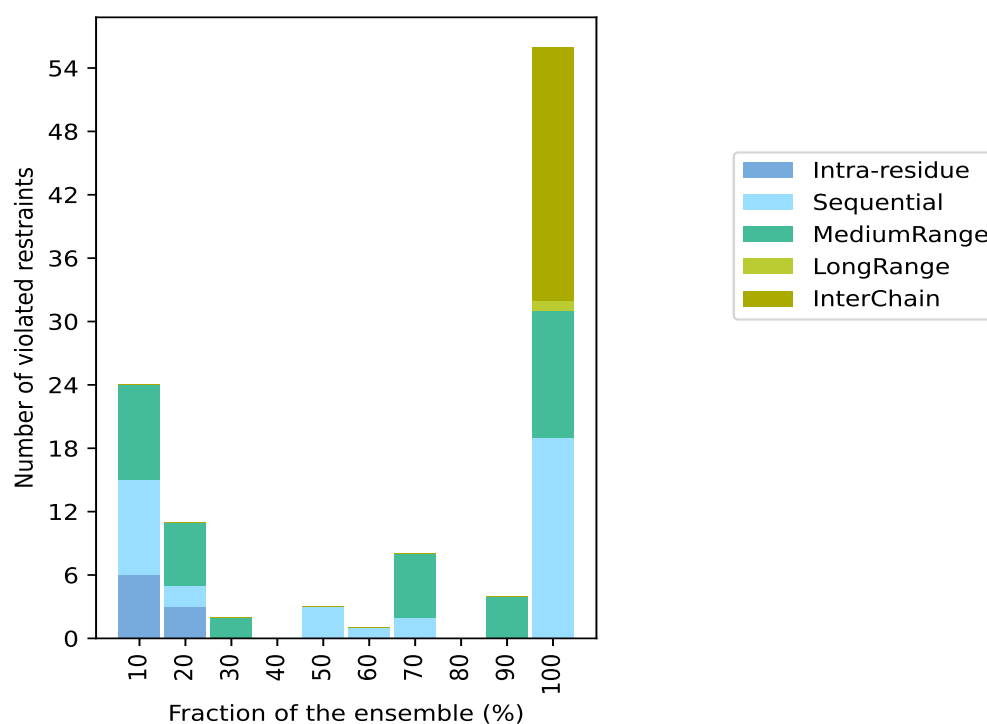
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| Number of violated restraints |                 |                 |                 |                 |       | Fraction of the ensemble |       |
|-------------------------------|-----------------|-----------------|-----------------|-----------------|-------|--------------------------|-------|
| IR <sup>1</sup>               | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total | Count <sup>6</sup>       | %     |
| 0                             | 0               | 0               | 0               | 0               | 0     | 4                        | 40.0  |
| 0                             | 3               | 0               | 0               | 0               | 3     | 5                        | 50.0  |
| 0                             | 1               | 0               | 0               | 0               | 1     | 6                        | 60.0  |
| 0                             | 2               | 6               | 0               | 0               | 8     | 7                        | 70.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 8                        | 80.0  |
| 0                             | 0               | 4               | 0               | 0               | 4     | 9                        | 90.0  |
| 0                             | 19              | 12              | 1               | 24              | 56    | 10                       | 100.0 |

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

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

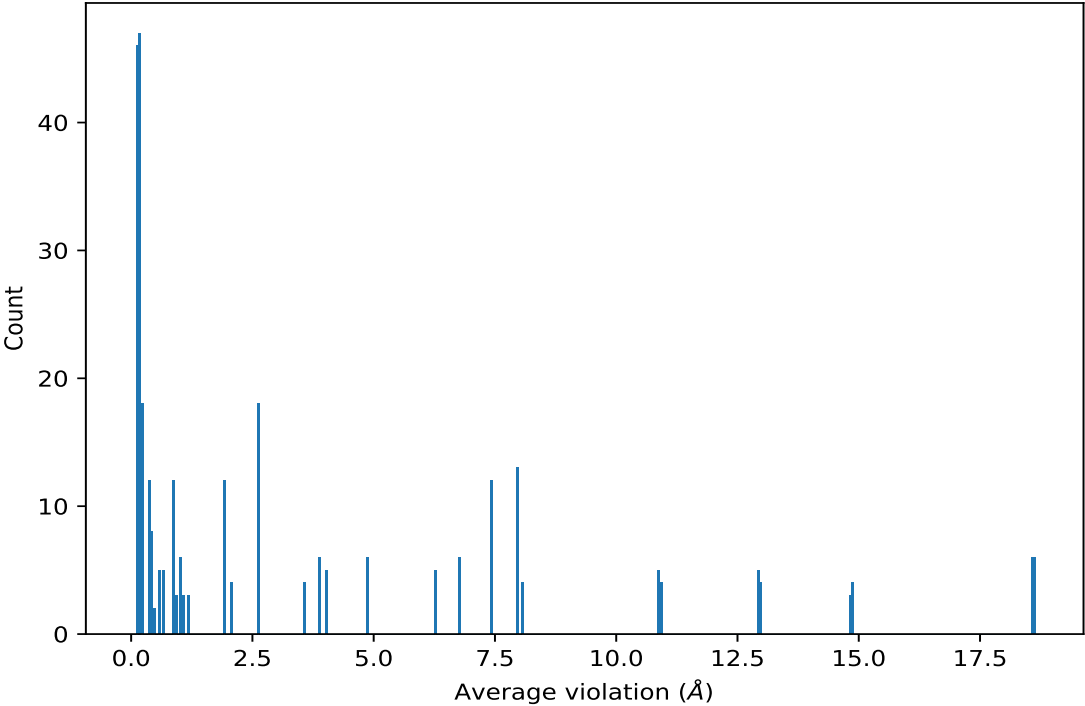


## 9.4 Most violated distance restraints in the ensemble [i](#)

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

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

in the ensemble



9.4.2 Table: Most violated distance restraints ⓘ

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

| Key     | Atom-1          | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,861) | 1:16:A:ILE:HD12 | 1:109:B:PHE:HD2  | 10                  | 18.64    | 1.09                | 18.99      |
| (1,861) | 1:16:A:ILE:HD12 | 1:109:B:PHE:HD1  | 10                  | 18.64    | 1.09                | 18.99      |
| (1,861) | 1:16:A:ILE:HD13 | 1:109:B:PHE:HD1  | 10                  | 18.64    | 1.09                | 18.99      |
| (1,861) | 1:16:A:ILE:HD13 | 1:109:B:PHE:HD2  | 10                  | 18.64    | 1.09                | 18.99      |
| (1,861) | 1:16:A:ILE:HD11 | 1:109:B:PHE:HD2  | 10                  | 18.64    | 1.09                | 18.99      |
| (1,861) | 1:16:A:ILE:HD11 | 1:109:B:PHE:HD1  | 10                  | 18.64    | 1.09                | 18.99      |
| (1,863) | 1:9:A:PHE:HD2   | 1:116:B:ILE:HD12 | 10                  | 18.59    | 1.1                 | 18.98      |
| (1,863) | 1:9:A:PHE:HD1   | 1:116:B:ILE:HD12 | 10                  | 18.59    | 1.1                 | 18.98      |
| (1,863) | 1:9:A:PHE:HD1   | 1:116:B:ILE:HD13 | 10                  | 18.59    | 1.1                 | 18.98      |
| (1,863) | 1:9:A:PHE:HD2   | 1:116:B:ILE:HD13 | 10                  | 18.59    | 1.1                 | 18.98      |
| (1,863) | 1:9:A:PHE:HD2   | 1:116:B:ILE:HD11 | 10                  | 18.59    | 1.1                 | 18.98      |
| (1,863) | 1:9:A:PHE:HD1   | 1:116:B:ILE:HD11 | 10                  | 18.59    | 1.1                 | 18.98      |
| (1,867) | 1:20:A:PHE:HD1  | 1:117:B:LEU:HD23 | 10                  | 14.85    | 0.2                 | 14.88      |
| (1,867) | 1:20:A:PHE:HD1  | 1:117:B:LEU:HD21 | 10                  | 14.85    | 0.2                 | 14.88      |
| (1,867) | 1:20:A:PHE:HD1  | 1:117:B:LEU:HD22 | 10                  | 14.85    | 0.2                 | 14.88      |

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| Key     | Atom-1          | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,867) | 1:20:A:PHE:HD2  | 1:117:B:LEU:HD21 | 10                  | 14.85    | 0.2                 | 14.88      |
| (1,869) | 1:17:A:LEU:HD23 | 1:120:B:PHE:HD1  | 10                  | 14.84    | 0.2                 | 14.83      |
| (1,869) | 1:17:A:LEU:HD21 | 1:120:B:PHE:HD1  | 10                  | 14.84    | 0.2                 | 14.83      |
| (1,869) | 1:17:A:LEU:HD22 | 1:120:B:PHE:HD1  | 10                  | 14.84    | 0.2                 | 14.83      |
| (1,860) | 1:21:A:ILE:HD13 | 1:120:B:PHE:HD1  | 10                  | 12.95    | 0.17                | 12.96      |
| (1,860) | 1:21:A:ILE:HD11 | 1:120:B:PHE:HD1  | 10                  | 12.95    | 0.17                | 12.96      |
| (1,860) | 1:21:A:ILE:HD11 | 1:120:B:PHE:HD2  | 10                  | 12.95    | 0.17                | 12.96      |
| (1,860) | 1:21:A:ILE:HD12 | 1:120:B:PHE:HD1  | 10                  | 12.95    | 0.17                | 12.96      |
| (1,858) | 1:20:A:PHE:HD1  | 1:121:B:ILE:HD13 | 10                  | 12.92    | 0.17                | 12.92      |
| (1,858) | 1:20:A:PHE:HD1  | 1:121:B:ILE:HD11 | 10                  | 12.92    | 0.17                | 12.92      |
| (1,858) | 1:20:A:PHE:HD2  | 1:121:B:ILE:HD11 | 10                  | 12.92    | 0.17                | 12.92      |
| (1,858) | 1:20:A:PHE:HD1  | 1:121:B:ILE:HD12 | 10                  | 12.92    | 0.17                | 12.92      |
| (1,858) | 1:20:A:PHE:HD2  | 1:121:B:ILE:HD13 | 10                  | 12.92    | 0.17                | 12.92      |
| (1,429) | 1:19:A:ILE:HD11 | 1:120:B:PHE:HD2  | 10                  | 10.9     | 0.43                | 10.93      |
| (1,429) | 1:19:A:ILE:HD12 | 1:120:B:PHE:HD2  | 10                  | 10.9     | 0.43                | 10.93      |
| (1,429) | 1:19:A:ILE:HD13 | 1:120:B:PHE:HD2  | 10                  | 10.9     | 0.43                | 10.93      |
| (1,429) | 1:19:A:ILE:HD11 | 1:120:B:PHE:HD1  | 10                  | 10.9     | 0.43                | 10.93      |
| (1,430) | 1:20:A:PHE:HD2  | 1:119:B:ILE:HD11 | 10                  | 10.86    | 0.46                | 10.95      |
| (1,430) | 1:20:A:PHE:HD2  | 1:119:B:ILE:HD12 | 10                  | 10.86    | 0.46                | 10.95      |
| (1,430) | 1:20:A:PHE:HD2  | 1:119:B:ILE:HD13 | 10                  | 10.86    | 0.46                | 10.95      |
| (1,430) | 1:20:A:PHE:HD1  | 1:119:B:ILE:HD12 | 10                  | 10.86    | 0.46                | 10.95      |
| (1,430) | 1:20:A:PHE:HD1  | 1:119:B:ILE:HD11 | 10                  | 10.86    | 0.46                | 10.95      |
| (1,873) | 1:12:A:ILE:HG23 | 1:110:B:PHE:HE1  | 10                  | 8.06     | 0.62                | 8.23       |
| (1,873) | 1:12:A:ILE:HG22 | 1:110:B:PHE:HE1  | 10                  | 8.06     | 0.62                | 8.23       |
| (1,873) | 1:12:A:ILE:HG22 | 1:110:B:PHE:HE2  | 10                  | 8.06     | 0.62                | 8.23       |
| (1,873) | 1:12:A:ILE:HG21 | 1:110:B:PHE:HE1  | 10                  | 8.06     | 0.62                | 8.23       |
| (1,431) | 1:18:A:LEU:HD11 | 1:120:B:PHE:HD2  | 10                  | 7.99     | 0.09                | 7.98       |
| (1,431) | 1:18:A:LEU:HD13 | 1:120:B:PHE:HD2  | 10                  | 7.99     | 0.09                | 7.98       |
| (1,431) | 1:18:A:LEU:HD13 | 1:120:B:PHE:HD1  | 10                  | 7.99     | 0.09                | 7.98       |
| (1,431) | 1:18:A:LEU:HD12 | 1:120:B:PHE:HD2  | 10                  | 7.99     | 0.09                | 7.98       |
| (1,875) | 1:10:A:PHE:HE1  | 1:112:B:ILE:HG23 | 10                  | 7.98     | 0.64                | 8.16       |
| (1,875) | 1:10:A:PHE:HE1  | 1:112:B:ILE:HG22 | 10                  | 7.98     | 0.64                | 8.16       |
| (1,875) | 1:10:A:PHE:HE2  | 1:112:B:ILE:HG22 | 10                  | 7.98     | 0.64                | 8.16       |
| (1,875) | 1:10:A:PHE:HE1  | 1:112:B:ILE:HG21 | 10                  | 7.98     | 0.64                | 8.16       |
| (1,432) | 1:20:A:PHE:HD2  | 1:118:B:LEU:HD11 | 10                  | 7.97     | 0.09                | 7.98       |
| (1,432) | 1:20:A:PHE:HD2  | 1:118:B:LEU:HD13 | 10                  | 7.97     | 0.09                | 7.98       |
| (1,432) | 1:20:A:PHE:HD1  | 1:118:B:LEU:HD13 | 10                  | 7.97     | 0.09                | 7.98       |
| (1,432) | 1:20:A:PHE:HD2  | 1:118:B:LEU:HD12 | 10                  | 7.97     | 0.09                | 7.98       |
| (1,432) | 1:20:A:PHE:HD1  | 1:118:B:LEU:HD12 | 10                  | 7.97     | 0.09                | 7.98       |
| (1,870) | 1:20:A:PHE:HB2  | 1:121:B:ILE:HD11 | 10                  | 7.41     | 0.06                | 7.42       |
| (1,870) | 1:20:A:PHE:HB2  | 1:121:B:ILE:HD12 | 10                  | 7.41     | 0.06                | 7.42       |
| (1,870) | 1:20:A:PHE:HB2  | 1:121:B:ILE:HD13 | 10                  | 7.41     | 0.06                | 7.42       |

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| Key     | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,870) | 1:20:A:PHE:HB3   | 1:121:B:ILE:HD11 | 10                  | 7.41     | 0.06                | 7.42       |
| (1,870) | 1:20:A:PHE:HB3   | 1:121:B:ILE:HD12 | 10                  | 7.41     | 0.06                | 7.42       |
| (1,870) | 1:20:A:PHE:HB3   | 1:121:B:ILE:HD13 | 10                  | 7.41     | 0.06                | 7.42       |
| (1,872) | 1:21:A:ILE:HD11  | 1:120:B:PHE:HB2  | 10                  | 7.41     | 0.1                 | 7.42       |
| (1,872) | 1:21:A:ILE:HD11  | 1:120:B:PHE:HB3  | 10                  | 7.41     | 0.1                 | 7.42       |
| (1,872) | 1:21:A:ILE:HD12  | 1:120:B:PHE:HB2  | 10                  | 7.41     | 0.1                 | 7.42       |
| (1,872) | 1:21:A:ILE:HD12  | 1:120:B:PHE:HB3  | 10                  | 7.41     | 0.1                 | 7.42       |
| (1,872) | 1:21:A:ILE:HD13  | 1:120:B:PHE:HB2  | 10                  | 7.41     | 0.1                 | 7.42       |
| (1,872) | 1:21:A:ILE:HD13  | 1:120:B:PHE:HB3  | 10                  | 7.41     | 0.1                 | 7.42       |
| (1,425) | 1:23:A:ILE:HD12  | 1:120:B:PHE:HD1  | 10                  | 6.78     | 0.36                | 6.72       |
| (1,425) | 1:23:A:ILE:HD13  | 1:120:B:PHE:HD1  | 10                  | 6.78     | 0.36                | 6.72       |
| (1,425) | 1:23:A:ILE:HD11  | 1:120:B:PHE:HD1  | 10                  | 6.78     | 0.36                | 6.72       |
| (1,426) | 1:20:A:PHE:HD1   | 1:123:B:ILE:HD12 | 10                  | 6.76     | 0.57                | 6.6        |
| (1,426) | 1:20:A:PHE:HD1   | 1:123:B:ILE:HD13 | 10                  | 6.76     | 0.57                | 6.6        |
| (1,426) | 1:20:A:PHE:HD1   | 1:123:B:ILE:HD11 | 10                  | 6.76     | 0.57                | 6.6        |
| (1,874) | 1:112:B:ILE:HG22 | 1:110:B:PHE:HD1  | 10                  | 6.29     | 0.43                | 6.44       |
| (1,874) | 1:112:B:ILE:HG21 | 1:110:B:PHE:HD1  | 10                  | 6.29     | 0.43                | 6.44       |
| (1,874) | 1:112:B:ILE:HG21 | 1:110:B:PHE:HD2  | 10                  | 6.29     | 0.43                | 6.44       |
| (1,874) | 1:112:B:ILE:HG23 | 1:110:B:PHE:HD1  | 10                  | 6.29     | 0.43                | 6.44       |
| (1,874) | 1:112:B:ILE:HG22 | 1:110:B:PHE:HD2  | 10                  | 6.29     | 0.43                | 6.44       |
| (1,866) | 1:21:A:ILE:HG21  | 1:120:B:PHE:HA   | 10                  | 4.87     | 0.15                | 4.92       |
| (1,866) | 1:21:A:ILE:HG22  | 1:120:B:PHE:HA   | 10                  | 4.87     | 0.15                | 4.92       |
| (1,866) | 1:21:A:ILE:HG23  | 1:120:B:PHE:HA   | 10                  | 4.87     | 0.15                | 4.92       |
| (1,864) | 1:20:A:PHE:HA    | 1:121:B:ILE:HG21 | 10                  | 4.87     | 0.11                | 4.91       |
| (1,864) | 1:20:A:PHE:HA    | 1:121:B:ILE:HG22 | 10                  | 4.87     | 0.11                | 4.91       |
| (1,864) | 1:20:A:PHE:HA    | 1:121:B:ILE:HG23 | 10                  | 4.87     | 0.11                | 4.91       |
| (1,862) | 1:116:B:ILE:HD13 | 1:109:B:PHE:HE1  | 10                  | 4.0      | 0.55                | 4.25       |
| (1,862) | 1:116:B:ILE:HD13 | 1:109:B:PHE:HD1  | 10                  | 4.0      | 0.55                | 4.25       |
| (1,862) | 1:116:B:ILE:HD11 | 1:109:B:PHE:HE1  | 10                  | 4.0      | 0.55                | 4.25       |
| (1,862) | 1:116:B:ILE:HD11 | 1:109:B:PHE:HD1  | 10                  | 4.0      | 0.55                | 4.25       |
| (1,862) | 1:116:B:ILE:HD12 | 1:109:B:PHE:HE1  | 10                  | 4.0      | 0.55                | 4.25       |
| (1,427) | 1:23:A:ILE:HD11  | 1:120:B:PHE:HA   | 10                  | 3.85     | 0.33                | 3.74       |
| (1,427) | 1:23:A:ILE:HD12  | 1:120:B:PHE:HA   | 10                  | 3.85     | 0.33                | 3.74       |
| (1,427) | 1:23:A:ILE:HD13  | 1:120:B:PHE:HA   | 10                  | 3.85     | 0.33                | 3.74       |
| (1,428) | 1:20:A:PHE:HA    | 1:123:B:ILE:HD11 | 10                  | 3.85     | 0.34                | 3.76       |
| (1,428) | 1:20:A:PHE:HA    | 1:123:B:ILE:HD12 | 10                  | 3.85     | 0.34                | 3.76       |
| (1,428) | 1:20:A:PHE:HA    | 1:123:B:ILE:HD13 | 10                  | 3.85     | 0.34                | 3.76       |
| (1,859) | 1:120:B:PHE:HD2  | 1:121:B:ILE:HD12 | 10                  | 3.56     | 0.73                | 3.26       |
| (1,859) | 1:120:B:PHE:HD2  | 1:121:B:ILE:HD11 | 10                  | 3.56     | 0.73                | 3.26       |
| (1,859) | 1:120:B:PHE:HD1  | 1:121:B:ILE:HD13 | 10                  | 3.56     | 0.73                | 3.26       |
| (1,859) | 1:120:B:PHE:HD1  | 1:121:B:ILE:HD12 | 10                  | 3.56     | 0.73                | 3.26       |
| (1,358) | 1:127:B:ILE:HG21 | 1:129:B:PHE:HD1  | 10                  | 2.62     | 0.02                | 2.61       |

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| Key     | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,358) | 1:127:B:ILE:HG21 | 1:129:B:PHE:HD2  | 10                  | 2.62     | 0.02                | 2.61       |
| (1,358) | 1:127:B:ILE:HG22 | 1:129:B:PHE:HD1  | 10                  | 2.62     | 0.02                | 2.61       |
| (1,358) | 1:127:B:ILE:HG22 | 1:129:B:PHE:HD2  | 10                  | 2.62     | 0.02                | 2.61       |
| (1,358) | 1:127:B:ILE:HG23 | 1:129:B:PHE:HD1  | 10                  | 2.62     | 0.02                | 2.61       |
| (1,358) | 1:127:B:ILE:HG23 | 1:129:B:PHE:HD2  | 10                  | 2.62     | 0.02                | 2.61       |
| (1,357) | 1:27:A:ILE:HG21  | 1:29:A:PHE:HD1   | 10                  | 2.62     | 0.02                | 2.62       |
| (1,357) | 1:27:A:ILE:HG21  | 1:29:A:PHE:HD2   | 10                  | 2.62     | 0.02                | 2.62       |
| (1,357) | 1:27:A:ILE:HG22  | 1:29:A:PHE:HD1   | 10                  | 2.62     | 0.02                | 2.62       |
| (1,357) | 1:27:A:ILE:HG22  | 1:29:A:PHE:HD2   | 10                  | 2.62     | 0.02                | 2.62       |
| (1,357) | 1:27:A:ILE:HG23  | 1:29:A:PHE:HD1   | 10                  | 2.62     | 0.02                | 2.62       |
| (1,357) | 1:27:A:ILE:HG23  | 1:29:A:PHE:HD2   | 10                  | 2.62     | 0.02                | 2.62       |
| (1,792) | 1:27:A:ILE:HG21  | 1:29:A:PHE:HD1   | 10                  | 2.62     | 0.02                | 2.62       |
| (1,792) | 1:27:A:ILE:HG21  | 1:29:A:PHE:HD2   | 10                  | 2.62     | 0.02                | 2.62       |
| (1,792) | 1:27:A:ILE:HG22  | 1:29:A:PHE:HD1   | 10                  | 2.62     | 0.02                | 2.62       |
| (1,792) | 1:27:A:ILE:HG22  | 1:29:A:PHE:HD2   | 10                  | 2.62     | 0.02                | 2.62       |
| (1,792) | 1:27:A:ILE:HG23  | 1:29:A:PHE:HD1   | 10                  | 2.62     | 0.02                | 2.62       |
| (1,792) | 1:27:A:ILE:HG23  | 1:29:A:PHE:HD2   | 10                  | 2.62     | 0.02                | 2.62       |
| (1,868) | 1:120:B:PHE:HD2  | 1:117:B:LEU:HD22 | 10                  | 2.06     | 0.77                | 1.77       |
| (1,868) | 1:120:B:PHE:HD2  | 1:117:B:LEU:HD23 | 10                  | 2.06     | 0.77                | 1.77       |
| (1,868) | 1:120:B:PHE:HD2  | 1:117:B:LEU:HD21 | 10                  | 2.06     | 0.77                | 1.77       |
| (1,868) | 1:120:B:PHE:HD1  | 1:117:B:LEU:HD23 | 10                  | 2.06     | 0.77                | 1.77       |
| (1,793) | 1:127:B:ILE:HG21 | 1:129:B:PHE:HD1  | 10                  | 1.91     | 0.01                | 1.9        |
| (1,793) | 1:127:B:ILE:HG21 | 1:129:B:PHE:HD2  | 10                  | 1.91     | 0.01                | 1.9        |
| (1,793) | 1:127:B:ILE:HG22 | 1:129:B:PHE:HD1  | 10                  | 1.91     | 0.01                | 1.9        |
| (1,793) | 1:127:B:ILE:HG22 | 1:129:B:PHE:HD2  | 10                  | 1.91     | 0.01                | 1.9        |
| (1,793) | 1:127:B:ILE:HG23 | 1:129:B:PHE:HD1  | 10                  | 1.91     | 0.01                | 1.9        |
| (1,793) | 1:127:B:ILE:HG23 | 1:129:B:PHE:HD2  | 10                  | 1.91     | 0.01                | 1.9        |
| (1,793) | 1:127:B:ILE:HG21 | 1:129:B:PHE:HD1  | 10                  | 1.91     | 0.01                | 1.9        |
| (1,793) | 1:127:B:ILE:HG21 | 1:129:B:PHE:HD2  | 10                  | 1.91     | 0.01                | 1.9        |
| (1,793) | 1:127:B:ILE:HG22 | 1:129:B:PHE:HD1  | 10                  | 1.91     | 0.01                | 1.9        |
| (1,793) | 1:127:B:ILE:HG22 | 1:129:B:PHE:HD2  | 10                  | 1.91     | 0.01                | 1.9        |
| (1,793) | 1:127:B:ILE:HG23 | 1:129:B:PHE:HD1  | 10                  | 1.91     | 0.01                | 1.9        |
| (1,793) | 1:127:B:ILE:HG23 | 1:129:B:PHE:HD2  | 10                  | 1.91     | 0.01                | 1.9        |
| (1,865) | 1:120:B:PHE:HA   | 1:121:B:ILE:HG21 | 10                  | 1.17     | 0.01                | 1.17       |
| (1,865) | 1:120:B:PHE:HA   | 1:121:B:ILE:HG22 | 10                  | 1.17     | 0.01                | 1.17       |
| (1,865) | 1:120:B:PHE:HA   | 1:121:B:ILE:HG23 | 10                  | 1.17     | 0.01                | 1.17       |
| (1,364) | 1:124:B:VAL:HA   | 1:125:B:LEU:HD21 | 10                  | 1.06     | 0.16                | 1.1        |
| (1,364) | 1:124:B:VAL:HA   | 1:125:B:LEU:HD22 | 10                  | 1.06     | 0.16                | 1.1        |
| (1,364) | 1:124:B:VAL:HA   | 1:125:B:LEU:HD23 | 10                  | 1.06     | 0.16                | 1.1        |
| (1,363) | 1:24:A:VAL:HA    | 1:25:A:LEU:HD21  | 10                  | 1.04     | 0.17                | 1.06       |
| (1,363) | 1:24:A:VAL:HA    | 1:25:A:LEU:HD22  | 10                  | 1.04     | 0.17                | 1.06       |
| (1,363) | 1:24:A:VAL:HA    | 1:25:A:LEU:HD23  | 10                  | 1.04     | 0.17                | 1.06       |

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| Key     | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,798) | 1:24:A:VAL:HA    | 1:25:A:LEU:HD21  | 10                  | 1.04     | 0.17                | 1.06       |
| (1,798) | 1:24:A:VAL:HA    | 1:25:A:LEU:HD22  | 10                  | 1.04     | 0.17                | 1.06       |
| (1,798) | 1:24:A:VAL:HA    | 1:25:A:LEU:HD23  | 10                  | 1.04     | 0.17                | 1.06       |
| (1,533) | 1:22:A:PHE:HD2   | 1:23:A:ILE:H     | 10                  | 0.94     | 0.25                | 0.82       |
| (1,534) | 1:122:B:PHE:HD2  | 1:123:B:ILE:H    | 10                  | 0.93     | 0.24                | 0.82       |
| (1,535) | 1:122:B:PHE:HD2  | 1:123:B:ILE:H    | 10                  | 0.93     | 0.24                | 0.82       |
| (1,830) | 1:18:A:LEU:HD21  | 1:22:A:PHE:HB2   | 10                  | 0.88     | 0.1                 | 0.88       |
| (1,830) | 1:18:A:LEU:HD21  | 1:22:A:PHE:HB3   | 10                  | 0.88     | 0.1                 | 0.88       |
| (1,830) | 1:18:A:LEU:HD22  | 1:22:A:PHE:HB2   | 10                  | 0.88     | 0.1                 | 0.88       |
| (1,830) | 1:18:A:LEU:HD22  | 1:22:A:PHE:HB3   | 10                  | 0.88     | 0.1                 | 0.88       |
| (1,830) | 1:18:A:LEU:HD23  | 1:22:A:PHE:HB2   | 10                  | 0.88     | 0.1                 | 0.88       |
| (1,830) | 1:18:A:LEU:HD23  | 1:22:A:PHE:HB3   | 10                  | 0.88     | 0.1                 | 0.88       |
| (1,871) | 1:120:B:PHE:HB2  | 1:121:B:ILE:HD11 | 10                  | 0.85     | 0.03                | 0.84       |
| (1,871) | 1:120:B:PHE:HB2  | 1:121:B:ILE:HD12 | 10                  | 0.85     | 0.03                | 0.84       |
| (1,871) | 1:120:B:PHE:HB2  | 1:121:B:ILE:HD13 | 10                  | 0.85     | 0.03                | 0.84       |
| (1,871) | 1:120:B:PHE:HB3  | 1:121:B:ILE:HD11 | 10                  | 0.85     | 0.03                | 0.84       |
| (1,871) | 1:120:B:PHE:HB3  | 1:121:B:ILE:HD12 | 10                  | 0.85     | 0.03                | 0.84       |
| (1,871) | 1:120:B:PHE:HB3  | 1:121:B:ILE:HD13 | 10                  | 0.85     | 0.03                | 0.84       |
| (1,421) | 1:14:A:THR:HG21  | 1:110:B:PHE:HE1  | 10                  | 0.68     | 0.23                | 0.6        |
| (1,421) | 1:14:A:THR:HG22  | 1:110:B:PHE:HE1  | 10                  | 0.68     | 0.23                | 0.6        |
| (1,421) | 1:14:A:THR:HG22  | 1:110:B:PHE:HE2  | 10                  | 0.68     | 0.23                | 0.6        |
| (1,421) | 1:14:A:THR:HG23  | 1:110:B:PHE:HE1  | 10                  | 0.68     | 0.23                | 0.6        |
| (1,421) | 1:14:A:THR:HG23  | 1:110:B:PHE:HE2  | 10                  | 0.68     | 0.23                | 0.6        |
| (1,422) | 1:10:A:PHE:HE1   | 1:114:B:THR:HG21 | 10                  | 0.59     | 0.07                | 0.57       |
| (1,422) | 1:10:A:PHE:HE1   | 1:114:B:THR:HG22 | 10                  | 0.59     | 0.07                | 0.57       |
| (1,422) | 1:10:A:PHE:HE2   | 1:114:B:THR:HG22 | 10                  | 0.59     | 0.07                | 0.57       |
| (1,422) | 1:10:A:PHE:HE2   | 1:114:B:THR:HG23 | 10                  | 0.59     | 0.07                | 0.57       |
| (1,422) | 1:10:A:PHE:HE1   | 1:114:B:THR:HG23 | 10                  | 0.59     | 0.07                | 0.57       |
| (2,4)   | 1:127:B:ILE:HA   | 1:131:B:GLY:H    | 10                  | 0.45     | 0.01                | 0.45       |
| (2,4)   | 1:127:B:ILE:HA   | 1:131:B:GLY:H    | 10                  | 0.45     | 0.01                | 0.45       |
| (1,799) | 1:124:B:VAL:HA   | 1:125:B:LEU:HD21 | 10                  | 0.43     | 0.14                | 0.46       |
| (1,799) | 1:124:B:VAL:HA   | 1:125:B:LEU:HD22 | 10                  | 0.43     | 0.14                | 0.46       |
| (1,799) | 1:124:B:VAL:HA   | 1:125:B:LEU:HD23 | 10                  | 0.43     | 0.14                | 0.46       |
| (1,799) | 1:124:B:VAL:HA   | 1:125:B:LEU:HD21 | 10                  | 0.43     | 0.14                | 0.46       |
| (1,799) | 1:124:B:VAL:HA   | 1:125:B:LEU:HD22 | 10                  | 0.43     | 0.14                | 0.46       |
| (1,799) | 1:124:B:VAL:HA   | 1:125:B:LEU:HD23 | 10                  | 0.43     | 0.14                | 0.46       |
| (3,4)   | 1:129:B:PHE:HA   | 1:132:B:TRP:H    | 10                  | 0.4      | 0.0                 | 0.4        |
| (3,4)   | 1:129:B:PHE:HA   | 1:132:B:TRP:H    | 10                  | 0.4      | 0.0                 | 0.4        |
| (1,831) | 1:118:B:LEU:HD21 | 1:122:B:PHE:HB2  | 10                  | 0.38     | 0.09                | 0.34       |
| (1,831) | 1:118:B:LEU:HD21 | 1:122:B:PHE:HB3  | 10                  | 0.38     | 0.09                | 0.34       |
| (1,831) | 1:118:B:LEU:HD22 | 1:122:B:PHE:HB2  | 10                  | 0.38     | 0.09                | 0.34       |
| (1,831) | 1:118:B:LEU:HD22 | 1:122:B:PHE:HB3  | 10                  | 0.38     | 0.09                | 0.34       |

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| Key     | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,831) | 1:118:B:LEU:HD23 | 1:122:B:PHE:HB2  | 10                  | 0.38     | 0.09                | 0.34       |
| (1,831) | 1:118:B:LEU:HD23 | 1:122:B:PHE:HB3  | 10                  | 0.38     | 0.09                | 0.34       |
| (1,831) | 1:118:B:LEU:HD21 | 1:122:B:PHE:HB2  | 10                  | 0.38     | 0.09                | 0.34       |
| (1,831) | 1:118:B:LEU:HD21 | 1:122:B:PHE:HB3  | 10                  | 0.38     | 0.09                | 0.34       |
| (1,831) | 1:118:B:LEU:HD22 | 1:122:B:PHE:HB2  | 10                  | 0.38     | 0.09                | 0.34       |
| (1,831) | 1:118:B:LEU:HD22 | 1:122:B:PHE:HB3  | 10                  | 0.38     | 0.09                | 0.34       |
| (1,831) | 1:118:B:LEU:HD23 | 1:122:B:PHE:HB2  | 10                  | 0.38     | 0.09                | 0.34       |
| (1,831) | 1:118:B:LEU:HD23 | 1:122:B:PHE:HB3  | 10                  | 0.38     | 0.09                | 0.34       |
| (1,436) | 1:18:A:LEU:HA    | 1:118:B:LEU:HD11 | 10                  | 0.24     | 0.02                | 0.24       |
| (1,436) | 1:18:A:LEU:HA    | 1:118:B:LEU:HD12 | 10                  | 0.24     | 0.02                | 0.24       |
| (1,436) | 1:18:A:LEU:HA    | 1:118:B:LEU:HD13 | 10                  | 0.24     | 0.02                | 0.24       |
| (1,436) | 1:18:A:LEU:HA    | 1:118:B:LEU:HD21 | 10                  | 0.24     | 0.02                | 0.24       |
| (1,436) | 1:18:A:LEU:HA    | 1:118:B:LEU:HD22 | 10                  | 0.24     | 0.02                | 0.24       |
| (1,436) | 1:18:A:LEU:HA    | 1:118:B:LEU:HD23 | 10                  | 0.24     | 0.02                | 0.24       |
| (1,435) | 1:18:A:LEU:HD11  | 1:118:B:LEU:HA   | 10                  | 0.23     | 0.02                | 0.23       |
| (1,435) | 1:18:A:LEU:HD12  | 1:118:B:LEU:HA   | 10                  | 0.23     | 0.02                | 0.23       |
| (1,435) | 1:18:A:LEU:HD13  | 1:118:B:LEU:HA   | 10                  | 0.23     | 0.02                | 0.23       |
| (1,435) | 1:18:A:LEU:HD21  | 1:118:B:LEU:HA   | 10                  | 0.23     | 0.02                | 0.23       |
| (1,435) | 1:18:A:LEU:HD22  | 1:118:B:LEU:HA   | 10                  | 0.23     | 0.02                | 0.23       |
| (1,435) | 1:18:A:LEU:HD23  | 1:118:B:LEU:HA   | 10                  | 0.23     | 0.02                | 0.23       |
| (1,416) | 1:121:B:ILE:HG21 | 1:122:B:PHE:HB2  | 10                  | 0.19     | 0.02                | 0.18       |
| (1,416) | 1:121:B:ILE:HG21 | 1:122:B:PHE:HB3  | 10                  | 0.19     | 0.02                | 0.18       |
| (1,416) | 1:121:B:ILE:HG22 | 1:122:B:PHE:HB2  | 10                  | 0.19     | 0.02                | 0.18       |
| (1,416) | 1:121:B:ILE:HG22 | 1:122:B:PHE:HB3  | 10                  | 0.19     | 0.02                | 0.18       |
| (1,416) | 1:121:B:ILE:HG23 | 1:122:B:PHE:HB2  | 10                  | 0.19     | 0.02                | 0.18       |
| (1,416) | 1:121:B:ILE:HG23 | 1:122:B:PHE:HB3  | 10                  | 0.19     | 0.02                | 0.18       |
| (1,415) | 1:21:A:ILE:HG21  | 1:22:A:PHE:HB2   | 10                  | 0.19     | 0.02                | 0.18       |
| (1,415) | 1:21:A:ILE:HG21  | 1:22:A:PHE:HB3   | 10                  | 0.19     | 0.02                | 0.18       |
| (1,415) | 1:21:A:ILE:HG22  | 1:22:A:PHE:HB2   | 10                  | 0.19     | 0.02                | 0.18       |
| (1,415) | 1:21:A:ILE:HG22  | 1:22:A:PHE:HB3   | 10                  | 0.19     | 0.02                | 0.18       |
| (1,415) | 1:21:A:ILE:HG23  | 1:22:A:PHE:HB2   | 10                  | 0.19     | 0.02                | 0.18       |
| (1,415) | 1:21:A:ILE:HG23  | 1:22:A:PHE:HB3   | 10                  | 0.19     | 0.02                | 0.18       |
| (1,852) | 1:21:A:ILE:HG21  | 1:22:A:PHE:HB2   | 10                  | 0.19     | 0.02                | 0.18       |
| (1,852) | 1:21:A:ILE:HG21  | 1:22:A:PHE:HB3   | 10                  | 0.19     | 0.02                | 0.18       |
| (1,852) | 1:21:A:ILE:HG22  | 1:22:A:PHE:HB2   | 10                  | 0.19     | 0.02                | 0.18       |
| (1,852) | 1:21:A:ILE:HG22  | 1:22:A:PHE:HB3   | 10                  | 0.19     | 0.02                | 0.18       |
| (1,852) | 1:21:A:ILE:HG23  | 1:22:A:PHE:HB2   | 10                  | 0.19     | 0.02                | 0.18       |
| (1,852) | 1:21:A:ILE:HG23  | 1:22:A:PHE:HB3   | 10                  | 0.19     | 0.02                | 0.18       |
| (1,253) | 1:17:A:LEU:HA    | 1:20:A:PHE:HB2   | 10                  | 0.14     | 0.03                | 0.14       |
| (1,253) | 1:17:A:LEU:HA    | 1:20:A:PHE:HB3   | 10                  | 0.14     | 0.03                | 0.14       |
| (1,692) | 1:17:A:LEU:HA    | 1:20:A:PHE:HB2   | 10                  | 0.14     | 0.03                | 0.14       |
| (1,692) | 1:17:A:LEU:HA    | 1:20:A:PHE:HB3   | 10                  | 0.14     | 0.03                | 0.14       |

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| Key     | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,155) | 1:31:A:GLY:HA3   | 1:32:A:TRP:H     | 10                  | 0.11     | 0.01                | 0.11       |
| (1,594) | 1:31:A:GLY:HA3   | 1:32:A:TRP:H     | 10                  | 0.11     | 0.01                | 0.11       |
| (1,277) | 1:4:A:ALA:HA     | 1:5:A:PRO:HD2    | 10                  | 0.11     | 0.0                 | 0.11       |
| (1,277) | 1:4:A:ALA:HA     | 1:5:A:PRO:HD3    | 10                  | 0.11     | 0.0                 | 0.11       |
| (1,278) | 1:104:B:ALA:HA   | 1:105:B:PRO:HD2  | 10                  | 0.11     | 0.0                 | 0.11       |
| (1,278) | 1:104:B:ALA:HA   | 1:105:B:PRO:HD3  | 10                  | 0.11     | 0.0                 | 0.11       |
| (1,716) | 1:4:A:ALA:HA     | 1:5:A:PRO:HD2    | 10                  | 0.11     | 0.0                 | 0.11       |
| (1,716) | 1:4:A:ALA:HA     | 1:5:A:PRO:HD3    | 10                  | 0.11     | 0.0                 | 0.11       |
| (1,156) | 1:131:B:GLY:HA3  | 1:132:B:TRP:H    | 10                  | 0.11     | 0.01                | 0.11       |
| (1,369) | 1:20:A:PHE:HA    | 1:23:A:ILE:HD11  | 9                   | 0.17     | 0.05                | 0.15       |
| (1,369) | 1:20:A:PHE:HA    | 1:23:A:ILE:HD12  | 9                   | 0.17     | 0.05                | 0.15       |
| (1,369) | 1:20:A:PHE:HA    | 1:23:A:ILE:HD13  | 9                   | 0.17     | 0.05                | 0.15       |
| (1,804) | 1:20:A:PHE:HA    | 1:23:A:ILE:HD11  | 9                   | 0.17     | 0.05                | 0.15       |
| (1,804) | 1:20:A:PHE:HA    | 1:23:A:ILE:HD12  | 9                   | 0.17     | 0.05                | 0.15       |
| (1,804) | 1:20:A:PHE:HA    | 1:23:A:ILE:HD13  | 9                   | 0.17     | 0.05                | 0.15       |
| (1,370) | 1:120:B:PHE:HA   | 1:123:B:ILE:HD11 | 9                   | 0.17     | 0.03                | 0.18       |
| (1,370) | 1:120:B:PHE:HA   | 1:123:B:ILE:HD12 | 9                   | 0.17     | 0.03                | 0.18       |
| (1,370) | 1:120:B:PHE:HA   | 1:123:B:ILE:HD13 | 9                   | 0.17     | 0.03                | 0.18       |
| (1,254) | 1:117:B:LEU:HA   | 1:120:B:PHE:HB2  | 9                   | 0.14     | 0.03                | 0.13       |
| (1,254) | 1:117:B:LEU:HA   | 1:120:B:PHE:HB3  | 9                   | 0.14     | 0.03                | 0.13       |
| (1,241) | 1:19:A:ILE:HA    | 1:22:A:PHE:H     | 7                   | 0.15     | 0.02                | 0.15       |
| (1,242) | 1:119:B:ILE:HA   | 1:122:B:PHE:H    | 7                   | 0.15     | 0.02                | 0.15       |
| (1,680) | 1:19:A:ILE:HA    | 1:22:A:PHE:H     | 7                   | 0.15     | 0.02                | 0.15       |
| (1,355) | 1:27:A:ILE:HG21  | 1:28:A:HIS:HB2   | 7                   | 0.14     | 0.03                | 0.16       |
| (1,355) | 1:27:A:ILE:HG22  | 1:28:A:HIS:HB2   | 7                   | 0.14     | 0.03                | 0.16       |
| (1,355) | 1:27:A:ILE:HG23  | 1:28:A:HIS:HB2   | 7                   | 0.14     | 0.03                | 0.16       |
| (1,790) | 1:27:A:ILE:HG21  | 1:28:A:HIS:HB2   | 7                   | 0.14     | 0.03                | 0.16       |
| (1,790) | 1:27:A:ILE:HG22  | 1:28:A:HIS:HB2   | 7                   | 0.14     | 0.03                | 0.16       |
| (1,790) | 1:27:A:ILE:HG23  | 1:28:A:HIS:HB2   | 7                   | 0.14     | 0.03                | 0.16       |
| (1,113) | 1:26:A:LEU:HA    | 1:29:A:PHE:H     | 7                   | 0.12     | 0.01                | 0.12       |
| (1,114) | 1:126:B:LEU:HA   | 1:129:B:PHE:H    | 7                   | 0.12     | 0.01                | 0.12       |
| (1,552) | 1:26:A:LEU:HA    | 1:29:A:PHE:H     | 7                   | 0.12     | 0.01                | 0.12       |
| (1,190) | 1:132:B:TRP:HB2  | 1:133:B:ARG:H    | 6                   | 0.22     | 0.08                | 0.26       |
| (1,190) | 1:132:B:TRP:HB3  | 1:133:B:ARG:H    | 6                   | 0.22     | 0.08                | 0.26       |
| (1,189) | 1:32:A:TRP:HB2   | 1:33:A:ARG:H     | 5                   | 0.22     | 0.06                | 0.25       |
| (1,189) | 1:32:A:TRP:HB3   | 1:33:A:ARG:H     | 5                   | 0.22     | 0.06                | 0.25       |
| (1,628) | 1:32:A:TRP:HB2   | 1:33:A:ARG:H     | 5                   | 0.22     | 0.06                | 0.25       |
| (1,628) | 1:32:A:TRP:HB3   | 1:33:A:ARG:H     | 5                   | 0.22     | 0.06                | 0.25       |
| (1,356) | 1:127:B:ILE:HG21 | 1:128:B:HIS:HB2  | 5                   | 0.15     | 0.02                | 0.16       |
| (1,356) | 1:127:B:ILE:HG22 | 1:128:B:HIS:HB2  | 5                   | 0.15     | 0.02                | 0.16       |
| (1,356) | 1:127:B:ILE:HG23 | 1:128:B:HIS:HB2  | 5                   | 0.15     | 0.02                | 0.16       |
| (1,343) | 1:25:A:LEU:HD11  | 1:29:A:PHE:HD1   | 3                   | 0.13     | 0.01                | 0.13       |

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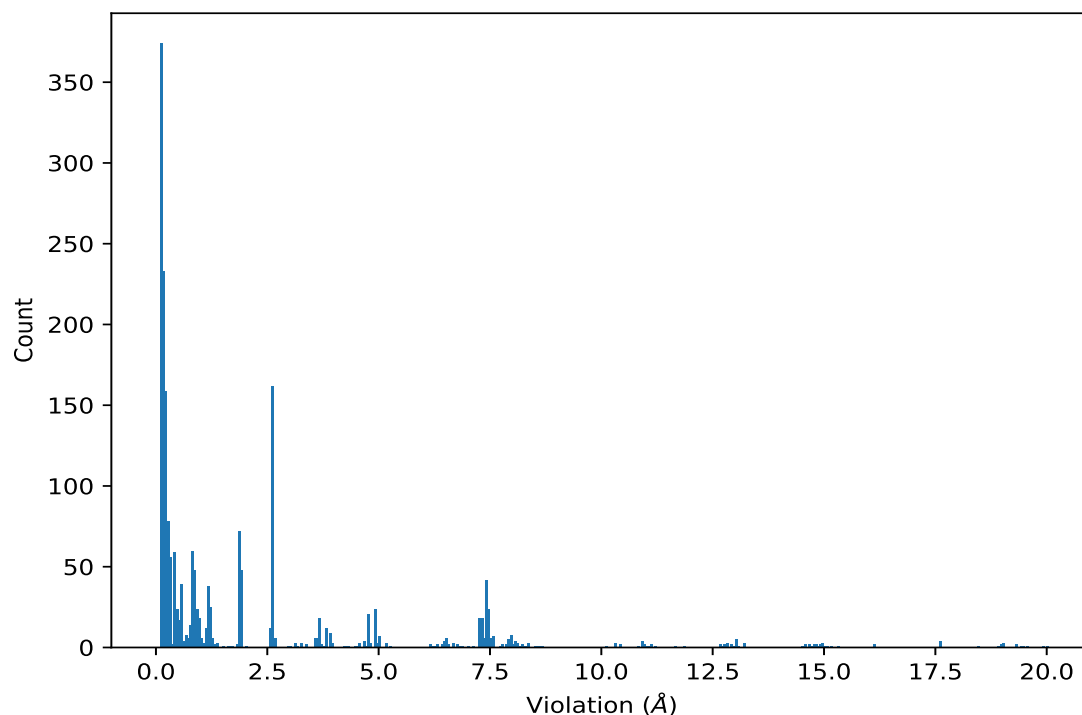
| Key     | Atom-1           | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (1,343) | 1:25:A:LEU:HD11  | 1:29:A:PHE:HD2  | 3                   | 0.13     | 0.01                | 0.13       |
| (1,343) | 1:25:A:LEU:HD12  | 1:29:A:PHE:HD1  | 3                   | 0.13     | 0.01                | 0.13       |
| (1,343) | 1:25:A:LEU:HD12  | 1:29:A:PHE:HD2  | 3                   | 0.13     | 0.01                | 0.13       |
| (1,343) | 1:25:A:LEU:HD13  | 1:29:A:PHE:HD1  | 3                   | 0.13     | 0.01                | 0.13       |
| (1,343) | 1:25:A:LEU:HD13  | 1:29:A:PHE:HD2  | 3                   | 0.13     | 0.01                | 0.13       |
| (1,778) | 1:25:A:LEU:HD11  | 1:29:A:PHE:HD1  | 3                   | 0.13     | 0.01                | 0.13       |
| (1,778) | 1:25:A:LEU:HD11  | 1:29:A:PHE:HD2  | 3                   | 0.13     | 0.01                | 0.13       |
| (1,778) | 1:25:A:LEU:HD12  | 1:29:A:PHE:HD1  | 3                   | 0.13     | 0.01                | 0.13       |
| (1,778) | 1:25:A:LEU:HD12  | 1:29:A:PHE:HD2  | 3                   | 0.13     | 0.01                | 0.13       |
| (1,778) | 1:25:A:LEU:HD13  | 1:29:A:PHE:HD1  | 3                   | 0.13     | 0.01                | 0.13       |
| (1,778) | 1:25:A:LEU:HD13  | 1:29:A:PHE:HD2  | 3                   | 0.13     | 0.01                | 0.13       |
| (1,225) | 1:34:A:ILE:H     | 1:34:A:ILE:HA   | 2                   | 0.16     | 0.01                | 0.16       |
| (1,664) | 1:34:A:ILE:H     | 1:34:A:ILE:HA   | 2                   | 0.16     | 0.01                | 0.16       |
| (1,375) | 1:20:A:PHE:HD1   | 1:23:A:ILE:HG21 | 2                   | 0.15     | 0.0                 | 0.15       |
| (1,375) | 1:20:A:PHE:HD1   | 1:23:A:ILE:HG22 | 2                   | 0.15     | 0.0                 | 0.15       |
| (1,375) | 1:20:A:PHE:HD1   | 1:23:A:ILE:HG23 | 2                   | 0.15     | 0.0                 | 0.15       |
| (1,375) | 1:20:A:PHE:HD2   | 1:23:A:ILE:HG21 | 2                   | 0.15     | 0.0                 | 0.15       |
| (1,375) | 1:20:A:PHE:HD2   | 1:23:A:ILE:HG22 | 2                   | 0.15     | 0.0                 | 0.15       |
| (1,375) | 1:20:A:PHE:HD2   | 1:23:A:ILE:HG23 | 2                   | 0.15     | 0.0                 | 0.15       |
| (1,810) | 1:20:A:PHE:HD1   | 1:23:A:ILE:HG21 | 2                   | 0.15     | 0.0                 | 0.15       |
| (1,810) | 1:20:A:PHE:HD1   | 1:23:A:ILE:HG22 | 2                   | 0.15     | 0.0                 | 0.15       |
| (1,810) | 1:20:A:PHE:HD1   | 1:23:A:ILE:HG23 | 2                   | 0.15     | 0.0                 | 0.15       |
| (1,810) | 1:20:A:PHE:HD2   | 1:23:A:ILE:HG21 | 2                   | 0.15     | 0.0                 | 0.15       |
| (1,810) | 1:20:A:PHE:HD2   | 1:23:A:ILE:HG22 | 2                   | 0.15     | 0.0                 | 0.15       |
| (1,810) | 1:20:A:PHE:HD2   | 1:23:A:ILE:HG23 | 2                   | 0.15     | 0.0                 | 0.15       |
| (1,226) | 1:134:B:ILE:H    | 1:134:B:ILE:HA  | 2                   | 0.14     | 0.03                | 0.14       |
| (1,273) | 1:26:A:LEU:HA    | 1:30:A:GLU:H    | 2                   | 0.12     | 0.02                | 0.12       |
| (1,274) | 1:126:B:LEU:HA   | 1:130:B:GLU:H   | 2                   | 0.12     | 0.02                | 0.12       |
| (1,712) | 1:26:A:LEU:HA    | 1:30:A:GLU:H    | 2                   | 0.12     | 0.02                | 0.12       |
| (1,344) | 1:125:B:LEU:HD11 | 1:129:B:PHE:HD1 | 2                   | 0.12     | 0.01                | 0.12       |
| (1,344) | 1:125:B:LEU:HD11 | 1:129:B:PHE:HD2 | 2                   | 0.12     | 0.01                | 0.12       |
| (1,344) | 1:125:B:LEU:HD12 | 1:129:B:PHE:HD1 | 2                   | 0.12     | 0.01                | 0.12       |
| (1,344) | 1:125:B:LEU:HD12 | 1:129:B:PHE:HD2 | 2                   | 0.12     | 0.01                | 0.12       |
| (1,344) | 1:125:B:LEU:HD13 | 1:129:B:PHE:HD1 | 2                   | 0.12     | 0.01                | 0.12       |
| (1,344) | 1:125:B:LEU:HD13 | 1:129:B:PHE:HD2 | 2                   | 0.12     | 0.01                | 0.12       |

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

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

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

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



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

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

| Key     | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (1,861) | 1:16:A:ILE:HD13 | 1:109:B:PHE:HD1  | 3        | 20.02         |
| (1,863) | 1:9:A:PHE:HD1   | 1:116:B:ILE:HD13 | 3        | 19.93         |
| (1,863) | 1:9:A:PHE:HD2   | 1:116:B:ILE:HD11 | 5        | 19.56         |
| (1,861) | 1:16:A:ILE:HD11 | 1:109:B:PHE:HD2  | 5        | 19.49         |
| (1,861) | 1:16:A:ILE:HD13 | 1:109:B:PHE:HD2  | 4        | 19.44         |
| (1,863) | 1:9:A:PHE:HD1   | 1:116:B:ILE:HD11 | 9        | 19.33         |
| (1,863) | 1:9:A:PHE:HD2   | 1:116:B:ILE:HD13 | 4        | 19.31         |
| (1,863) | 1:9:A:PHE:HD2   | 1:116:B:ILE:HD12 | 1        | 19.04         |
| (1,861) | 1:16:A:ILE:HD12 | 1:109:B:PHE:HD2  | 1        | 19.03         |
| (1,861) | 1:16:A:ILE:HD11 | 1:109:B:PHE:HD2  | 7        | 19.02         |

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| Key     | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (1,861) | 1:16:A:ILE:HD13 | 1:109:B:PHE:HD2  | 8        | 18.96         |
| (1,861) | 1:16:A:ILE:HD11 | 1:109:B:PHE:HD1  | 9        | 18.95         |
| (1,863) | 1:9:A:PHE:HD2   | 1:116:B:ILE:HD11 | 7        | 18.92         |
| (1,863) | 1:9:A:PHE:HD2   | 1:116:B:ILE:HD13 | 8        | 18.46         |
| (1,861) | 1:16:A:ILE:HD12 | 1:109:B:PHE:HD1  | 2        | 17.65         |
| (1,861) | 1:16:A:ILE:HD13 | 1:109:B:PHE:HD2  | 6        | 17.65         |
| (1,863) | 1:9:A:PHE:HD2   | 1:116:B:ILE:HD13 | 6        | 17.64         |
| (1,863) | 1:9:A:PHE:HD1   | 1:116:B:ILE:HD12 | 2        | 17.6          |
| (1,861) | 1:16:A:ILE:HD11 | 1:109:B:PHE:HD1  | 10       | 16.15         |
| (1,863) | 1:9:A:PHE:HD1   | 1:116:B:ILE:HD11 | 10       | 16.13         |
| (1,869) | 1:17:A:LEU:HD23 | 1:120:B:PHE:HD1  | 7        | 15.3          |
| (1,867) | 1:20:A:PHE:HD1  | 1:117:B:LEU:HD23 | 7        | 15.15         |
| (1,867) | 1:20:A:PHE:HD2  | 1:117:B:LEU:HD21 | 10       | 15.08         |
| (1,867) | 1:20:A:PHE:HD1  | 1:117:B:LEU:HD21 | 2        | 15.0          |
| (1,869) | 1:17:A:LEU:HD21 | 1:120:B:PHE:HD1  | 2        | 14.96         |
| (1,869) | 1:17:A:LEU:HD23 | 1:120:B:PHE:HD1  | 4        | 14.96         |
| (1,867) | 1:20:A:PHE:HD2  | 1:117:B:LEU:HD21 | 6        | 14.96         |
| (1,867) | 1:20:A:PHE:HD1  | 1:117:B:LEU:HD23 | 4        | 14.95         |
| (1,869) | 1:17:A:LEU:HD21 | 1:120:B:PHE:HD1  | 10       | 14.9          |
| (1,869) | 1:17:A:LEU:HD22 | 1:120:B:PHE:HD1  | 3        | 14.86         |
| (1,869) | 1:17:A:LEU:HD23 | 1:120:B:PHE:HD1  | 1        | 14.8          |
| (1,867) | 1:20:A:PHE:HD1  | 1:117:B:LEU:HD23 | 1        | 14.8          |
| (1,867) | 1:20:A:PHE:HD1  | 1:117:B:LEU:HD22 | 3        | 14.77         |
| (1,869) | 1:17:A:LEU:HD21 | 1:120:B:PHE:HD1  | 6        | 14.75         |
| (1,867) | 1:20:A:PHE:HD1  | 1:117:B:LEU:HD23 | 8        | 14.74         |
| (1,869) | 1:17:A:LEU:HD22 | 1:120:B:PHE:HD1  | 9        | 14.7          |
| (1,869) | 1:17:A:LEU:HD23 | 1:120:B:PHE:HD1  | 8        | 14.66         |
| (1,867) | 1:20:A:PHE:HD1  | 1:117:B:LEU:HD22 | 5        | 14.57         |
| (1,869) | 1:17:A:LEU:HD22 | 1:120:B:PHE:HD1  | 5        | 14.55         |
| (1,867) | 1:20:A:PHE:HD1  | 1:117:B:LEU:HD22 | 9        | 14.51         |
| (1,860) | 1:21:A:ILE:HD11 | 1:120:B:PHE:HD1  | 4        | 13.23         |
| (1,858) | 1:20:A:PHE:HD1  | 1:121:B:ILE:HD11 | 4        | 13.23         |
| (1,860) | 1:21:A:ILE:HD12 | 1:120:B:PHE:HD1  | 9        | 13.21         |
| (1,858) | 1:20:A:PHE:HD1  | 1:121:B:ILE:HD13 | 2        | 13.05         |
| (1,860) | 1:21:A:ILE:HD11 | 1:120:B:PHE:HD1  | 3        | 13.03         |
| (1,858) | 1:20:A:PHE:HD1  | 1:121:B:ILE:HD11 | 3        | 13.02         |
| (1,860) | 1:21:A:ILE:HD13 | 1:120:B:PHE:HD1  | 1        | 13.01         |
| (1,858) | 1:20:A:PHE:HD1  | 1:121:B:ILE:HD13 | 1        | 13.01         |
| (1,858) | 1:20:A:PHE:HD1  | 1:121:B:ILE:HD11 | 8        | 13.01         |
| (1,860) | 1:21:A:ILE:HD13 | 1:120:B:PHE:HD1  | 2        | 12.98         |
| (1,860) | 1:21:A:ILE:HD11 | 1:120:B:PHE:HD1  | 8        | 12.95         |
| (1,860) | 1:21:A:ILE:HD13 | 1:120:B:PHE:HD1  | 10       | 12.92         |

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| Key     | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (1,858) | 1:20:A:PHE:HD2  | 1:121:B:ILE:HD13 | 10       | 12.84         |
| (1,858) | 1:20:A:PHE:HD1  | 1:121:B:ILE:HD13 | 5        | 12.82         |
| (1,858) | 1:20:A:PHE:HD1  | 1:121:B:ILE:HD12 | 9        | 12.8          |
| (1,860) | 1:21:A:ILE:HD13 | 1:120:B:PHE:HD1  | 5        | 12.77         |
| (1,860) | 1:21:A:ILE:HD11 | 1:120:B:PHE:HD1  | 6        | 12.75         |
| (1,858) | 1:20:A:PHE:HD2  | 1:121:B:ILE:HD11 | 6        | 12.74         |
| (1,860) | 1:21:A:ILE:HD11 | 1:120:B:PHE:HD2  | 7        | 12.69         |
| (1,858) | 1:20:A:PHE:HD1  | 1:121:B:ILE:HD11 | 7        | 12.65         |
| (1,429) | 1:19:A:ILE:HD11 | 1:120:B:PHE:HD1  | 7        | 11.87         |
| (1,430) | 1:20:A:PHE:HD2  | 1:119:B:ILE:HD11 | 7        | 11.7          |
| (1,430) | 1:20:A:PHE:HD2  | 1:119:B:ILE:HD13 | 5        | 11.24         |
| (1,430) | 1:20:A:PHE:HD2  | 1:119:B:ILE:HD12 | 2        | 11.13         |
| (1,429) | 1:19:A:ILE:HD13 | 1:120:B:PHE:HD2  | 5        | 11.12         |
| (1,429) | 1:19:A:ILE:HD12 | 1:120:B:PHE:HD2  | 2        | 11.1          |
| (1,430) | 1:20:A:PHE:HD2  | 1:119:B:ILE:HD11 | 3        | 11.02         |
| (1,430) | 1:20:A:PHE:HD2  | 1:119:B:ILE:HD13 | 8        | 10.99         |
| (1,429) | 1:19:A:ILE:HD11 | 1:120:B:PHE:HD2  | 3        | 10.99         |
| (1,429) | 1:19:A:ILE:HD11 | 1:120:B:PHE:HD2  | 1        | 10.95         |
| (1,429) | 1:19:A:ILE:HD13 | 1:120:B:PHE:HD2  | 4        | 10.92         |
| (1,430) | 1:20:A:PHE:HD2  | 1:119:B:ILE:HD11 | 1        | 10.91         |
| (1,429) | 1:19:A:ILE:HD13 | 1:120:B:PHE:HD2  | 8        | 10.9          |
| (1,430) | 1:20:A:PHE:HD2  | 1:119:B:ILE:HD13 | 4        | 10.8          |
| (1,429) | 1:19:A:ILE:HD12 | 1:120:B:PHE:HD2  | 6        | 10.41         |
| (1,429) | 1:19:A:ILE:HD11 | 1:120:B:PHE:HD1  | 9        | 10.4          |
| (1,430) | 1:20:A:PHE:HD1  | 1:119:B:ILE:HD12 | 6        | 10.33         |
| (1,430) | 1:20:A:PHE:HD1  | 1:119:B:ILE:HD11 | 10       | 10.32         |
| (1,429) | 1:19:A:ILE:HD11 | 1:120:B:PHE:HD2  | 10       | 10.32         |
| (1,430) | 1:20:A:PHE:HD1  | 1:119:B:ILE:HD11 | 9        | 10.11         |
| (1,873) | 1:12:A:ILE:HG22 | 1:110:B:PHE:HE2  | 9        | 8.65          |
| (1,873) | 1:12:A:ILE:HG21 | 1:110:B:PHE:HE1  | 6        | 8.62          |
| (1,875) | 1:10:A:PHE:HE1  | 1:112:B:ILE:HG22 | 9        | 8.55          |
| (1,875) | 1:10:A:PHE:HE1  | 1:112:B:ILE:HG21 | 6        | 8.54          |
| (1,426) | 1:20:A:PHE:HD1  | 1:123:B:ILE:HD12 | 7        | 8.38          |
| (1,875) | 1:10:A:PHE:HE2  | 1:112:B:ILE:HG22 | 4        | 8.37          |
| (1,873) | 1:12:A:ILE:HG22 | 1:110:B:PHE:HE1  | 4        | 8.35          |
| (1,875) | 1:10:A:PHE:HE1  | 1:112:B:ILE:HG23 | 1        | 8.3           |
| (1,873) | 1:12:A:ILE:HG23 | 1:110:B:PHE:HE1  | 1        | 8.27          |
| (1,873) | 1:12:A:ILE:HG22 | 1:110:B:PHE:HE2  | 3        | 8.23          |
| (1,873) | 1:12:A:ILE:HG22 | 1:110:B:PHE:HE1  | 8        | 8.22          |
| (1,875) | 1:10:A:PHE:HE2  | 1:112:B:ILE:HG22 | 3        | 8.19          |
| (1,875) | 1:10:A:PHE:HE2  | 1:112:B:ILE:HG22 | 5        | 8.14          |
| (1,432) | 1:20:A:PHE:HD2  | 1:118:B:LEU:HD13 | 8        | 8.1           |

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| Key     | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (1,431) | 1:18:A:LEU:HD12 | 1:120:B:PHE:HD2  | 9        | 8.1           |
| (1,432) | 1:20:A:PHE:HD1  | 1:118:B:LEU:HD13 | 5        | 8.08          |
| (1,431) | 1:18:A:LEU:HD11 | 1:120:B:PHE:HD2  | 1        | 8.07          |
| (1,431) | 1:18:A:LEU:HD13 | 1:120:B:PHE:HD2  | 8        | 8.07          |
| (1,432) | 1:20:A:PHE:HD2  | 1:118:B:LEU:HD11 | 1        | 8.05          |
| (1,873) | 1:12:A:ILE:HG22 | 1:110:B:PHE:HE2  | 5        | 8.03          |
| (1,431) | 1:18:A:LEU:HD13 | 1:120:B:PHE:HD1  | 5        | 8.03          |
| (1,432) | 1:20:A:PHE:HD2  | 1:118:B:LEU:HD13 | 2        | 7.99          |
| (1,432) | 1:20:A:PHE:HD1  | 1:118:B:LEU:HD12 | 9        | 7.99          |
| (1,431) | 1:18:A:LEU:HD13 | 1:120:B:PHE:HD2  | 6        | 7.99          |
| (1,432) | 1:20:A:PHE:HD2  | 1:118:B:LEU:HD11 | 3        | 7.98          |
| (1,431) | 1:18:A:LEU:HD11 | 1:120:B:PHE:HD2  | 3        | 7.97          |
| (1,432) | 1:20:A:PHE:HD2  | 1:118:B:LEU:HD12 | 10       | 7.96          |
| (1,431) | 1:18:A:LEU:HD13 | 1:120:B:PHE:HD2  | 2        | 7.96          |
| (1,431) | 1:18:A:LEU:HD12 | 1:120:B:PHE:HD2  | 10       | 7.96          |
| (1,873) | 1:12:A:ILE:HG22 | 1:110:B:PHE:HE1  | 2        | 7.94          |
| (1,431) | 1:18:A:LEU:HD13 | 1:120:B:PHE:HD2  | 4        | 7.94          |
| (1,875) | 1:10:A:PHE:HE1  | 1:112:B:ILE:HG23 | 10       | 7.93          |
| (1,432) | 1:20:A:PHE:HD2  | 1:118:B:LEU:HD12 | 7        | 7.93          |
| (1,873) | 1:12:A:ILE:HG23 | 1:110:B:PHE:HE1  | 10       | 7.91          |
| (1,875) | 1:10:A:PHE:HE1  | 1:112:B:ILE:HG22 | 2        | 7.86          |
| (1,432) | 1:20:A:PHE:HD2  | 1:118:B:LEU:HD13 | 4        | 7.86          |
| (1,432) | 1:20:A:PHE:HD2  | 1:118:B:LEU:HD13 | 6        | 7.78          |
| (1,431) | 1:18:A:LEU:HD12 | 1:120:B:PHE:HD2  | 7        | 7.78          |
| (1,875) | 1:10:A:PHE:HE1  | 1:112:B:ILE:HG22 | 8        | 7.72          |
| (1,872) | 1:21:A:ILE:HD11 | 1:120:B:PHE:HB2  | 9        | 7.59          |
| (1,872) | 1:21:A:ILE:HD11 | 1:120:B:PHE:HB3  | 9        | 7.59          |
| (1,872) | 1:21:A:ILE:HD12 | 1:120:B:PHE:HB2  | 9        | 7.59          |
| (1,872) | 1:21:A:ILE:HD12 | 1:120:B:PHE:HB3  | 9        | 7.59          |
| (1,872) | 1:21:A:ILE:HD13 | 1:120:B:PHE:HB2  | 9        | 7.59          |
| (1,872) | 1:21:A:ILE:HD13 | 1:120:B:PHE:HB3  | 9        | 7.59          |
| (1,425) | 1:23:A:ILE:HD12 | 1:120:B:PHE:HD1  | 7        | 7.57          |
| (1,872) | 1:21:A:ILE:HD11 | 1:120:B:PHE:HB2  | 4        | 7.52          |
| (1,872) | 1:21:A:ILE:HD11 | 1:120:B:PHE:HB3  | 4        | 7.52          |
| (1,872) | 1:21:A:ILE:HD12 | 1:120:B:PHE:HB2  | 4        | 7.52          |
| (1,872) | 1:21:A:ILE:HD12 | 1:120:B:PHE:HB3  | 4        | 7.52          |
| (1,872) | 1:21:A:ILE:HD13 | 1:120:B:PHE:HB2  | 4        | 7.52          |
| (1,872) | 1:21:A:ILE:HD13 | 1:120:B:PHE:HB3  | 4        | 7.52          |
| (1,870) | 1:20:A:PHE:HB2  | 1:121:B:ILE:HD11 | 4        | 7.49          |
| (1,870) | 1:20:A:PHE:HB2  | 1:121:B:ILE:HD12 | 4        | 7.49          |
| (1,870) | 1:20:A:PHE:HB2  | 1:121:B:ILE:HD13 | 4        | 7.49          |
| (1,870) | 1:20:A:PHE:HB3  | 1:121:B:ILE:HD11 | 4        | 7.49          |

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| Key     | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (1,870) | 1:20:A:PHE:HB3  | 1:121:B:ILE:HD12 | 4        | 7.49          |
| (1,870) | 1:20:A:PHE:HB3  | 1:121:B:ILE:HD13 | 4        | 7.49          |
| (1,870) | 1:20:A:PHE:HB2  | 1:121:B:ILE:HD11 | 2        | 7.48          |
| (1,870) | 1:20:A:PHE:HB2  | 1:121:B:ILE:HD12 | 2        | 7.48          |
| (1,870) | 1:20:A:PHE:HB2  | 1:121:B:ILE:HD13 | 2        | 7.48          |
| (1,870) | 1:20:A:PHE:HB3  | 1:121:B:ILE:HD11 | 2        | 7.48          |
| (1,870) | 1:20:A:PHE:HB3  | 1:121:B:ILE:HD12 | 2        | 7.48          |
| (1,870) | 1:20:A:PHE:HB3  | 1:121:B:ILE:HD13 | 2        | 7.48          |
| (1,870) | 1:20:A:PHE:HB2  | 1:121:B:ILE:HD11 | 5        | 7.45          |
| (1,870) | 1:20:A:PHE:HB2  | 1:121:B:ILE:HD12 | 5        | 7.45          |
| (1,870) | 1:20:A:PHE:HB2  | 1:121:B:ILE:HD13 | 5        | 7.45          |
| (1,870) | 1:20:A:PHE:HB3  | 1:121:B:ILE:HD11 | 5        | 7.45          |
| (1,870) | 1:20:A:PHE:HB3  | 1:121:B:ILE:HD12 | 5        | 7.45          |
| (1,870) | 1:20:A:PHE:HB3  | 1:121:B:ILE:HD13 | 5        | 7.45          |
| (1,870) | 1:20:A:PHE:HB2  | 1:121:B:ILE:HD11 | 8        | 7.45          |
| (1,870) | 1:20:A:PHE:HB2  | 1:121:B:ILE:HD12 | 8        | 7.45          |
| (1,870) | 1:20:A:PHE:HB2  | 1:121:B:ILE:HD13 | 8        | 7.45          |
| (1,870) | 1:20:A:PHE:HB3  | 1:121:B:ILE:HD11 | 8        | 7.45          |
| (1,870) | 1:20:A:PHE:HB3  | 1:121:B:ILE:HD12 | 8        | 7.45          |
| (1,870) | 1:20:A:PHE:HB3  | 1:121:B:ILE:HD13 | 8        | 7.45          |
| (1,872) | 1:21:A:ILE:HD11 | 1:120:B:PHE:HB2  | 1        | 7.43          |
| (1,872) | 1:21:A:ILE:HD11 | 1:120:B:PHE:HB3  | 1        | 7.43          |
| (1,872) | 1:21:A:ILE:HD12 | 1:120:B:PHE:HB2  | 1        | 7.43          |
| (1,872) | 1:21:A:ILE:HD12 | 1:120:B:PHE:HB3  | 1        | 7.43          |
| (1,872) | 1:21:A:ILE:HD13 | 1:120:B:PHE:HB2  | 1        | 7.43          |
| (1,872) | 1:21:A:ILE:HD13 | 1:120:B:PHE:HB3  | 1        | 7.43          |
| (1,872) | 1:21:A:ILE:HD11 | 1:120:B:PHE:HB2  | 2        | 7.43          |
| (1,872) | 1:21:A:ILE:HD11 | 1:120:B:PHE:HB3  | 2        | 7.43          |
| (1,872) | 1:21:A:ILE:HD12 | 1:120:B:PHE:HB2  | 2        | 7.43          |
| (1,872) | 1:21:A:ILE:HD12 | 1:120:B:PHE:HB3  | 2        | 7.43          |
| (1,872) | 1:21:A:ILE:HD13 | 1:120:B:PHE:HB2  | 2        | 7.43          |
| (1,872) | 1:21:A:ILE:HD13 | 1:120:B:PHE:HB3  | 2        | 7.43          |
| (1,870) | 1:20:A:PHE:HB2  | 1:121:B:ILE:HD11 | 1        | 7.43          |
| (1,870) | 1:20:A:PHE:HB2  | 1:121:B:ILE:HD12 | 1        | 7.43          |
| (1,870) | 1:20:A:PHE:HB2  | 1:121:B:ILE:HD13 | 1        | 7.43          |
| (1,870) | 1:20:A:PHE:HB3  | 1:121:B:ILE:HD11 | 1        | 7.43          |
| (1,870) | 1:20:A:PHE:HB3  | 1:121:B:ILE:HD12 | 1        | 7.43          |
| (1,870) | 1:20:A:PHE:HB3  | 1:121:B:ILE:HD13 | 1        | 7.43          |
| (1,872) | 1:21:A:ILE:HD11 | 1:120:B:PHE:HB2  | 8        | 7.42          |
| (1,872) | 1:21:A:ILE:HD11 | 1:120:B:PHE:HB3  | 8        | 7.42          |
| (1,872) | 1:21:A:ILE:HD12 | 1:120:B:PHE:HB2  | 8        | 7.42          |
| (1,872) | 1:21:A:ILE:HD12 | 1:120:B:PHE:HB3  | 8        | 7.42          |

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| Key     | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (1,872) | 1:21:A:ILE:HD13 | 1:120:B:PHE:HB2  | 8        | 7.42          |
| (1,872) | 1:21:A:ILE:HD13 | 1:120:B:PHE:HB3  | 8        | 7.42          |
| (1,872) | 1:21:A:ILE:HD11 | 1:120:B:PHE:HB2  | 3        | 7.41          |
| (1,872) | 1:21:A:ILE:HD11 | 1:120:B:PHE:HB3  | 3        | 7.41          |
| (1,872) | 1:21:A:ILE:HD12 | 1:120:B:PHE:HB2  | 3        | 7.41          |
| (1,872) | 1:21:A:ILE:HD12 | 1:120:B:PHE:HB3  | 3        | 7.41          |
| (1,872) | 1:21:A:ILE:HD13 | 1:120:B:PHE:HB2  | 3        | 7.41          |
| (1,872) | 1:21:A:ILE:HD13 | 1:120:B:PHE:HB3  | 3        | 7.41          |
| (1,872) | 1:21:A:ILE:HD11 | 1:120:B:PHE:HB2  | 5        | 7.41          |
| (1,872) | 1:21:A:ILE:HD11 | 1:120:B:PHE:HB3  | 5        | 7.41          |
| (1,872) | 1:21:A:ILE:HD12 | 1:120:B:PHE:HB2  | 5        | 7.41          |
| (1,872) | 1:21:A:ILE:HD12 | 1:120:B:PHE:HB3  | 5        | 7.41          |
| (1,872) | 1:21:A:ILE:HD13 | 1:120:B:PHE:HB2  | 5        | 7.41          |
| (1,872) | 1:21:A:ILE:HD13 | 1:120:B:PHE:HB3  | 5        | 7.41          |
| (1,870) | 1:20:A:PHE:HB2  | 1:121:B:ILE:HD11 | 3        | 7.41          |
| (1,870) | 1:20:A:PHE:HB2  | 1:121:B:ILE:HD12 | 3        | 7.41          |
| (1,870) | 1:20:A:PHE:HB2  | 1:121:B:ILE:HD13 | 3        | 7.41          |
| (1,870) | 1:20:A:PHE:HB3  | 1:121:B:ILE:HD11 | 3        | 7.41          |
| (1,870) | 1:20:A:PHE:HB3  | 1:121:B:ILE:HD12 | 3        | 7.41          |
| (1,870) | 1:20:A:PHE:HB3  | 1:121:B:ILE:HD13 | 3        | 7.41          |
| (1,870) | 1:20:A:PHE:HB2  | 1:121:B:ILE:HD11 | 9        | 7.38          |
| (1,870) | 1:20:A:PHE:HB2  | 1:121:B:ILE:HD12 | 9        | 7.38          |
| (1,870) | 1:20:A:PHE:HB2  | 1:121:B:ILE:HD13 | 9        | 7.38          |
| (1,870) | 1:20:A:PHE:HB3  | 1:121:B:ILE:HD11 | 9        | 7.38          |
| (1,870) | 1:20:A:PHE:HB3  | 1:121:B:ILE:HD12 | 9        | 7.38          |
| (1,870) | 1:20:A:PHE:HB3  | 1:121:B:ILE:HD13 | 9        | 7.38          |
| (1,870) | 1:20:A:PHE:HB2  | 1:121:B:ILE:HD11 | 10       | 7.35          |
| (1,870) | 1:20:A:PHE:HB2  | 1:121:B:ILE:HD12 | 10       | 7.35          |
| (1,870) | 1:20:A:PHE:HB2  | 1:121:B:ILE:HD13 | 10       | 7.35          |
| (1,870) | 1:20:A:PHE:HB3  | 1:121:B:ILE:HD11 | 10       | 7.35          |
| (1,870) | 1:20:A:PHE:HB3  | 1:121:B:ILE:HD12 | 10       | 7.35          |
| (1,870) | 1:20:A:PHE:HB3  | 1:121:B:ILE:HD13 | 10       | 7.35          |
| (1,870) | 1:20:A:PHE:HB2  | 1:121:B:ILE:HD11 | 6        | 7.34          |
| (1,870) | 1:20:A:PHE:HB2  | 1:121:B:ILE:HD12 | 6        | 7.34          |
| (1,870) | 1:20:A:PHE:HB2  | 1:121:B:ILE:HD13 | 6        | 7.34          |
| (1,870) | 1:20:A:PHE:HB3  | 1:121:B:ILE:HD11 | 6        | 7.34          |
| (1,870) | 1:20:A:PHE:HB3  | 1:121:B:ILE:HD12 | 6        | 7.34          |
| (1,870) | 1:20:A:PHE:HB3  | 1:121:B:ILE:HD13 | 6        | 7.34          |
| (1,872) | 1:21:A:ILE:HD11 | 1:120:B:PHE:HB2  | 10       | 7.33          |
| (1,872) | 1:21:A:ILE:HD11 | 1:120:B:PHE:HB3  | 10       | 7.33          |
| (1,872) | 1:21:A:ILE:HD12 | 1:120:B:PHE:HB2  | 10       | 7.33          |
| (1,872) | 1:21:A:ILE:HD12 | 1:120:B:PHE:HB3  | 10       | 7.33          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,872) | 1:21:A:ILE:HD13  | 1:120:B:PHE:HB2  | 10       | 7.33          |
| (1,872) | 1:21:A:ILE:HD13  | 1:120:B:PHE:HB3  | 10       | 7.33          |
| (1,870) | 1:20:A:PHE:HB2   | 1:121:B:ILE:HD11 | 7        | 7.29          |
| (1,870) | 1:20:A:PHE:HB2   | 1:121:B:ILE:HD12 | 7        | 7.29          |
| (1,870) | 1:20:A:PHE:HB2   | 1:121:B:ILE:HD13 | 7        | 7.29          |
| (1,870) | 1:20:A:PHE:HB3   | 1:121:B:ILE:HD11 | 7        | 7.29          |
| (1,870) | 1:20:A:PHE:HB3   | 1:121:B:ILE:HD12 | 7        | 7.29          |
| (1,870) | 1:20:A:PHE:HB3   | 1:121:B:ILE:HD13 | 7        | 7.29          |
| (1,872) | 1:21:A:ILE:HD11  | 1:120:B:PHE:HB2  | 6        | 7.28          |
| (1,872) | 1:21:A:ILE:HD11  | 1:120:B:PHE:HB3  | 6        | 7.28          |
| (1,872) | 1:21:A:ILE:HD12  | 1:120:B:PHE:HB2  | 6        | 7.28          |
| (1,872) | 1:21:A:ILE:HD12  | 1:120:B:PHE:HB3  | 6        | 7.28          |
| (1,872) | 1:21:A:ILE:HD13  | 1:120:B:PHE:HB2  | 6        | 7.28          |
| (1,872) | 1:21:A:ILE:HD13  | 1:120:B:PHE:HB3  | 6        | 7.28          |
| (1,872) | 1:21:A:ILE:HD11  | 1:120:B:PHE:HB2  | 7        | 7.25          |
| (1,872) | 1:21:A:ILE:HD11  | 1:120:B:PHE:HB3  | 7        | 7.25          |
| (1,872) | 1:21:A:ILE:HD12  | 1:120:B:PHE:HB2  | 7        | 7.25          |
| (1,872) | 1:21:A:ILE:HD12  | 1:120:B:PHE:HB3  | 7        | 7.25          |
| (1,872) | 1:21:A:ILE:HD13  | 1:120:B:PHE:HB2  | 7        | 7.25          |
| (1,872) | 1:21:A:ILE:HD13  | 1:120:B:PHE:HB3  | 7        | 7.25          |
| (1,425) | 1:23:A:ILE:HD12  | 1:120:B:PHE:HD1  | 6        | 7.12          |
| (1,425) | 1:23:A:ILE:HD13  | 1:120:B:PHE:HD1  | 10       | 7.02          |
| (1,426) | 1:20:A:PHE:HD1   | 1:123:B:ILE:HD13 | 2        | 6.89          |
| (1,425) | 1:23:A:ILE:HD13  | 1:120:B:PHE:HD1  | 2        | 6.85          |
| (1,426) | 1:20:A:PHE:HD1   | 1:123:B:ILE:HD13 | 3        | 6.77          |
| (1,425) | 1:23:A:ILE:HD13  | 1:120:B:PHE:HD1  | 3        | 6.77          |
| (1,426) | 1:20:A:PHE:HD1   | 1:123:B:ILE:HD11 | 6        | 6.68          |
| (1,425) | 1:23:A:ILE:HD11  | 1:120:B:PHE:HD1  | 5        | 6.67          |
| (1,426) | 1:20:A:PHE:HD1   | 1:123:B:ILE:HD11 | 5        | 6.66          |
| (1,874) | 1:112:B:ILE:HG22 | 1:110:B:PHE:HD1  | 7        | 6.56          |
| (1,425) | 1:23:A:ILE:HD11  | 1:120:B:PHE:HD1  | 4        | 6.56          |
| (1,874) | 1:112:B:ILE:HG21 | 1:110:B:PHE:HD2  | 3        | 6.54          |
| (1,426) | 1:20:A:PHE:HD1   | 1:123:B:ILE:HD11 | 4        | 6.53          |
| (1,426) | 1:20:A:PHE:HD1   | 1:123:B:ILE:HD13 | 8        | 6.53          |
| (1,426) | 1:20:A:PHE:HD1   | 1:123:B:ILE:HD12 | 10       | 6.53          |
| (1,874) | 1:112:B:ILE:HG23 | 1:110:B:PHE:HD1  | 6        | 6.52          |
| (1,425) | 1:23:A:ILE:HD12  | 1:120:B:PHE:HD1  | 1        | 6.5           |
| (1,426) | 1:20:A:PHE:HD1   | 1:123:B:ILE:HD12 | 1        | 6.49          |
| (1,425) | 1:23:A:ILE:HD13  | 1:120:B:PHE:HD1  | 8        | 6.49          |
| (1,874) | 1:112:B:ILE:HG21 | 1:110:B:PHE:HD1  | 4        | 6.47          |
| (1,874) | 1:112:B:ILE:HG21 | 1:110:B:PHE:HD1  | 8        | 6.47          |
| (1,874) | 1:112:B:ILE:HG22 | 1:110:B:PHE:HD1  | 1        | 6.42          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,874) | 1:112:B:ILE:HG21 | 1:110:B:PHE:HD1  | 5        | 6.4           |
| (1,873) | 1:12:A:ILE:HG22  | 1:110:B:PHE:HE1  | 7        | 6.33          |
| (1,874) | 1:112:B:ILE:HG22 | 1:110:B:PHE:HD2  | 10       | 6.31          |
| (1,425) | 1:23:A:ILE:HD12  | 1:120:B:PHE:HD1  | 9        | 6.26          |
| (1,875) | 1:10:A:PHE:HE1   | 1:112:B:ILE:HG22 | 7        | 6.22          |
| (1,874) | 1:112:B:ILE:HG21 | 1:110:B:PHE:HD1  | 2        | 6.19          |
| (1,426) | 1:20:A:PHE:HD1   | 1:123:B:ILE:HD12 | 9        | 6.15          |
| (1,859) | 1:120:B:PHE:HD1  | 1:121:B:ILE:HD12 | 9        | 5.25          |
| (1,866) | 1:21:A:ILE:HG21  | 1:120:B:PHE:HA   | 9        | 5.15          |
| (1,866) | 1:21:A:ILE:HG22  | 1:120:B:PHE:HA   | 9        | 5.15          |
| (1,866) | 1:21:A:ILE:HG23  | 1:120:B:PHE:HA   | 9        | 5.15          |
| (1,874) | 1:112:B:ILE:HG21 | 1:110:B:PHE:HD1  | 9        | 5.04          |
| (1,864) | 1:20:A:PHE:HA    | 1:121:B:ILE:HG21 | 2        | 5.01          |
| (1,864) | 1:20:A:PHE:HA    | 1:121:B:ILE:HG22 | 2        | 5.01          |
| (1,864) | 1:20:A:PHE:HA    | 1:121:B:ILE:HG23 | 2        | 5.01          |
| (1,864) | 1:20:A:PHE:HA    | 1:121:B:ILE:HG21 | 9        | 5.0           |
| (1,864) | 1:20:A:PHE:HA    | 1:121:B:ILE:HG22 | 9        | 5.0           |
| (1,864) | 1:20:A:PHE:HA    | 1:121:B:ILE:HG23 | 9        | 5.0           |
| (1,866) | 1:21:A:ILE:HG21  | 1:120:B:PHE:HA   | 2        | 4.97          |
| (1,866) | 1:21:A:ILE:HG22  | 1:120:B:PHE:HA   | 2        | 4.97          |
| (1,866) | 1:21:A:ILE:HG23  | 1:120:B:PHE:HA   | 2        | 4.97          |
| (1,864) | 1:20:A:PHE:HA    | 1:121:B:ILE:HG21 | 8        | 4.94          |
| (1,864) | 1:20:A:PHE:HA    | 1:121:B:ILE:HG22 | 8        | 4.94          |
| (1,864) | 1:20:A:PHE:HA    | 1:121:B:ILE:HG23 | 8        | 4.94          |
| (1,866) | 1:21:A:ILE:HG21  | 1:120:B:PHE:HA   | 1        | 4.93          |
| (1,866) | 1:21:A:ILE:HG22  | 1:120:B:PHE:HA   | 1        | 4.93          |
| (1,866) | 1:21:A:ILE:HG23  | 1:120:B:PHE:HA   | 1        | 4.93          |
| (1,866) | 1:21:A:ILE:HG21  | 1:120:B:PHE:HA   | 3        | 4.93          |
| (1,866) | 1:21:A:ILE:HG22  | 1:120:B:PHE:HA   | 3        | 4.93          |
| (1,866) | 1:21:A:ILE:HG23  | 1:120:B:PHE:HA   | 3        | 4.93          |
| (1,866) | 1:21:A:ILE:HG21  | 1:120:B:PHE:HA   | 4        | 4.93          |
| (1,866) | 1:21:A:ILE:HG22  | 1:120:B:PHE:HA   | 4        | 4.93          |
| (1,866) | 1:21:A:ILE:HG23  | 1:120:B:PHE:HA   | 4        | 4.93          |
| (1,864) | 1:20:A:PHE:HA    | 1:121:B:ILE:HG21 | 1        | 4.93          |
| (1,864) | 1:20:A:PHE:HA    | 1:121:B:ILE:HG22 | 1        | 4.93          |
| (1,864) | 1:20:A:PHE:HA    | 1:121:B:ILE:HG23 | 1        | 4.93          |
| (1,866) | 1:21:A:ILE:HG21  | 1:120:B:PHE:HA   | 8        | 4.92          |
| (1,866) | 1:21:A:ILE:HG22  | 1:120:B:PHE:HA   | 8        | 4.92          |
| (1,866) | 1:21:A:ILE:HG23  | 1:120:B:PHE:HA   | 8        | 4.92          |
| (1,864) | 1:20:A:PHE:HA    | 1:121:B:ILE:HG21 | 3        | 4.92          |
| (1,864) | 1:20:A:PHE:HA    | 1:121:B:ILE:HG22 | 3        | 4.92          |
| (1,864) | 1:20:A:PHE:HA    | 1:121:B:ILE:HG23 | 3        | 4.92          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,864) | 1:20:A:PHE:HA    | 1:121:B:ILE:HG21 | 4        | 4.9           |
| (1,864) | 1:20:A:PHE:HA    | 1:121:B:ILE:HG22 | 4        | 4.9           |
| (1,864) | 1:20:A:PHE:HA    | 1:121:B:ILE:HG23 | 4        | 4.9           |
| (1,864) | 1:20:A:PHE:HA    | 1:121:B:ILE:HG21 | 5        | 4.81          |
| (1,864) | 1:20:A:PHE:HA    | 1:121:B:ILE:HG22 | 5        | 4.81          |
| (1,864) | 1:20:A:PHE:HA    | 1:121:B:ILE:HG23 | 5        | 4.81          |
| (1,866) | 1:21:A:ILE:HG21  | 1:120:B:PHE:HA   | 5        | 4.8           |
| (1,866) | 1:21:A:ILE:HG22  | 1:120:B:PHE:HA   | 5        | 4.8           |
| (1,866) | 1:21:A:ILE:HG23  | 1:120:B:PHE:HA   | 5        | 4.8           |
| (1,428) | 1:20:A:PHE:HA    | 1:123:B:ILE:HD11 | 7        | 4.8           |
| (1,428) | 1:20:A:PHE:HA    | 1:123:B:ILE:HD12 | 7        | 4.8           |
| (1,428) | 1:20:A:PHE:HA    | 1:123:B:ILE:HD13 | 7        | 4.8           |
| (1,864) | 1:20:A:PHE:HA    | 1:121:B:ILE:HG21 | 6        | 4.79          |
| (1,864) | 1:20:A:PHE:HA    | 1:121:B:ILE:HG22 | 6        | 4.79          |
| (1,864) | 1:20:A:PHE:HA    | 1:121:B:ILE:HG23 | 6        | 4.79          |
| (1,866) | 1:21:A:ILE:HG21  | 1:120:B:PHE:HA   | 6        | 4.78          |
| (1,866) | 1:21:A:ILE:HG22  | 1:120:B:PHE:HA   | 6        | 4.78          |
| (1,866) | 1:21:A:ILE:HG23  | 1:120:B:PHE:HA   | 6        | 4.78          |
| (1,427) | 1:23:A:ILE:HD11  | 1:120:B:PHE:HA   | 7        | 4.78          |
| (1,427) | 1:23:A:ILE:HD12  | 1:120:B:PHE:HA   | 7        | 4.78          |
| (1,427) | 1:23:A:ILE:HD13  | 1:120:B:PHE:HA   | 7        | 4.78          |
| (1,866) | 1:21:A:ILE:HG21  | 1:120:B:PHE:HA   | 10       | 4.76          |
| (1,866) | 1:21:A:ILE:HG22  | 1:120:B:PHE:HA   | 10       | 4.76          |
| (1,866) | 1:21:A:ILE:HG23  | 1:120:B:PHE:HA   | 10       | 4.76          |
| (1,864) | 1:20:A:PHE:HA    | 1:121:B:ILE:HG21 | 10       | 4.75          |
| (1,864) | 1:20:A:PHE:HA    | 1:121:B:ILE:HG22 | 10       | 4.75          |
| (1,864) | 1:20:A:PHE:HA    | 1:121:B:ILE:HG23 | 10       | 4.75          |
| (1,859) | 1:120:B:PHE:HD1  | 1:121:B:ILE:HD13 | 7        | 4.74          |
| (1,864) | 1:20:A:PHE:HA    | 1:121:B:ILE:HG21 | 7        | 4.67          |
| (1,864) | 1:20:A:PHE:HA    | 1:121:B:ILE:HG22 | 7        | 4.67          |
| (1,864) | 1:20:A:PHE:HA    | 1:121:B:ILE:HG23 | 7        | 4.67          |
| (1,862) | 1:116:B:ILE:HD12 | 1:109:B:PHE:HE1  | 10       | 4.65          |
| (1,866) | 1:21:A:ILE:HG21  | 1:120:B:PHE:HA   | 7        | 4.58          |
| (1,866) | 1:21:A:ILE:HG22  | 1:120:B:PHE:HA   | 7        | 4.58          |
| (1,866) | 1:21:A:ILE:HG23  | 1:120:B:PHE:HA   | 7        | 4.58          |
| (1,862) | 1:116:B:ILE:HD11 | 1:109:B:PHE:HE1  | 5        | 4.5           |
| (1,862) | 1:116:B:ILE:HD13 | 1:109:B:PHE:HE1  | 8        | 4.45          |
| (1,862) | 1:116:B:ILE:HD13 | 1:109:B:PHE:HE1  | 1        | 4.35          |
| (1,862) | 1:116:B:ILE:HD13 | 1:109:B:PHE:HE1  | 6        | 4.28          |
| (1,862) | 1:116:B:ILE:HD11 | 1:109:B:PHE:HD1  | 7        | 4.22          |
| (1,427) | 1:23:A:ILE:HD11  | 1:120:B:PHE:HA   | 9        | 3.97          |
| (1,427) | 1:23:A:ILE:HD12  | 1:120:B:PHE:HA   | 9        | 3.97          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,427) | 1:23:A:ILE:HD13  | 1:120:B:PHE:HA   | 9        | 3.97          |
| (1,428) | 1:20:A:PHE:HA    | 1:123:B:ILE:HD11 | 2        | 3.92          |
| (1,428) | 1:20:A:PHE:HA    | 1:123:B:ILE:HD12 | 2        | 3.92          |
| (1,428) | 1:20:A:PHE:HA    | 1:123:B:ILE:HD13 | 2        | 3.92          |
| (1,428) | 1:20:A:PHE:HA    | 1:123:B:ILE:HD11 | 9        | 3.92          |
| (1,428) | 1:20:A:PHE:HA    | 1:123:B:ILE:HD12 | 9        | 3.92          |
| (1,428) | 1:20:A:PHE:HA    | 1:123:B:ILE:HD13 | 9        | 3.92          |
| (1,427) | 1:23:A:ILE:HD11  | 1:120:B:PHE:HA   | 2        | 3.92          |
| (1,427) | 1:23:A:ILE:HD12  | 1:120:B:PHE:HA   | 2        | 3.92          |
| (1,427) | 1:23:A:ILE:HD13  | 1:120:B:PHE:HA   | 2        | 3.92          |
| (1,428) | 1:20:A:PHE:HA    | 1:123:B:ILE:HD11 | 5        | 3.84          |
| (1,428) | 1:20:A:PHE:HA    | 1:123:B:ILE:HD12 | 5        | 3.84          |
| (1,428) | 1:20:A:PHE:HA    | 1:123:B:ILE:HD13 | 5        | 3.84          |
| (1,427) | 1:23:A:ILE:HD11  | 1:120:B:PHE:HA   | 5        | 3.84          |
| (1,427) | 1:23:A:ILE:HD12  | 1:120:B:PHE:HA   | 5        | 3.84          |
| (1,427) | 1:23:A:ILE:HD13  | 1:120:B:PHE:HA   | 5        | 3.84          |
| (1,428) | 1:20:A:PHE:HA    | 1:123:B:ILE:HD11 | 3        | 3.83          |
| (1,428) | 1:20:A:PHE:HA    | 1:123:B:ILE:HD12 | 3        | 3.83          |
| (1,428) | 1:20:A:PHE:HA    | 1:123:B:ILE:HD13 | 3        | 3.83          |
| (1,427) | 1:23:A:ILE:HD11  | 1:120:B:PHE:HA   | 3        | 3.82          |
| (1,427) | 1:23:A:ILE:HD12  | 1:120:B:PHE:HA   | 3        | 3.82          |
| (1,427) | 1:23:A:ILE:HD13  | 1:120:B:PHE:HA   | 3        | 3.82          |
| (1,862) | 1:116:B:ILE:HD13 | 1:109:B:PHE:HD1  | 3        | 3.77          |
| (1,868) | 1:120:B:PHE:HD1  | 1:117:B:LEU:HD23 | 7        | 3.73          |
| (1,862) | 1:116:B:ILE:HD13 | 1:109:B:PHE:HE1  | 4        | 3.7           |
| (1,428) | 1:20:A:PHE:HA    | 1:123:B:ILE:HD11 | 8        | 3.68          |
| (1,428) | 1:20:A:PHE:HA    | 1:123:B:ILE:HD12 | 8        | 3.68          |
| (1,428) | 1:20:A:PHE:HA    | 1:123:B:ILE:HD13 | 8        | 3.68          |
| (1,428) | 1:20:A:PHE:HA    | 1:123:B:ILE:HD11 | 6        | 3.66          |
| (1,428) | 1:20:A:PHE:HA    | 1:123:B:ILE:HD12 | 6        | 3.66          |
| (1,428) | 1:20:A:PHE:HA    | 1:123:B:ILE:HD13 | 6        | 3.66          |
| (1,427) | 1:23:A:ILE:HD11  | 1:120:B:PHE:HA   | 1        | 3.66          |
| (1,427) | 1:23:A:ILE:HD12  | 1:120:B:PHE:HA   | 1        | 3.66          |
| (1,427) | 1:23:A:ILE:HD13  | 1:120:B:PHE:HA   | 1        | 3.66          |
| (1,427) | 1:23:A:ILE:HD11  | 1:120:B:PHE:HA   | 4        | 3.66          |
| (1,427) | 1:23:A:ILE:HD12  | 1:120:B:PHE:HA   | 4        | 3.66          |
| (1,427) | 1:23:A:ILE:HD13  | 1:120:B:PHE:HA   | 4        | 3.66          |
| (1,427) | 1:23:A:ILE:HD11  | 1:120:B:PHE:HA   | 6        | 3.66          |
| (1,427) | 1:23:A:ILE:HD12  | 1:120:B:PHE:HA   | 6        | 3.66          |
| (1,427) | 1:23:A:ILE:HD13  | 1:120:B:PHE:HA   | 6        | 3.66          |
| (1,427) | 1:23:A:ILE:HD11  | 1:120:B:PHE:HA   | 8        | 3.66          |
| (1,427) | 1:23:A:ILE:HD12  | 1:120:B:PHE:HA   | 8        | 3.66          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,427) | 1:23:A:ILE:HD13  | 1:120:B:PHE:HA   | 8        | 3.66          |
| (1,428) | 1:20:A:PHE:HA    | 1:123:B:ILE:HD11 | 1        | 3.65          |
| (1,428) | 1:20:A:PHE:HA    | 1:123:B:ILE:HD12 | 1        | 3.65          |
| (1,428) | 1:20:A:PHE:HA    | 1:123:B:ILE:HD13 | 1        | 3.65          |
| (1,428) | 1:20:A:PHE:HA    | 1:123:B:ILE:HD11 | 4        | 3.63          |
| (1,428) | 1:20:A:PHE:HA    | 1:123:B:ILE:HD12 | 4        | 3.63          |
| (1,428) | 1:20:A:PHE:HA    | 1:123:B:ILE:HD13 | 4        | 3.63          |
| (1,428) | 1:20:A:PHE:HA    | 1:123:B:ILE:HD11 | 10       | 3.57          |
| (1,428) | 1:20:A:PHE:HA    | 1:123:B:ILE:HD12 | 10       | 3.57          |
| (1,428) | 1:20:A:PHE:HA    | 1:123:B:ILE:HD13 | 10       | 3.57          |
| (1,427) | 1:23:A:ILE:HD11  | 1:120:B:PHE:HA   | 10       | 3.56          |
| (1,427) | 1:23:A:ILE:HD12  | 1:120:B:PHE:HA   | 10       | 3.56          |
| (1,427) | 1:23:A:ILE:HD13  | 1:120:B:PHE:HA   | 10       | 3.56          |
| (1,868) | 1:120:B:PHE:HD2  | 1:117:B:LEU:HD21 | 9        | 3.39          |
| (1,859) | 1:120:B:PHE:HD2  | 1:121:B:ILE:HD11 | 5        | 3.38          |
| (1,859) | 1:120:B:PHE:HD2  | 1:121:B:ILE:HD12 | 8        | 3.29          |
| (1,859) | 1:120:B:PHE:HD2  | 1:121:B:ILE:HD12 | 6        | 3.27          |
| (1,859) | 1:120:B:PHE:HD2  | 1:121:B:ILE:HD12 | 1        | 3.25          |
| (1,859) | 1:120:B:PHE:HD2  | 1:121:B:ILE:HD12 | 3        | 3.16          |
| (1,859) | 1:120:B:PHE:HD2  | 1:121:B:ILE:HD12 | 2        | 3.14          |
| (1,862) | 1:116:B:ILE:HD13 | 1:109:B:PHE:HD1  | 2        | 3.12          |
| (1,859) | 1:120:B:PHE:HD2  | 1:121:B:ILE:HD11 | 10       | 3.12          |
| (1,859) | 1:120:B:PHE:HD2  | 1:121:B:ILE:HD12 | 4        | 3.02          |
| (1,862) | 1:116:B:ILE:HD11 | 1:109:B:PHE:HD1  | 9        | 2.99          |
| (1,358) | 1:127:B:ILE:HG21 | 1:129:B:PHE:HD1  | 8        | 2.66          |
| (1,358) | 1:127:B:ILE:HG21 | 1:129:B:PHE:HD2  | 8        | 2.66          |
| (1,358) | 1:127:B:ILE:HG22 | 1:129:B:PHE:HD1  | 8        | 2.66          |
| (1,358) | 1:127:B:ILE:HG22 | 1:129:B:PHE:HD2  | 8        | 2.66          |
| (1,358) | 1:127:B:ILE:HG23 | 1:129:B:PHE:HD1  | 8        | 2.66          |
| (1,358) | 1:127:B:ILE:HG23 | 1:129:B:PHE:HD2  | 8        | 2.66          |
| (1,792) | 1:27:A:ILE:HG21  | 1:29:A:PHE:HD1   | 8        | 2.65          |
| (1,792) | 1:27:A:ILE:HG21  | 1:29:A:PHE:HD2   | 8        | 2.65          |
| (1,792) | 1:27:A:ILE:HG22  | 1:29:A:PHE:HD1   | 8        | 2.65          |
| (1,792) | 1:27:A:ILE:HG22  | 1:29:A:PHE:HD2   | 8        | 2.65          |
| (1,792) | 1:27:A:ILE:HG23  | 1:29:A:PHE:HD1   | 8        | 2.65          |
| (1,792) | 1:27:A:ILE:HG23  | 1:29:A:PHE:HD2   | 8        | 2.65          |
| (1,357) | 1:27:A:ILE:HG21  | 1:29:A:PHE:HD1   | 8        | 2.65          |
| (1,357) | 1:27:A:ILE:HG21  | 1:29:A:PHE:HD2   | 8        | 2.65          |
| (1,357) | 1:27:A:ILE:HG22  | 1:29:A:PHE:HD1   | 8        | 2.65          |
| (1,357) | 1:27:A:ILE:HG22  | 1:29:A:PHE:HD2   | 8        | 2.65          |
| (1,357) | 1:27:A:ILE:HG23  | 1:29:A:PHE:HD1   | 8        | 2.65          |
| (1,357) | 1:27:A:ILE:HG23  | 1:29:A:PHE:HD2   | 8        | 2.65          |

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| Key     | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|---------|------------------|-----------------|----------|---------------|
| (1,792) | 1:27:A:ILE:HG21  | 1:29:A:PHE:HD1  | 9        | 2.64          |
| (1,792) | 1:27:A:ILE:HG21  | 1:29:A:PHE:HD2  | 9        | 2.64          |
| (1,792) | 1:27:A:ILE:HG22  | 1:29:A:PHE:HD1  | 9        | 2.64          |
| (1,792) | 1:27:A:ILE:HG22  | 1:29:A:PHE:HD2  | 9        | 2.64          |
| (1,792) | 1:27:A:ILE:HG23  | 1:29:A:PHE:HD1  | 9        | 2.64          |
| (1,792) | 1:27:A:ILE:HG23  | 1:29:A:PHE:HD2  | 9        | 2.64          |
| (1,358) | 1:127:B:ILE:HG21 | 1:129:B:PHE:HD1 | 2        | 2.64          |
| (1,358) | 1:127:B:ILE:HG21 | 1:129:B:PHE:HD2 | 2        | 2.64          |
| (1,358) | 1:127:B:ILE:HG22 | 1:129:B:PHE:HD1 | 2        | 2.64          |
| (1,358) | 1:127:B:ILE:HG22 | 1:129:B:PHE:HD2 | 2        | 2.64          |
| (1,358) | 1:127:B:ILE:HG23 | 1:129:B:PHE:HD1 | 2        | 2.64          |
| (1,358) | 1:127:B:ILE:HG23 | 1:129:B:PHE:HD2 | 2        | 2.64          |
| (1,358) | 1:127:B:ILE:HG21 | 1:129:B:PHE:HD1 | 9        | 2.64          |
| (1,358) | 1:127:B:ILE:HG21 | 1:129:B:PHE:HD2 | 9        | 2.64          |
| (1,358) | 1:127:B:ILE:HG22 | 1:129:B:PHE:HD1 | 9        | 2.64          |
| (1,358) | 1:127:B:ILE:HG22 | 1:129:B:PHE:HD2 | 9        | 2.64          |
| (1,358) | 1:127:B:ILE:HG23 | 1:129:B:PHE:HD1 | 9        | 2.64          |
| (1,358) | 1:127:B:ILE:HG23 | 1:129:B:PHE:HD2 | 9        | 2.64          |
| (1,357) | 1:27:A:ILE:HG21  | 1:29:A:PHE:HD1  | 9        | 2.64          |
| (1,357) | 1:27:A:ILE:HG21  | 1:29:A:PHE:HD2  | 9        | 2.64          |
| (1,357) | 1:27:A:ILE:HG22  | 1:29:A:PHE:HD1  | 9        | 2.64          |
| (1,357) | 1:27:A:ILE:HG22  | 1:29:A:PHE:HD2  | 9        | 2.64          |
| (1,357) | 1:27:A:ILE:HG23  | 1:29:A:PHE:HD1  | 9        | 2.64          |
| (1,357) | 1:27:A:ILE:HG23  | 1:29:A:PHE:HD2  | 9        | 2.64          |
| (1,792) | 1:27:A:ILE:HG21  | 1:29:A:PHE:HD1  | 2        | 2.63          |
| (1,792) | 1:27:A:ILE:HG21  | 1:29:A:PHE:HD2  | 2        | 2.63          |
| (1,792) | 1:27:A:ILE:HG22  | 1:29:A:PHE:HD1  | 2        | 2.63          |
| (1,792) | 1:27:A:ILE:HG22  | 1:29:A:PHE:HD2  | 2        | 2.63          |
| (1,792) | 1:27:A:ILE:HG23  | 1:29:A:PHE:HD1  | 2        | 2.63          |
| (1,792) | 1:27:A:ILE:HG23  | 1:29:A:PHE:HD2  | 2        | 2.63          |
| (1,792) | 1:27:A:ILE:HG21  | 1:29:A:PHE:HD1  | 4        | 2.63          |
| (1,792) | 1:27:A:ILE:HG21  | 1:29:A:PHE:HD2  | 4        | 2.63          |
| (1,792) | 1:27:A:ILE:HG22  | 1:29:A:PHE:HD1  | 4        | 2.63          |
| (1,792) | 1:27:A:ILE:HG22  | 1:29:A:PHE:HD2  | 4        | 2.63          |
| (1,792) | 1:27:A:ILE:HG23  | 1:29:A:PHE:HD1  | 4        | 2.63          |
| (1,792) | 1:27:A:ILE:HG23  | 1:29:A:PHE:HD2  | 4        | 2.63          |
| (1,357) | 1:27:A:ILE:HG21  | 1:29:A:PHE:HD1  | 2        | 2.63          |
| (1,357) | 1:27:A:ILE:HG21  | 1:29:A:PHE:HD2  | 2        | 2.63          |
| (1,357) | 1:27:A:ILE:HG22  | 1:29:A:PHE:HD1  | 2        | 2.63          |
| (1,357) | 1:27:A:ILE:HG22  | 1:29:A:PHE:HD2  | 2        | 2.63          |
| (1,357) | 1:27:A:ILE:HG23  | 1:29:A:PHE:HD1  | 2        | 2.63          |
| (1,357) | 1:27:A:ILE:HG23  | 1:29:A:PHE:HD2  | 2        | 2.63          |

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| Key     | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|---------|------------------|-----------------|----------|---------------|
| (1,357) | 1:27:A:ILE:HG21  | 1:29:A:PHE:HD1  | 4        | 2.63          |
| (1,357) | 1:27:A:ILE:HG21  | 1:29:A:PHE:HD2  | 4        | 2.63          |
| (1,357) | 1:27:A:ILE:HG22  | 1:29:A:PHE:HD1  | 4        | 2.63          |
| (1,357) | 1:27:A:ILE:HG22  | 1:29:A:PHE:HD2  | 4        | 2.63          |
| (1,357) | 1:27:A:ILE:HG23  | 1:29:A:PHE:HD1  | 4        | 2.63          |
| (1,357) | 1:27:A:ILE:HG23  | 1:29:A:PHE:HD2  | 4        | 2.63          |
| (1,792) | 1:27:A:ILE:HG21  | 1:29:A:PHE:HD1  | 3        | 2.62          |
| (1,792) | 1:27:A:ILE:HG21  | 1:29:A:PHE:HD2  | 3        | 2.62          |
| (1,792) | 1:27:A:ILE:HG22  | 1:29:A:PHE:HD1  | 3        | 2.62          |
| (1,792) | 1:27:A:ILE:HG22  | 1:29:A:PHE:HD2  | 3        | 2.62          |
| (1,792) | 1:27:A:ILE:HG23  | 1:29:A:PHE:HD1  | 3        | 2.62          |
| (1,792) | 1:27:A:ILE:HG23  | 1:29:A:PHE:HD2  | 3        | 2.62          |
| (1,792) | 1:27:A:ILE:HG21  | 1:29:A:PHE:HD1  | 6        | 2.62          |
| (1,792) | 1:27:A:ILE:HG21  | 1:29:A:PHE:HD2  | 6        | 2.62          |
| (1,792) | 1:27:A:ILE:HG22  | 1:29:A:PHE:HD1  | 6        | 2.62          |
| (1,792) | 1:27:A:ILE:HG22  | 1:29:A:PHE:HD2  | 6        | 2.62          |
| (1,792) | 1:27:A:ILE:HG23  | 1:29:A:PHE:HD1  | 6        | 2.62          |
| (1,792) | 1:27:A:ILE:HG23  | 1:29:A:PHE:HD2  | 6        | 2.62          |
| (1,358) | 1:127:B:ILE:HG21 | 1:129:B:PHE:HD1 | 3        | 2.62          |
| (1,358) | 1:127:B:ILE:HG21 | 1:129:B:PHE:HD2 | 3        | 2.62          |
| (1,358) | 1:127:B:ILE:HG22 | 1:129:B:PHE:HD1 | 3        | 2.62          |
| (1,358) | 1:127:B:ILE:HG22 | 1:129:B:PHE:HD2 | 3        | 2.62          |
| (1,358) | 1:127:B:ILE:HG23 | 1:129:B:PHE:HD1 | 3        | 2.62          |
| (1,358) | 1:127:B:ILE:HG23 | 1:129:B:PHE:HD2 | 3        | 2.62          |
| (1,357) | 1:27:A:ILE:HG21  | 1:29:A:PHE:HD1  | 3        | 2.62          |
| (1,357) | 1:27:A:ILE:HG21  | 1:29:A:PHE:HD2  | 3        | 2.62          |
| (1,357) | 1:27:A:ILE:HG22  | 1:29:A:PHE:HD1  | 3        | 2.62          |
| (1,357) | 1:27:A:ILE:HG22  | 1:29:A:PHE:HD2  | 3        | 2.62          |
| (1,357) | 1:27:A:ILE:HG23  | 1:29:A:PHE:HD1  | 3        | 2.62          |
| (1,357) | 1:27:A:ILE:HG23  | 1:29:A:PHE:HD2  | 3        | 2.62          |
| (1,357) | 1:27:A:ILE:HG21  | 1:29:A:PHE:HD1  | 6        | 2.62          |
| (1,357) | 1:27:A:ILE:HG21  | 1:29:A:PHE:HD2  | 6        | 2.62          |
| (1,357) | 1:27:A:ILE:HG22  | 1:29:A:PHE:HD1  | 6        | 2.62          |
| (1,357) | 1:27:A:ILE:HG22  | 1:29:A:PHE:HD2  | 6        | 2.62          |
| (1,357) | 1:27:A:ILE:HG23  | 1:29:A:PHE:HD1  | 6        | 2.62          |
| (1,357) | 1:27:A:ILE:HG23  | 1:29:A:PHE:HD2  | 6        | 2.62          |
| (1,792) | 1:27:A:ILE:HG21  | 1:29:A:PHE:HD1  | 1        | 2.61          |
| (1,792) | 1:27:A:ILE:HG21  | 1:29:A:PHE:HD2  | 1        | 2.61          |
| (1,792) | 1:27:A:ILE:HG22  | 1:29:A:PHE:HD1  | 1        | 2.61          |
| (1,792) | 1:27:A:ILE:HG22  | 1:29:A:PHE:HD2  | 1        | 2.61          |
| (1,792) | 1:27:A:ILE:HG23  | 1:29:A:PHE:HD1  | 1        | 2.61          |
| (1,792) | 1:27:A:ILE:HG23  | 1:29:A:PHE:HD2  | 1        | 2.61          |

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| Key     | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|---------|------------------|-----------------|----------|---------------|
| (1,792) | 1:27:A:ILE:HG21  | 1:29:A:PHE:HD1  | 5        | 2.61          |
| (1,792) | 1:27:A:ILE:HG21  | 1:29:A:PHE:HD2  | 5        | 2.61          |
| (1,792) | 1:27:A:ILE:HG22  | 1:29:A:PHE:HD1  | 5        | 2.61          |
| (1,792) | 1:27:A:ILE:HG22  | 1:29:A:PHE:HD2  | 5        | 2.61          |
| (1,792) | 1:27:A:ILE:HG23  | 1:29:A:PHE:HD1  | 5        | 2.61          |
| (1,792) | 1:27:A:ILE:HG23  | 1:29:A:PHE:HD2  | 5        | 2.61          |
| (1,792) | 1:27:A:ILE:HG21  | 1:29:A:PHE:HD1  | 10       | 2.61          |
| (1,792) | 1:27:A:ILE:HG21  | 1:29:A:PHE:HD2  | 10       | 2.61          |
| (1,792) | 1:27:A:ILE:HG22  | 1:29:A:PHE:HD1  | 10       | 2.61          |
| (1,792) | 1:27:A:ILE:HG22  | 1:29:A:PHE:HD2  | 10       | 2.61          |
| (1,792) | 1:27:A:ILE:HG23  | 1:29:A:PHE:HD1  | 10       | 2.61          |
| (1,792) | 1:27:A:ILE:HG23  | 1:29:A:PHE:HD2  | 10       | 2.61          |
| (1,358) | 1:127:B:ILE:HG21 | 1:129:B:PHE:HD1 | 1        | 2.61          |
| (1,358) | 1:127:B:ILE:HG21 | 1:129:B:PHE:HD2 | 1        | 2.61          |
| (1,358) | 1:127:B:ILE:HG22 | 1:129:B:PHE:HD1 | 1        | 2.61          |
| (1,358) | 1:127:B:ILE:HG22 | 1:129:B:PHE:HD2 | 1        | 2.61          |
| (1,358) | 1:127:B:ILE:HG23 | 1:129:B:PHE:HD1 | 1        | 2.61          |
| (1,358) | 1:127:B:ILE:HG23 | 1:129:B:PHE:HD2 | 1        | 2.61          |
| (1,358) | 1:127:B:ILE:HG21 | 1:129:B:PHE:HD1 | 4        | 2.61          |
| (1,358) | 1:127:B:ILE:HG21 | 1:129:B:PHE:HD2 | 4        | 2.61          |
| (1,358) | 1:127:B:ILE:HG22 | 1:129:B:PHE:HD1 | 4        | 2.61          |
| (1,358) | 1:127:B:ILE:HG22 | 1:129:B:PHE:HD2 | 4        | 2.61          |
| (1,358) | 1:127:B:ILE:HG23 | 1:129:B:PHE:HD1 | 4        | 2.61          |
| (1,358) | 1:127:B:ILE:HG23 | 1:129:B:PHE:HD2 | 4        | 2.61          |
| (1,358) | 1:127:B:ILE:HG21 | 1:129:B:PHE:HD1 | 5        | 2.61          |
| (1,358) | 1:127:B:ILE:HG21 | 1:129:B:PHE:HD2 | 5        | 2.61          |
| (1,358) | 1:127:B:ILE:HG22 | 1:129:B:PHE:HD1 | 5        | 2.61          |
| (1,358) | 1:127:B:ILE:HG22 | 1:129:B:PHE:HD2 | 5        | 2.61          |
| (1,358) | 1:127:B:ILE:HG23 | 1:129:B:PHE:HD1 | 5        | 2.61          |
| (1,358) | 1:127:B:ILE:HG23 | 1:129:B:PHE:HD2 | 5        | 2.61          |
| (1,358) | 1:127:B:ILE:HG21 | 1:129:B:PHE:HD1 | 6        | 2.61          |
| (1,358) | 1:127:B:ILE:HG21 | 1:129:B:PHE:HD2 | 6        | 2.61          |
| (1,358) | 1:127:B:ILE:HG22 | 1:129:B:PHE:HD1 | 6        | 2.61          |
| (1,358) | 1:127:B:ILE:HG22 | 1:129:B:PHE:HD2 | 6        | 2.61          |
| (1,358) | 1:127:B:ILE:HG23 | 1:129:B:PHE:HD1 | 6        | 2.61          |
| (1,358) | 1:127:B:ILE:HG23 | 1:129:B:PHE:HD2 | 6        | 2.61          |
| (1,358) | 1:127:B:ILE:HG21 | 1:129:B:PHE:HD1 | 7        | 2.61          |
| (1,358) | 1:127:B:ILE:HG21 | 1:129:B:PHE:HD2 | 7        | 2.61          |
| (1,358) | 1:127:B:ILE:HG22 | 1:129:B:PHE:HD1 | 7        | 2.61          |
| (1,358) | 1:127:B:ILE:HG22 | 1:129:B:PHE:HD2 | 7        | 2.61          |
| (1,358) | 1:127:B:ILE:HG23 | 1:129:B:PHE:HD1 | 7        | 2.61          |
| (1,358) | 1:127:B:ILE:HG23 | 1:129:B:PHE:HD2 | 7        | 2.61          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,358) | 1:127:B:ILE:HG21 | 1:129:B:PHE:HD1  | 10       | 2.61          |
| (1,358) | 1:127:B:ILE:HG21 | 1:129:B:PHE:HD2  | 10       | 2.61          |
| (1,358) | 1:127:B:ILE:HG22 | 1:129:B:PHE:HD1  | 10       | 2.61          |
| (1,358) | 1:127:B:ILE:HG22 | 1:129:B:PHE:HD2  | 10       | 2.61          |
| (1,358) | 1:127:B:ILE:HG23 | 1:129:B:PHE:HD1  | 10       | 2.61          |
| (1,358) | 1:127:B:ILE:HG23 | 1:129:B:PHE:HD2  | 10       | 2.61          |
| (1,357) | 1:27:A:ILE:HG21  | 1:29:A:PHE:HD1   | 1        | 2.61          |
| (1,357) | 1:27:A:ILE:HG21  | 1:29:A:PHE:HD2   | 1        | 2.61          |
| (1,357) | 1:27:A:ILE:HG22  | 1:29:A:PHE:HD1   | 1        | 2.61          |
| (1,357) | 1:27:A:ILE:HG22  | 1:29:A:PHE:HD2   | 1        | 2.61          |
| (1,357) | 1:27:A:ILE:HG23  | 1:29:A:PHE:HD1   | 1        | 2.61          |
| (1,357) | 1:27:A:ILE:HG23  | 1:29:A:PHE:HD2   | 1        | 2.61          |
| (1,357) | 1:27:A:ILE:HG21  | 1:29:A:PHE:HD1   | 5        | 2.61          |
| (1,357) | 1:27:A:ILE:HG21  | 1:29:A:PHE:HD2   | 5        | 2.61          |
| (1,357) | 1:27:A:ILE:HG22  | 1:29:A:PHE:HD1   | 5        | 2.61          |
| (1,357) | 1:27:A:ILE:HG22  | 1:29:A:PHE:HD2   | 5        | 2.61          |
| (1,357) | 1:27:A:ILE:HG23  | 1:29:A:PHE:HD1   | 5        | 2.61          |
| (1,357) | 1:27:A:ILE:HG23  | 1:29:A:PHE:HD2   | 5        | 2.61          |
| (1,357) | 1:27:A:ILE:HG21  | 1:29:A:PHE:HD1   | 10       | 2.61          |
| (1,357) | 1:27:A:ILE:HG21  | 1:29:A:PHE:HD2   | 10       | 2.61          |
| (1,357) | 1:27:A:ILE:HG22  | 1:29:A:PHE:HD1   | 10       | 2.61          |
| (1,357) | 1:27:A:ILE:HG22  | 1:29:A:PHE:HD2   | 10       | 2.61          |
| (1,357) | 1:27:A:ILE:HG23  | 1:29:A:PHE:HD1   | 10       | 2.61          |
| (1,357) | 1:27:A:ILE:HG23  | 1:29:A:PHE:HD2   | 10       | 2.61          |
| (1,792) | 1:27:A:ILE:HG21  | 1:29:A:PHE:HD1   | 7        | 2.59          |
| (1,792) | 1:27:A:ILE:HG21  | 1:29:A:PHE:HD2   | 7        | 2.59          |
| (1,792) | 1:27:A:ILE:HG22  | 1:29:A:PHE:HD1   | 7        | 2.59          |
| (1,792) | 1:27:A:ILE:HG22  | 1:29:A:PHE:HD2   | 7        | 2.59          |
| (1,792) | 1:27:A:ILE:HG23  | 1:29:A:PHE:HD1   | 7        | 2.59          |
| (1,792) | 1:27:A:ILE:HG23  | 1:29:A:PHE:HD2   | 7        | 2.59          |
| (1,357) | 1:27:A:ILE:HG21  | 1:29:A:PHE:HD1   | 7        | 2.59          |
| (1,357) | 1:27:A:ILE:HG21  | 1:29:A:PHE:HD2   | 7        | 2.59          |
| (1,357) | 1:27:A:ILE:HG22  | 1:29:A:PHE:HD1   | 7        | 2.59          |
| (1,357) | 1:27:A:ILE:HG22  | 1:29:A:PHE:HD2   | 7        | 2.59          |
| (1,357) | 1:27:A:ILE:HG23  | 1:29:A:PHE:HD1   | 7        | 2.59          |
| (1,357) | 1:27:A:ILE:HG23  | 1:29:A:PHE:HD2   | 7        | 2.59          |
| (1,868) | 1:120:B:PHE:HD2  | 1:117:B:LEU:HD23 | 6        | 2.0           |
| (1,793) | 1:127:B:ILE:HG21 | 1:129:B:PHE:HD1  | 8        | 1.94          |
| (1,793) | 1:127:B:ILE:HG21 | 1:129:B:PHE:HD2  | 8        | 1.94          |
| (1,793) | 1:127:B:ILE:HG22 | 1:129:B:PHE:HD1  | 8        | 1.94          |
| (1,793) | 1:127:B:ILE:HG22 | 1:129:B:PHE:HD2  | 8        | 1.94          |
| (1,793) | 1:127:B:ILE:HG23 | 1:129:B:PHE:HD1  | 8        | 1.94          |

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| Key     | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|---------|------------------|-----------------|----------|---------------|
| (1,793) | 1:127:B:ILE:HG23 | 1:129:B:PHE:HD2 | 8        | 1.94          |
| (1,793) | 1:127:B:ILE:HG21 | 1:129:B:PHE:HD1 | 8        | 1.94          |
| (1,793) | 1:127:B:ILE:HG21 | 1:129:B:PHE:HD2 | 8        | 1.94          |
| (1,793) | 1:127:B:ILE:HG22 | 1:129:B:PHE:HD1 | 8        | 1.94          |
| (1,793) | 1:127:B:ILE:HG22 | 1:129:B:PHE:HD2 | 8        | 1.94          |
| (1,793) | 1:127:B:ILE:HG23 | 1:129:B:PHE:HD1 | 8        | 1.94          |
| (1,793) | 1:127:B:ILE:HG23 | 1:129:B:PHE:HD2 | 8        | 1.94          |
| (1,793) | 1:127:B:ILE:HG21 | 1:129:B:PHE:HD1 | 2        | 1.92          |
| (1,793) | 1:127:B:ILE:HG21 | 1:129:B:PHE:HD2 | 2        | 1.92          |
| (1,793) | 1:127:B:ILE:HG22 | 1:129:B:PHE:HD1 | 2        | 1.92          |
| (1,793) | 1:127:B:ILE:HG22 | 1:129:B:PHE:HD2 | 2        | 1.92          |
| (1,793) | 1:127:B:ILE:HG23 | 1:129:B:PHE:HD1 | 2        | 1.92          |
| (1,793) | 1:127:B:ILE:HG23 | 1:129:B:PHE:HD2 | 2        | 1.92          |
| (1,793) | 1:127:B:ILE:HG21 | 1:129:B:PHE:HD1 | 2        | 1.92          |
| (1,793) | 1:127:B:ILE:HG21 | 1:129:B:PHE:HD2 | 2        | 1.92          |
| (1,793) | 1:127:B:ILE:HG22 | 1:129:B:PHE:HD1 | 2        | 1.92          |
| (1,793) | 1:127:B:ILE:HG22 | 1:129:B:PHE:HD2 | 2        | 1.92          |
| (1,793) | 1:127:B:ILE:HG23 | 1:129:B:PHE:HD1 | 2        | 1.92          |
| (1,793) | 1:127:B:ILE:HG23 | 1:129:B:PHE:HD2 | 2        | 1.92          |
| (1,793) | 1:127:B:ILE:HG21 | 1:129:B:PHE:HD1 | 9        | 1.92          |
| (1,793) | 1:127:B:ILE:HG21 | 1:129:B:PHE:HD2 | 9        | 1.92          |
| (1,793) | 1:127:B:ILE:HG22 | 1:129:B:PHE:HD1 | 9        | 1.92          |
| (1,793) | 1:127:B:ILE:HG22 | 1:129:B:PHE:HD2 | 9        | 1.92          |
| (1,793) | 1:127:B:ILE:HG23 | 1:129:B:PHE:HD1 | 9        | 1.92          |
| (1,793) | 1:127:B:ILE:HG23 | 1:129:B:PHE:HD2 | 9        | 1.92          |
| (1,793) | 1:127:B:ILE:HG21 | 1:129:B:PHE:HD1 | 9        | 1.92          |
| (1,793) | 1:127:B:ILE:HG21 | 1:129:B:PHE:HD2 | 9        | 1.92          |
| (1,793) | 1:127:B:ILE:HG22 | 1:129:B:PHE:HD1 | 9        | 1.92          |
| (1,793) | 1:127:B:ILE:HG22 | 1:129:B:PHE:HD2 | 9        | 1.92          |
| (1,793) | 1:127:B:ILE:HG23 | 1:129:B:PHE:HD1 | 9        | 1.92          |
| (1,793) | 1:127:B:ILE:HG23 | 1:129:B:PHE:HD2 | 9        | 1.92          |
| (1,793) | 1:127:B:ILE:HG21 | 1:129:B:PHE:HD1 | 3        | 1.91          |
| (1,793) | 1:127:B:ILE:HG21 | 1:129:B:PHE:HD2 | 3        | 1.91          |
| (1,793) | 1:127:B:ILE:HG22 | 1:129:B:PHE:HD1 | 3        | 1.91          |
| (1,793) | 1:127:B:ILE:HG22 | 1:129:B:PHE:HD2 | 3        | 1.91          |
| (1,793) | 1:127:B:ILE:HG23 | 1:129:B:PHE:HD1 | 3        | 1.91          |
| (1,793) | 1:127:B:ILE:HG23 | 1:129:B:PHE:HD2 | 3        | 1.91          |
| (1,793) | 1:127:B:ILE:HG21 | 1:129:B:PHE:HD1 | 3        | 1.91          |
| (1,793) | 1:127:B:ILE:HG21 | 1:129:B:PHE:HD2 | 3        | 1.91          |
| (1,793) | 1:127:B:ILE:HG22 | 1:129:B:PHE:HD1 | 3        | 1.91          |
| (1,793) | 1:127:B:ILE:HG22 | 1:129:B:PHE:HD2 | 3        | 1.91          |
| (1,793) | 1:127:B:ILE:HG23 | 1:129:B:PHE:HD1 | 3        | 1.91          |

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| Key     | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|---------|------------------|-----------------|----------|---------------|
| (1,793) | 1:127:B:ILE:HG23 | 1:129:B:PHE:HD2 | 3        | 1.91          |
| (1,793) | 1:127:B:ILE:HG21 | 1:129:B:PHE:HD1 | 1        | 1.9           |
| (1,793) | 1:127:B:ILE:HG21 | 1:129:B:PHE:HD2 | 1        | 1.9           |
| (1,793) | 1:127:B:ILE:HG22 | 1:129:B:PHE:HD1 | 1        | 1.9           |
| (1,793) | 1:127:B:ILE:HG22 | 1:129:B:PHE:HD2 | 1        | 1.9           |
| (1,793) | 1:127:B:ILE:HG23 | 1:129:B:PHE:HD1 | 1        | 1.9           |
| (1,793) | 1:127:B:ILE:HG23 | 1:129:B:PHE:HD2 | 1        | 1.9           |
| (1,793) | 1:127:B:ILE:HG21 | 1:129:B:PHE:HD1 | 1        | 1.9           |
| (1,793) | 1:127:B:ILE:HG21 | 1:129:B:PHE:HD2 | 1        | 1.9           |
| (1,793) | 1:127:B:ILE:HG22 | 1:129:B:PHE:HD1 | 1        | 1.9           |
| (1,793) | 1:127:B:ILE:HG22 | 1:129:B:PHE:HD2 | 1        | 1.9           |
| (1,793) | 1:127:B:ILE:HG23 | 1:129:B:PHE:HD1 | 1        | 1.9           |
| (1,793) | 1:127:B:ILE:HG23 | 1:129:B:PHE:HD2 | 1        | 1.9           |
| (1,793) | 1:127:B:ILE:HG21 | 1:129:B:PHE:HD1 | 4        | 1.9           |
| (1,793) | 1:127:B:ILE:HG21 | 1:129:B:PHE:HD2 | 4        | 1.9           |
| (1,793) | 1:127:B:ILE:HG22 | 1:129:B:PHE:HD1 | 4        | 1.9           |
| (1,793) | 1:127:B:ILE:HG22 | 1:129:B:PHE:HD2 | 4        | 1.9           |
| (1,793) | 1:127:B:ILE:HG23 | 1:129:B:PHE:HD1 | 4        | 1.9           |
| (1,793) | 1:127:B:ILE:HG23 | 1:129:B:PHE:HD2 | 4        | 1.9           |
| (1,793) | 1:127:B:ILE:HG21 | 1:129:B:PHE:HD1 | 4        | 1.9           |
| (1,793) | 1:127:B:ILE:HG21 | 1:129:B:PHE:HD2 | 4        | 1.9           |
| (1,793) | 1:127:B:ILE:HG22 | 1:129:B:PHE:HD1 | 4        | 1.9           |
| (1,793) | 1:127:B:ILE:HG22 | 1:129:B:PHE:HD2 | 4        | 1.9           |
| (1,793) | 1:127:B:ILE:HG23 | 1:129:B:PHE:HD1 | 4        | 1.9           |
| (1,793) | 1:127:B:ILE:HG23 | 1:129:B:PHE:HD2 | 4        | 1.9           |
| (1,793) | 1:127:B:ILE:HG21 | 1:129:B:PHE:HD1 | 5        | 1.9           |
| (1,793) | 1:127:B:ILE:HG21 | 1:129:B:PHE:HD2 | 5        | 1.9           |
| (1,793) | 1:127:B:ILE:HG22 | 1:129:B:PHE:HD1 | 5        | 1.9           |
| (1,793) | 1:127:B:ILE:HG22 | 1:129:B:PHE:HD2 | 5        | 1.9           |
| (1,793) | 1:127:B:ILE:HG23 | 1:129:B:PHE:HD1 | 5        | 1.9           |
| (1,793) | 1:127:B:ILE:HG23 | 1:129:B:PHE:HD2 | 5        | 1.9           |
| (1,793) | 1:127:B:ILE:HG21 | 1:129:B:PHE:HD1 | 5        | 1.9           |
| (1,793) | 1:127:B:ILE:HG21 | 1:129:B:PHE:HD2 | 5        | 1.9           |
| (1,793) | 1:127:B:ILE:HG22 | 1:129:B:PHE:HD1 | 5        | 1.9           |
| (1,793) | 1:127:B:ILE:HG22 | 1:129:B:PHE:HD2 | 5        | 1.9           |
| (1,793) | 1:127:B:ILE:HG23 | 1:129:B:PHE:HD1 | 5        | 1.9           |
| (1,793) | 1:127:B:ILE:HG23 | 1:129:B:PHE:HD2 | 5        | 1.9           |
| (1,793) | 1:127:B:ILE:HG21 | 1:129:B:PHE:HD1 | 6        | 1.9           |
| (1,793) | 1:127:B:ILE:HG21 | 1:129:B:PHE:HD2 | 6        | 1.9           |
| (1,793) | 1:127:B:ILE:HG22 | 1:129:B:PHE:HD1 | 6        | 1.9           |
| (1,793) | 1:127:B:ILE:HG22 | 1:129:B:PHE:HD2 | 6        | 1.9           |
| (1,793) | 1:127:B:ILE:HG23 | 1:129:B:PHE:HD1 | 6        | 1.9           |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,793) | 1:127:B:ILE:HG23 | 1:129:B:PHE:HD2  | 6        | 1.9           |
| (1,793) | 1:127:B:ILE:HG21 | 1:129:B:PHE:HD1  | 6        | 1.9           |
| (1,793) | 1:127:B:ILE:HG21 | 1:129:B:PHE:HD2  | 6        | 1.9           |
| (1,793) | 1:127:B:ILE:HG22 | 1:129:B:PHE:HD1  | 6        | 1.9           |
| (1,793) | 1:127:B:ILE:HG22 | 1:129:B:PHE:HD2  | 6        | 1.9           |
| (1,793) | 1:127:B:ILE:HG23 | 1:129:B:PHE:HD1  | 6        | 1.9           |
| (1,793) | 1:127:B:ILE:HG23 | 1:129:B:PHE:HD2  | 6        | 1.9           |
| (1,793) | 1:127:B:ILE:HG21 | 1:129:B:PHE:HD1  | 7        | 1.9           |
| (1,793) | 1:127:B:ILE:HG21 | 1:129:B:PHE:HD2  | 7        | 1.9           |
| (1,793) | 1:127:B:ILE:HG22 | 1:129:B:PHE:HD1  | 7        | 1.9           |
| (1,793) | 1:127:B:ILE:HG22 | 1:129:B:PHE:HD2  | 7        | 1.9           |
| (1,793) | 1:127:B:ILE:HG23 | 1:129:B:PHE:HD1  | 7        | 1.9           |
| (1,793) | 1:127:B:ILE:HG23 | 1:129:B:PHE:HD2  | 7        | 1.9           |
| (1,793) | 1:127:B:ILE:HG21 | 1:129:B:PHE:HD1  | 7        | 1.9           |
| (1,793) | 1:127:B:ILE:HG21 | 1:129:B:PHE:HD2  | 7        | 1.9           |
| (1,793) | 1:127:B:ILE:HG22 | 1:129:B:PHE:HD1  | 7        | 1.9           |
| (1,793) | 1:127:B:ILE:HG22 | 1:129:B:PHE:HD2  | 7        | 1.9           |
| (1,793) | 1:127:B:ILE:HG23 | 1:129:B:PHE:HD1  | 7        | 1.9           |
| (1,793) | 1:127:B:ILE:HG23 | 1:129:B:PHE:HD2  | 7        | 1.9           |
| (1,793) | 1:127:B:ILE:HG21 | 1:129:B:PHE:HD1  | 10       | 1.9           |
| (1,793) | 1:127:B:ILE:HG21 | 1:129:B:PHE:HD2  | 10       | 1.9           |
| (1,793) | 1:127:B:ILE:HG22 | 1:129:B:PHE:HD1  | 10       | 1.9           |
| (1,793) | 1:127:B:ILE:HG22 | 1:129:B:PHE:HD2  | 10       | 1.9           |
| (1,793) | 1:127:B:ILE:HG23 | 1:129:B:PHE:HD1  | 10       | 1.9           |
| (1,793) | 1:127:B:ILE:HG23 | 1:129:B:PHE:HD2  | 10       | 1.9           |
| (1,793) | 1:127:B:ILE:HG21 | 1:129:B:PHE:HD1  | 10       | 1.9           |
| (1,793) | 1:127:B:ILE:HG21 | 1:129:B:PHE:HD2  | 10       | 1.9           |
| (1,793) | 1:127:B:ILE:HG22 | 1:129:B:PHE:HD1  | 10       | 1.9           |
| (1,793) | 1:127:B:ILE:HG22 | 1:129:B:PHE:HD2  | 10       | 1.9           |
| (1,793) | 1:127:B:ILE:HG23 | 1:129:B:PHE:HD1  | 10       | 1.9           |
| (1,793) | 1:127:B:ILE:HG23 | 1:129:B:PHE:HD2  | 10       | 1.9           |
| (1,868) | 1:120:B:PHE:HD2  | 1:117:B:LEU:HD23 | 10       | 1.82          |
| (1,868) | 1:120:B:PHE:HD2  | 1:117:B:LEU:HD21 | 5        | 1.81          |
| (1,868) | 1:120:B:PHE:HD2  | 1:117:B:LEU:HD22 | 8        | 1.73          |
| (1,868) | 1:120:B:PHE:HD2  | 1:117:B:LEU:HD23 | 2        | 1.7           |
| (1,868) | 1:120:B:PHE:HD2  | 1:117:B:LEU:HD22 | 4        | 1.62          |
| (1,868) | 1:120:B:PHE:HD2  | 1:117:B:LEU:HD22 | 1        | 1.53          |
| (1,535) | 1:122:B:PHE:HD2  | 1:123:B:ILE:H    | 5        | 1.39          |
| (1,534) | 1:122:B:PHE:HD2  | 1:123:B:ILE:H    | 5        | 1.39          |
| (1,533) | 1:22:A:PHE:HD2   | 1:23:A:ILE:H     | 5        | 1.39          |
| (1,421) | 1:14:A:THR:HG23  | 1:110:B:PHE:HE2  | 9        | 1.34          |
| (1,868) | 1:120:B:PHE:HD2  | 1:117:B:LEU:HD21 | 3        | 1.31          |

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| Key     | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (1,535) | 1:122:B:PHE:HD2 | 1:123:B:ILE:H    | 6        | 1.29          |
| (1,534) | 1:122:B:PHE:HD2 | 1:123:B:ILE:H    | 6        | 1.29          |
| (1,533) | 1:22:A:PHE:HD2  | 1:23:A:ILE:H     | 6        | 1.28          |
| (1,364) | 1:124:B:VAL:HA  | 1:125:B:LEU:HD21 | 8        | 1.25          |
| (1,364) | 1:124:B:VAL:HA  | 1:125:B:LEU:HD22 | 8        | 1.25          |
| (1,364) | 1:124:B:VAL:HA  | 1:125:B:LEU:HD23 | 8        | 1.25          |
| (1,798) | 1:24:A:VAL:HA   | 1:25:A:LEU:HD21  | 8        | 1.24          |
| (1,798) | 1:24:A:VAL:HA   | 1:25:A:LEU:HD22  | 8        | 1.24          |
| (1,798) | 1:24:A:VAL:HA   | 1:25:A:LEU:HD23  | 8        | 1.24          |
| (1,364) | 1:124:B:VAL:HA  | 1:125:B:LEU:HD21 | 2        | 1.24          |
| (1,364) | 1:124:B:VAL:HA  | 1:125:B:LEU:HD22 | 2        | 1.24          |
| (1,364) | 1:124:B:VAL:HA  | 1:125:B:LEU:HD23 | 2        | 1.24          |
| (1,363) | 1:24:A:VAL:HA   | 1:25:A:LEU:HD21  | 8        | 1.24          |
| (1,363) | 1:24:A:VAL:HA   | 1:25:A:LEU:HD22  | 8        | 1.24          |
| (1,363) | 1:24:A:VAL:HA   | 1:25:A:LEU:HD23  | 8        | 1.24          |
| (1,798) | 1:24:A:VAL:HA   | 1:25:A:LEU:HD21  | 2        | 1.22          |
| (1,798) | 1:24:A:VAL:HA   | 1:25:A:LEU:HD22  | 2        | 1.22          |
| (1,798) | 1:24:A:VAL:HA   | 1:25:A:LEU:HD23  | 2        | 1.22          |
| (1,798) | 1:24:A:VAL:HA   | 1:25:A:LEU:HD21  | 9        | 1.22          |
| (1,798) | 1:24:A:VAL:HA   | 1:25:A:LEU:HD22  | 9        | 1.22          |
| (1,798) | 1:24:A:VAL:HA   | 1:25:A:LEU:HD23  | 9        | 1.22          |
| (1,363) | 1:24:A:VAL:HA   | 1:25:A:LEU:HD21  | 2        | 1.22          |
| (1,363) | 1:24:A:VAL:HA   | 1:25:A:LEU:HD22  | 2        | 1.22          |
| (1,363) | 1:24:A:VAL:HA   | 1:25:A:LEU:HD23  | 2        | 1.22          |
| (1,363) | 1:24:A:VAL:HA   | 1:25:A:LEU:HD21  | 9        | 1.22          |
| (1,363) | 1:24:A:VAL:HA   | 1:25:A:LEU:HD22  | 9        | 1.22          |
| (1,363) | 1:24:A:VAL:HA   | 1:25:A:LEU:HD23  | 9        | 1.22          |
| (1,865) | 1:120:B:PHE:HA  | 1:121:B:ILE:HG21 | 9        | 1.21          |
| (1,865) | 1:120:B:PHE:HA  | 1:121:B:ILE:HG22 | 9        | 1.21          |
| (1,865) | 1:120:B:PHE:HA  | 1:121:B:ILE:HG23 | 9        | 1.21          |
| (1,533) | 1:22:A:PHE:HD2  | 1:23:A:ILE:H     | 10       | 1.21          |
| (1,364) | 1:124:B:VAL:HA  | 1:125:B:LEU:HD21 | 9        | 1.2           |
| (1,364) | 1:124:B:VAL:HA  | 1:125:B:LEU:HD22 | 9        | 1.2           |
| (1,364) | 1:124:B:VAL:HA  | 1:125:B:LEU:HD23 | 9        | 1.2           |
| (1,364) | 1:124:B:VAL:HA  | 1:125:B:LEU:HD21 | 1        | 1.19          |
| (1,364) | 1:124:B:VAL:HA  | 1:125:B:LEU:HD22 | 1        | 1.19          |
| (1,364) | 1:124:B:VAL:HA  | 1:125:B:LEU:HD23 | 1        | 1.19          |
| (1,865) | 1:120:B:PHE:HA  | 1:121:B:ILE:HG21 | 1        | 1.17          |
| (1,865) | 1:120:B:PHE:HA  | 1:121:B:ILE:HG22 | 1        | 1.17          |
| (1,865) | 1:120:B:PHE:HA  | 1:121:B:ILE:HG23 | 1        | 1.17          |
| (1,865) | 1:120:B:PHE:HA  | 1:121:B:ILE:HG21 | 2        | 1.17          |
| (1,865) | 1:120:B:PHE:HA  | 1:121:B:ILE:HG22 | 2        | 1.17          |

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| Key     | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (1,865) | 1:120:B:PHE:HA  | 1:121:B:ILE:HG23 | 2        | 1.17          |
| (1,865) | 1:120:B:PHE:HA  | 1:121:B:ILE:HG21 | 3        | 1.17          |
| (1,865) | 1:120:B:PHE:HA  | 1:121:B:ILE:HG22 | 3        | 1.17          |
| (1,865) | 1:120:B:PHE:HA  | 1:121:B:ILE:HG23 | 3        | 1.17          |
| (1,865) | 1:120:B:PHE:HA  | 1:121:B:ILE:HG21 | 6        | 1.17          |
| (1,865) | 1:120:B:PHE:HA  | 1:121:B:ILE:HG22 | 6        | 1.17          |
| (1,865) | 1:120:B:PHE:HA  | 1:121:B:ILE:HG23 | 6        | 1.17          |
| (1,865) | 1:120:B:PHE:HA  | 1:121:B:ILE:HG21 | 8        | 1.17          |
| (1,865) | 1:120:B:PHE:HA  | 1:121:B:ILE:HG22 | 8        | 1.17          |
| (1,865) | 1:120:B:PHE:HA  | 1:121:B:ILE:HG23 | 8        | 1.17          |
| (1,865) | 1:120:B:PHE:HA  | 1:121:B:ILE:HG21 | 10       | 1.17          |
| (1,865) | 1:120:B:PHE:HA  | 1:121:B:ILE:HG22 | 10       | 1.17          |
| (1,865) | 1:120:B:PHE:HA  | 1:121:B:ILE:HG23 | 10       | 1.17          |
| (1,798) | 1:24:A:VAL:HA   | 1:25:A:LEU:HD21  | 1        | 1.17          |
| (1,798) | 1:24:A:VAL:HA   | 1:25:A:LEU:HD22  | 1        | 1.17          |
| (1,798) | 1:24:A:VAL:HA   | 1:25:A:LEU:HD23  | 1        | 1.17          |
| (1,535) | 1:122:B:PHE:HD2 | 1:123:B:ILE:H    | 10       | 1.17          |
| (1,534) | 1:122:B:PHE:HD2 | 1:123:B:ILE:H    | 10       | 1.17          |
| (1,363) | 1:24:A:VAL:HA   | 1:25:A:LEU:HD21  | 1        | 1.17          |
| (1,363) | 1:24:A:VAL:HA   | 1:25:A:LEU:HD22  | 1        | 1.17          |
| (1,363) | 1:24:A:VAL:HA   | 1:25:A:LEU:HD23  | 1        | 1.17          |
| (1,865) | 1:120:B:PHE:HA  | 1:121:B:ILE:HG21 | 4        | 1.16          |
| (1,865) | 1:120:B:PHE:HA  | 1:121:B:ILE:HG22 | 4        | 1.16          |
| (1,865) | 1:120:B:PHE:HA  | 1:121:B:ILE:HG23 | 4        | 1.16          |
| (1,865) | 1:120:B:PHE:HA  | 1:121:B:ILE:HG21 | 5        | 1.16          |
| (1,865) | 1:120:B:PHE:HA  | 1:121:B:ILE:HG22 | 5        | 1.16          |
| (1,865) | 1:120:B:PHE:HA  | 1:121:B:ILE:HG23 | 5        | 1.16          |
| (1,865) | 1:120:B:PHE:HA  | 1:121:B:ILE:HG21 | 7        | 1.15          |
| (1,865) | 1:120:B:PHE:HA  | 1:121:B:ILE:HG22 | 7        | 1.15          |
| (1,865) | 1:120:B:PHE:HA  | 1:121:B:ILE:HG23 | 7        | 1.15          |
| (1,364) | 1:124:B:VAL:HA  | 1:125:B:LEU:HD21 | 3        | 1.14          |
| (1,364) | 1:124:B:VAL:HA  | 1:125:B:LEU:HD22 | 3        | 1.14          |
| (1,364) | 1:124:B:VAL:HA  | 1:125:B:LEU:HD23 | 3        | 1.14          |
| (1,798) | 1:24:A:VAL:HA   | 1:25:A:LEU:HD21  | 3        | 1.13          |
| (1,798) | 1:24:A:VAL:HA   | 1:25:A:LEU:HD22  | 3        | 1.13          |
| (1,798) | 1:24:A:VAL:HA   | 1:25:A:LEU:HD23  | 3        | 1.13          |
| (1,363) | 1:24:A:VAL:HA   | 1:25:A:LEU:HD21  | 3        | 1.13          |
| (1,363) | 1:24:A:VAL:HA   | 1:25:A:LEU:HD22  | 3        | 1.13          |
| (1,363) | 1:24:A:VAL:HA   | 1:25:A:LEU:HD23  | 3        | 1.13          |
| (1,364) | 1:124:B:VAL:HA  | 1:125:B:LEU:HD21 | 5        | 1.05          |
| (1,364) | 1:124:B:VAL:HA  | 1:125:B:LEU:HD22 | 5        | 1.05          |
| (1,364) | 1:124:B:VAL:HA  | 1:125:B:LEU:HD23 | 5        | 1.05          |

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| Key     | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (1,830) | 1:18:A:LEU:HD21 | 1:22:A:PHE:HB2   | 6        | 1.04          |
| (1,830) | 1:18:A:LEU:HD21 | 1:22:A:PHE:HB3   | 6        | 1.04          |
| (1,830) | 1:18:A:LEU:HD22 | 1:22:A:PHE:HB2   | 6        | 1.04          |
| (1,830) | 1:18:A:LEU:HD22 | 1:22:A:PHE:HB3   | 6        | 1.04          |
| (1,830) | 1:18:A:LEU:HD23 | 1:22:A:PHE:HB2   | 6        | 1.04          |
| (1,830) | 1:18:A:LEU:HD23 | 1:22:A:PHE:HB3   | 6        | 1.04          |
| (1,798) | 1:24:A:VAL:HA   | 1:25:A:LEU:HD21  | 5        | 0.99          |
| (1,798) | 1:24:A:VAL:HA   | 1:25:A:LEU:HD22  | 5        | 0.99          |
| (1,798) | 1:24:A:VAL:HA   | 1:25:A:LEU:HD23  | 5        | 0.99          |
| (1,363) | 1:24:A:VAL:HA   | 1:25:A:LEU:HD21  | 5        | 0.99          |
| (1,363) | 1:24:A:VAL:HA   | 1:25:A:LEU:HD22  | 5        | 0.99          |
| (1,363) | 1:24:A:VAL:HA   | 1:25:A:LEU:HD23  | 5        | 0.99          |
| (1,830) | 1:18:A:LEU:HD21 | 1:22:A:PHE:HB2   | 3        | 0.98          |
| (1,830) | 1:18:A:LEU:HD21 | 1:22:A:PHE:HB3   | 3        | 0.98          |
| (1,830) | 1:18:A:LEU:HD22 | 1:22:A:PHE:HB2   | 3        | 0.98          |
| (1,830) | 1:18:A:LEU:HD22 | 1:22:A:PHE:HB3   | 3        | 0.98          |
| (1,830) | 1:18:A:LEU:HD23 | 1:22:A:PHE:HB2   | 3        | 0.98          |
| (1,830) | 1:18:A:LEU:HD23 | 1:22:A:PHE:HB3   | 3        | 0.98          |
| (1,830) | 1:18:A:LEU:HD21 | 1:22:A:PHE:HB2   | 10       | 0.96          |
| (1,830) | 1:18:A:LEU:HD21 | 1:22:A:PHE:HB3   | 10       | 0.96          |
| (1,830) | 1:18:A:LEU:HD22 | 1:22:A:PHE:HB2   | 10       | 0.96          |
| (1,830) | 1:18:A:LEU:HD22 | 1:22:A:PHE:HB3   | 10       | 0.96          |
| (1,830) | 1:18:A:LEU:HD23 | 1:22:A:PHE:HB2   | 10       | 0.96          |
| (1,830) | 1:18:A:LEU:HD23 | 1:22:A:PHE:HB3   | 10       | 0.96          |
| (1,798) | 1:24:A:VAL:HA   | 1:25:A:LEU:HD21  | 7        | 0.95          |
| (1,798) | 1:24:A:VAL:HA   | 1:25:A:LEU:HD22  | 7        | 0.95          |
| (1,798) | 1:24:A:VAL:HA   | 1:25:A:LEU:HD23  | 7        | 0.95          |
| (1,363) | 1:24:A:VAL:HA   | 1:25:A:LEU:HD21  | 7        | 0.95          |
| (1,363) | 1:24:A:VAL:HA   | 1:25:A:LEU:HD22  | 7        | 0.95          |
| (1,363) | 1:24:A:VAL:HA   | 1:25:A:LEU:HD23  | 7        | 0.95          |
| (1,830) | 1:18:A:LEU:HD21 | 1:22:A:PHE:HB2   | 2        | 0.92          |
| (1,830) | 1:18:A:LEU:HD21 | 1:22:A:PHE:HB3   | 2        | 0.92          |
| (1,830) | 1:18:A:LEU:HD22 | 1:22:A:PHE:HB2   | 2        | 0.92          |
| (1,830) | 1:18:A:LEU:HD22 | 1:22:A:PHE:HB3   | 2        | 0.92          |
| (1,830) | 1:18:A:LEU:HD23 | 1:22:A:PHE:HB2   | 2        | 0.92          |
| (1,830) | 1:18:A:LEU:HD23 | 1:22:A:PHE:HB3   | 2        | 0.92          |
| (1,364) | 1:124:B:VAL:HA  | 1:125:B:LEU:HD21 | 6        | 0.92          |
| (1,364) | 1:124:B:VAL:HA  | 1:125:B:LEU:HD22 | 6        | 0.92          |
| (1,364) | 1:124:B:VAL:HA  | 1:125:B:LEU:HD23 | 6        | 0.92          |
| (1,364) | 1:124:B:VAL:HA  | 1:125:B:LEU:HD21 | 7        | 0.92          |
| (1,364) | 1:124:B:VAL:HA  | 1:125:B:LEU:HD22 | 7        | 0.92          |
| (1,364) | 1:124:B:VAL:HA  | 1:125:B:LEU:HD23 | 7        | 0.92          |

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| Key     | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (1,798) | 1:24:A:VAL:HA   | 1:25:A:LEU:HD21  | 6        | 0.91          |
| (1,798) | 1:24:A:VAL:HA   | 1:25:A:LEU:HD22  | 6        | 0.91          |
| (1,798) | 1:24:A:VAL:HA   | 1:25:A:LEU:HD23  | 6        | 0.91          |
| (1,363) | 1:24:A:VAL:HA   | 1:25:A:LEU:HD21  | 6        | 0.91          |
| (1,363) | 1:24:A:VAL:HA   | 1:25:A:LEU:HD22  | 6        | 0.91          |
| (1,363) | 1:24:A:VAL:HA   | 1:25:A:LEU:HD23  | 6        | 0.91          |
| (1,871) | 1:120:B:PHE:HB2 | 1:121:B:ILE:HD11 | 8        | 0.89          |
| (1,871) | 1:120:B:PHE:HB2 | 1:121:B:ILE:HD12 | 8        | 0.89          |
| (1,871) | 1:120:B:PHE:HB2 | 1:121:B:ILE:HD13 | 8        | 0.89          |
| (1,871) | 1:120:B:PHE:HB3 | 1:121:B:ILE:HD11 | 8        | 0.89          |
| (1,871) | 1:120:B:PHE:HB3 | 1:121:B:ILE:HD12 | 8        | 0.89          |
| (1,871) | 1:120:B:PHE:HB3 | 1:121:B:ILE:HD13 | 8        | 0.89          |
| (1,830) | 1:18:A:LEU:HD21 | 1:22:A:PHE:HB2   | 5        | 0.89          |
| (1,830) | 1:18:A:LEU:HD21 | 1:22:A:PHE:HB3   | 5        | 0.89          |
| (1,830) | 1:18:A:LEU:HD22 | 1:22:A:PHE:HB2   | 5        | 0.89          |
| (1,830) | 1:18:A:LEU:HD22 | 1:22:A:PHE:HB3   | 5        | 0.89          |
| (1,830) | 1:18:A:LEU:HD23 | 1:22:A:PHE:HB2   | 5        | 0.89          |
| (1,830) | 1:18:A:LEU:HD23 | 1:22:A:PHE:HB3   | 5        | 0.89          |
| (1,871) | 1:120:B:PHE:HB2 | 1:121:B:ILE:HD11 | 1        | 0.88          |
| (1,871) | 1:120:B:PHE:HB2 | 1:121:B:ILE:HD12 | 1        | 0.88          |
| (1,871) | 1:120:B:PHE:HB2 | 1:121:B:ILE:HD13 | 1        | 0.88          |
| (1,871) | 1:120:B:PHE:HB3 | 1:121:B:ILE:HD11 | 1        | 0.88          |
| (1,871) | 1:120:B:PHE:HB3 | 1:121:B:ILE:HD12 | 1        | 0.88          |
| (1,871) | 1:120:B:PHE:HB3 | 1:121:B:ILE:HD13 | 1        | 0.88          |
| (1,830) | 1:18:A:LEU:HD21 | 1:22:A:PHE:HB2   | 7        | 0.88          |
| (1,830) | 1:18:A:LEU:HD21 | 1:22:A:PHE:HB3   | 7        | 0.88          |
| (1,830) | 1:18:A:LEU:HD22 | 1:22:A:PHE:HB2   | 7        | 0.88          |
| (1,830) | 1:18:A:LEU:HD22 | 1:22:A:PHE:HB3   | 7        | 0.88          |
| (1,830) | 1:18:A:LEU:HD23 | 1:22:A:PHE:HB2   | 7        | 0.88          |
| (1,830) | 1:18:A:LEU:HD23 | 1:22:A:PHE:HB3   | 7        | 0.88          |
| (1,871) | 1:120:B:PHE:HB2 | 1:121:B:ILE:HD11 | 2        | 0.87          |
| (1,871) | 1:120:B:PHE:HB2 | 1:121:B:ILE:HD12 | 2        | 0.87          |
| (1,871) | 1:120:B:PHE:HB2 | 1:121:B:ILE:HD13 | 2        | 0.87          |
| (1,871) | 1:120:B:PHE:HB3 | 1:121:B:ILE:HD11 | 2        | 0.87          |
| (1,871) | 1:120:B:PHE:HB3 | 1:121:B:ILE:HD12 | 2        | 0.87          |
| (1,871) | 1:120:B:PHE:HB3 | 1:121:B:ILE:HD13 | 2        | 0.87          |
| (1,871) | 1:120:B:PHE:HB2 | 1:121:B:ILE:HD11 | 9        | 0.87          |
| (1,871) | 1:120:B:PHE:HB2 | 1:121:B:ILE:HD12 | 9        | 0.87          |
| (1,871) | 1:120:B:PHE:HB2 | 1:121:B:ILE:HD13 | 9        | 0.87          |
| (1,871) | 1:120:B:PHE:HB3 | 1:121:B:ILE:HD11 | 9        | 0.87          |
| (1,871) | 1:120:B:PHE:HB3 | 1:121:B:ILE:HD12 | 9        | 0.87          |
| (1,871) | 1:120:B:PHE:HB3 | 1:121:B:ILE:HD13 | 9        | 0.87          |

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| Key     | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (1,830) | 1:18:A:LEU:HD21 | 1:22:A:PHE:HB2   | 1        | 0.87          |
| (1,830) | 1:18:A:LEU:HD21 | 1:22:A:PHE:HB3   | 1        | 0.87          |
| (1,830) | 1:18:A:LEU:HD22 | 1:22:A:PHE:HB2   | 1        | 0.87          |
| (1,830) | 1:18:A:LEU:HD22 | 1:22:A:PHE:HB3   | 1        | 0.87          |
| (1,830) | 1:18:A:LEU:HD23 | 1:22:A:PHE:HB2   | 1        | 0.87          |
| (1,830) | 1:18:A:LEU:HD23 | 1:22:A:PHE:HB3   | 1        | 0.87          |
| (1,830) | 1:18:A:LEU:HD21 | 1:22:A:PHE:HB2   | 8        | 0.86          |
| (1,830) | 1:18:A:LEU:HD21 | 1:22:A:PHE:HB3   | 8        | 0.86          |
| (1,830) | 1:18:A:LEU:HD22 | 1:22:A:PHE:HB2   | 8        | 0.86          |
| (1,830) | 1:18:A:LEU:HD22 | 1:22:A:PHE:HB3   | 8        | 0.86          |
| (1,830) | 1:18:A:LEU:HD23 | 1:22:A:PHE:HB2   | 8        | 0.86          |
| (1,830) | 1:18:A:LEU:HD23 | 1:22:A:PHE:HB3   | 8        | 0.86          |
| (1,535) | 1:122:B:PHE:HD2 | 1:123:B:ILE:H    | 4        | 0.85          |
| (1,534) | 1:122:B:PHE:HD2 | 1:123:B:ILE:H    | 4        | 0.85          |
| (1,533) | 1:22:A:PHE:HD2  | 1:23:A:ILE:H     | 4        | 0.85          |
| (1,364) | 1:124:B:VAL:HA  | 1:125:B:LEU:HD21 | 4        | 0.85          |
| (1,364) | 1:124:B:VAL:HA  | 1:125:B:LEU:HD22 | 4        | 0.85          |
| (1,364) | 1:124:B:VAL:HA  | 1:125:B:LEU:HD23 | 4        | 0.85          |
| (1,871) | 1:120:B:PHE:HB2 | 1:121:B:ILE:HD11 | 5        | 0.84          |
| (1,871) | 1:120:B:PHE:HB2 | 1:121:B:ILE:HD12 | 5        | 0.84          |
| (1,871) | 1:120:B:PHE:HB2 | 1:121:B:ILE:HD13 | 5        | 0.84          |
| (1,871) | 1:120:B:PHE:HB3 | 1:121:B:ILE:HD11 | 5        | 0.84          |
| (1,871) | 1:120:B:PHE:HB3 | 1:121:B:ILE:HD12 | 5        | 0.84          |
| (1,871) | 1:120:B:PHE:HB3 | 1:121:B:ILE:HD13 | 5        | 0.84          |
| (1,871) | 1:120:B:PHE:HB2 | 1:121:B:ILE:HD11 | 3        | 0.83          |
| (1,871) | 1:120:B:PHE:HB2 | 1:121:B:ILE:HD12 | 3        | 0.83          |
| (1,871) | 1:120:B:PHE:HB2 | 1:121:B:ILE:HD13 | 3        | 0.83          |
| (1,871) | 1:120:B:PHE:HB3 | 1:121:B:ILE:HD11 | 3        | 0.83          |
| (1,871) | 1:120:B:PHE:HB3 | 1:121:B:ILE:HD12 | 3        | 0.83          |
| (1,871) | 1:120:B:PHE:HB3 | 1:121:B:ILE:HD13 | 3        | 0.83          |
| (1,871) | 1:120:B:PHE:HB2 | 1:121:B:ILE:HD11 | 4        | 0.83          |
| (1,871) | 1:120:B:PHE:HB2 | 1:121:B:ILE:HD12 | 4        | 0.83          |
| (1,871) | 1:120:B:PHE:HB2 | 1:121:B:ILE:HD13 | 4        | 0.83          |
| (1,871) | 1:120:B:PHE:HB3 | 1:121:B:ILE:HD11 | 4        | 0.83          |
| (1,871) | 1:120:B:PHE:HB3 | 1:121:B:ILE:HD12 | 4        | 0.83          |
| (1,871) | 1:120:B:PHE:HB3 | 1:121:B:ILE:HD13 | 4        | 0.83          |
| (1,871) | 1:120:B:PHE:HB2 | 1:121:B:ILE:HD11 | 7        | 0.83          |
| (1,871) | 1:120:B:PHE:HB2 | 1:121:B:ILE:HD12 | 7        | 0.83          |
| (1,871) | 1:120:B:PHE:HB2 | 1:121:B:ILE:HD13 | 7        | 0.83          |
| (1,871) | 1:120:B:PHE:HB3 | 1:121:B:ILE:HD11 | 7        | 0.83          |
| (1,871) | 1:120:B:PHE:HB3 | 1:121:B:ILE:HD12 | 7        | 0.83          |
| (1,871) | 1:120:B:PHE:HB3 | 1:121:B:ILE:HD13 | 7        | 0.83          |

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| Key     | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (1,535) | 1:122:B:PHE:HD2 | 1:123:B:ILE:H    | 3        | 0.83          |
| (1,534) | 1:122:B:PHE:HD2 | 1:123:B:ILE:H    | 3        | 0.83          |
| (1,533) | 1:22:A:PHE:HD2  | 1:23:A:ILE:H     | 3        | 0.83          |
| (1,364) | 1:124:B:VAL:HA  | 1:125:B:LEU:HD21 | 10       | 0.83          |
| (1,364) | 1:124:B:VAL:HA  | 1:125:B:LEU:HD22 | 10       | 0.83          |
| (1,364) | 1:124:B:VAL:HA  | 1:125:B:LEU:HD23 | 10       | 0.83          |
| (1,871) | 1:120:B:PHE:HB2 | 1:121:B:ILE:HD11 | 6        | 0.82          |
| (1,871) | 1:120:B:PHE:HB2 | 1:121:B:ILE:HD12 | 6        | 0.82          |
| (1,871) | 1:120:B:PHE:HB2 | 1:121:B:ILE:HD13 | 6        | 0.82          |
| (1,871) | 1:120:B:PHE:HB3 | 1:121:B:ILE:HD11 | 6        | 0.82          |
| (1,871) | 1:120:B:PHE:HB3 | 1:121:B:ILE:HD12 | 6        | 0.82          |
| (1,871) | 1:120:B:PHE:HB3 | 1:121:B:ILE:HD13 | 6        | 0.82          |
| (1,535) | 1:122:B:PHE:HD2 | 1:123:B:ILE:H    | 2        | 0.82          |
| (1,534) | 1:122:B:PHE:HD2 | 1:123:B:ILE:H    | 2        | 0.82          |
| (1,533) | 1:22:A:PHE:HD2  | 1:23:A:ILE:H     | 9        | 0.82          |
| (1,871) | 1:120:B:PHE:HB2 | 1:121:B:ILE:HD11 | 10       | 0.81          |
| (1,871) | 1:120:B:PHE:HB2 | 1:121:B:ILE:HD12 | 10       | 0.81          |
| (1,871) | 1:120:B:PHE:HB2 | 1:121:B:ILE:HD13 | 10       | 0.81          |
| (1,871) | 1:120:B:PHE:HB3 | 1:121:B:ILE:HD11 | 10       | 0.81          |
| (1,871) | 1:120:B:PHE:HB3 | 1:121:B:ILE:HD12 | 10       | 0.81          |
| (1,871) | 1:120:B:PHE:HB3 | 1:121:B:ILE:HD13 | 10       | 0.81          |
| (1,533) | 1:22:A:PHE:HD2  | 1:23:A:ILE:H     | 2        | 0.81          |
| (1,798) | 1:24:A:VAL:HA   | 1:25:A:LEU:HD21  | 4        | 0.8           |
| (1,798) | 1:24:A:VAL:HA   | 1:25:A:LEU:HD22  | 4        | 0.8           |
| (1,798) | 1:24:A:VAL:HA   | 1:25:A:LEU:HD23  | 4        | 0.8           |
| (1,533) | 1:22:A:PHE:HD2  | 1:23:A:ILE:H     | 8        | 0.8           |
| (1,421) | 1:14:A:THR:HG22 | 1:110:B:PHE:HE1  | 7        | 0.8           |
| (1,363) | 1:24:A:VAL:HA   | 1:25:A:LEU:HD21  | 4        | 0.8           |
| (1,363) | 1:24:A:VAL:HA   | 1:25:A:LEU:HD22  | 4        | 0.8           |
| (1,363) | 1:24:A:VAL:HA   | 1:25:A:LEU:HD23  | 4        | 0.8           |
| (1,535) | 1:122:B:PHE:HD2 | 1:123:B:ILE:H    | 8        | 0.78          |
| (1,535) | 1:122:B:PHE:HD2 | 1:123:B:ILE:H    | 9        | 0.78          |
| (1,534) | 1:122:B:PHE:HD2 | 1:123:B:ILE:H    | 8        | 0.78          |
| (1,534) | 1:122:B:PHE:HD2 | 1:123:B:ILE:H    | 9        | 0.78          |
| (1,535) | 1:122:B:PHE:HD2 | 1:123:B:ILE:H    | 1        | 0.77          |
| (1,534) | 1:122:B:PHE:HD2 | 1:123:B:ILE:H    | 1        | 0.77          |
| (1,533) | 1:22:A:PHE:HD2  | 1:23:A:ILE:H     | 1        | 0.77          |
| (1,422) | 1:10:A:PHE:HE1  | 1:114:B:THR:HG22 | 7        | 0.77          |
| (1,798) | 1:24:A:VAL:HA   | 1:25:A:LEU:HD21  | 10       | 0.76          |
| (1,798) | 1:24:A:VAL:HA   | 1:25:A:LEU:HD22  | 10       | 0.76          |
| (1,798) | 1:24:A:VAL:HA   | 1:25:A:LEU:HD23  | 10       | 0.76          |
| (1,363) | 1:24:A:VAL:HA   | 1:25:A:LEU:HD21  | 10       | 0.76          |

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| Key     | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (1,363) | 1:24:A:VAL:HA   | 1:25:A:LEU:HD22  | 10       | 0.76          |
| (1,363) | 1:24:A:VAL:HA   | 1:25:A:LEU:HD23  | 10       | 0.76          |
| (1,830) | 1:18:A:LEU:HD21 | 1:22:A:PHE:HB2   | 9        | 0.74          |
| (1,830) | 1:18:A:LEU:HD21 | 1:22:A:PHE:HB3   | 9        | 0.74          |
| (1,830) | 1:18:A:LEU:HD22 | 1:22:A:PHE:HB2   | 9        | 0.74          |
| (1,830) | 1:18:A:LEU:HD22 | 1:22:A:PHE:HB3   | 9        | 0.74          |
| (1,830) | 1:18:A:LEU:HD23 | 1:22:A:PHE:HB2   | 9        | 0.74          |
| (1,830) | 1:18:A:LEU:HD23 | 1:22:A:PHE:HB3   | 9        | 0.74          |
| (1,830) | 1:18:A:LEU:HD21 | 1:22:A:PHE:HB2   | 4        | 0.7           |
| (1,830) | 1:18:A:LEU:HD21 | 1:22:A:PHE:HB3   | 4        | 0.7           |
| (1,830) | 1:18:A:LEU:HD22 | 1:22:A:PHE:HB2   | 4        | 0.7           |
| (1,830) | 1:18:A:LEU:HD22 | 1:22:A:PHE:HB3   | 4        | 0.7           |
| (1,830) | 1:18:A:LEU:HD23 | 1:22:A:PHE:HB2   | 4        | 0.7           |
| (1,830) | 1:18:A:LEU:HD23 | 1:22:A:PHE:HB3   | 4        | 0.7           |
| (1,421) | 1:14:A:THR:HG22 | 1:110:B:PHE:HE1  | 2        | 0.68          |
| (1,422) | 1:10:A:PHE:HE1  | 1:114:B:THR:HG22 | 2        | 0.66          |
| (1,535) | 1:122:B:PHE:HD2 | 1:123:B:ILE:H    | 7        | 0.63          |
| (1,534) | 1:122:B:PHE:HD2 | 1:123:B:ILE:H    | 7        | 0.63          |
| (1,422) | 1:10:A:PHE:HE1  | 1:114:B:THR:HG21 | 8        | 0.63          |
| (1,421) | 1:14:A:THR:HG22 | 1:110:B:PHE:HE2  | 3        | 0.62          |
| (1,799) | 1:124:B:VAL:HA  | 1:125:B:LEU:HD21 | 8        | 0.6           |
| (1,799) | 1:124:B:VAL:HA  | 1:125:B:LEU:HD22 | 8        | 0.6           |
| (1,799) | 1:124:B:VAL:HA  | 1:125:B:LEU:HD23 | 8        | 0.6           |
| (1,799) | 1:124:B:VAL:HA  | 1:125:B:LEU:HD21 | 8        | 0.6           |
| (1,799) | 1:124:B:VAL:HA  | 1:125:B:LEU:HD22 | 8        | 0.6           |
| (1,799) | 1:124:B:VAL:HA  | 1:125:B:LEU:HD23 | 8        | 0.6           |
| (1,533) | 1:22:A:PHE:HD2  | 1:23:A:ILE:H     | 7        | 0.6           |
| (1,422) | 1:10:A:PHE:HE2  | 1:114:B:THR:HG23 | 4        | 0.6           |
| (1,421) | 1:14:A:THR:HG23 | 1:110:B:PHE:HE1  | 10       | 0.6           |
| (1,799) | 1:124:B:VAL:HA  | 1:125:B:LEU:HD21 | 2        | 0.59          |
| (1,799) | 1:124:B:VAL:HA  | 1:125:B:LEU:HD22 | 2        | 0.59          |
| (1,799) | 1:124:B:VAL:HA  | 1:125:B:LEU:HD23 | 2        | 0.59          |
| (1,799) | 1:124:B:VAL:HA  | 1:125:B:LEU:HD21 | 2        | 0.59          |
| (1,799) | 1:124:B:VAL:HA  | 1:125:B:LEU:HD22 | 2        | 0.59          |
| (1,799) | 1:124:B:VAL:HA  | 1:125:B:LEU:HD23 | 2        | 0.59          |
| (1,421) | 1:14:A:THR:HG23 | 1:110:B:PHE:HE1  | 4        | 0.59          |
| (1,422) | 1:10:A:PHE:HE2  | 1:114:B:THR:HG22 | 3        | 0.58          |
| (1,421) | 1:14:A:THR:HG22 | 1:110:B:PHE:HE2  | 5        | 0.58          |
| (1,421) | 1:14:A:THR:HG21 | 1:110:B:PHE:HE1  | 8        | 0.58          |
| (1,799) | 1:124:B:VAL:HA  | 1:125:B:LEU:HD21 | 9        | 0.56          |
| (1,799) | 1:124:B:VAL:HA  | 1:125:B:LEU:HD22 | 9        | 0.56          |
| (1,799) | 1:124:B:VAL:HA  | 1:125:B:LEU:HD23 | 9        | 0.56          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,799) | 1:124:B:VAL:HA   | 1:125:B:LEU:HD21 | 9        | 0.56          |
| (1,799) | 1:124:B:VAL:HA   | 1:125:B:LEU:HD22 | 9        | 0.56          |
| (1,799) | 1:124:B:VAL:HA   | 1:125:B:LEU:HD23 | 9        | 0.56          |
| (1,422) | 1:10:A:PHE:HE2   | 1:114:B:THR:HG22 | 5        | 0.56          |
| (1,422) | 1:10:A:PHE:HE1   | 1:114:B:THR:HG23 | 10       | 0.56          |
| (1,831) | 1:118:B:LEU:HD21 | 1:122:B:PHE:HB2  | 9        | 0.55          |
| (1,831) | 1:118:B:LEU:HD21 | 1:122:B:PHE:HB3  | 9        | 0.55          |
| (1,831) | 1:118:B:LEU:HD22 | 1:122:B:PHE:HB2  | 9        | 0.55          |
| (1,831) | 1:118:B:LEU:HD22 | 1:122:B:PHE:HB3  | 9        | 0.55          |
| (1,831) | 1:118:B:LEU:HD23 | 1:122:B:PHE:HB2  | 9        | 0.55          |
| (1,831) | 1:118:B:LEU:HD23 | 1:122:B:PHE:HB3  | 9        | 0.55          |
| (1,831) | 1:118:B:LEU:HD21 | 1:122:B:PHE:HB2  | 9        | 0.55          |
| (1,831) | 1:118:B:LEU:HD21 | 1:122:B:PHE:HB3  | 9        | 0.55          |
| (1,831) | 1:118:B:LEU:HD22 | 1:122:B:PHE:HB2  | 9        | 0.55          |
| (1,831) | 1:118:B:LEU:HD22 | 1:122:B:PHE:HB3  | 9        | 0.55          |
| (1,831) | 1:118:B:LEU:HD23 | 1:122:B:PHE:HB2  | 9        | 0.55          |
| (1,831) | 1:118:B:LEU:HD23 | 1:122:B:PHE:HB3  | 9        | 0.55          |
| (1,799) | 1:124:B:VAL:HA   | 1:125:B:LEU:HD21 | 1        | 0.54          |
| (1,799) | 1:124:B:VAL:HA   | 1:125:B:LEU:HD22 | 1        | 0.54          |
| (1,799) | 1:124:B:VAL:HA   | 1:125:B:LEU:HD23 | 1        | 0.54          |
| (1,799) | 1:124:B:VAL:HA   | 1:125:B:LEU:HD21 | 1        | 0.54          |
| (1,799) | 1:124:B:VAL:HA   | 1:125:B:LEU:HD22 | 1        | 0.54          |
| (1,799) | 1:124:B:VAL:HA   | 1:125:B:LEU:HD23 | 1        | 0.54          |
| (1,422) | 1:10:A:PHE:HE1   | 1:114:B:THR:HG23 | 9        | 0.53          |
| (1,422) | 1:10:A:PHE:HE1   | 1:114:B:THR:HG21 | 1        | 0.52          |
| (1,422) | 1:10:A:PHE:HE1   | 1:114:B:THR:HG22 | 6        | 0.52          |
| (1,421) | 1:14:A:THR:HG22  | 1:110:B:PHE:HE1  | 6        | 0.52          |
| (1,799) | 1:124:B:VAL:HA   | 1:125:B:LEU:HD21 | 3        | 0.5           |
| (1,799) | 1:124:B:VAL:HA   | 1:125:B:LEU:HD22 | 3        | 0.5           |
| (1,799) | 1:124:B:VAL:HA   | 1:125:B:LEU:HD23 | 3        | 0.5           |
| (1,799) | 1:124:B:VAL:HA   | 1:125:B:LEU:HD21 | 3        | 0.5           |
| (1,799) | 1:124:B:VAL:HA   | 1:125:B:LEU:HD22 | 3        | 0.5           |
| (1,799) | 1:124:B:VAL:HA   | 1:125:B:LEU:HD23 | 3        | 0.5           |
| (1,421) | 1:14:A:THR:HG21  | 1:110:B:PHE:HE1  | 1        | 0.5           |
| (1,831) | 1:118:B:LEU:HD21 | 1:122:B:PHE:HB2  | 6        | 0.48          |
| (1,831) | 1:118:B:LEU:HD21 | 1:122:B:PHE:HB3  | 6        | 0.48          |
| (1,831) | 1:118:B:LEU:HD22 | 1:122:B:PHE:HB2  | 6        | 0.48          |
| (1,831) | 1:118:B:LEU:HD22 | 1:122:B:PHE:HB3  | 6        | 0.48          |
| (1,831) | 1:118:B:LEU:HD23 | 1:122:B:PHE:HB2  | 6        | 0.48          |
| (1,831) | 1:118:B:LEU:HD23 | 1:122:B:PHE:HB3  | 6        | 0.48          |
| (1,831) | 1:118:B:LEU:HD21 | 1:122:B:PHE:HB2  | 6        | 0.48          |
| (1,831) | 1:118:B:LEU:HD21 | 1:122:B:PHE:HB3  | 6        | 0.48          |

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| Key     | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|---------|------------------|-----------------|----------|---------------|
| (1,831) | 1:118:B:LEU:HD22 | 1:122:B:PHE:HB2 | 6        | 0.48          |
| (1,831) | 1:118:B:LEU:HD22 | 1:122:B:PHE:HB3 | 6        | 0.48          |
| (1,831) | 1:118:B:LEU:HD23 | 1:122:B:PHE:HB2 | 6        | 0.48          |
| (1,831) | 1:118:B:LEU:HD23 | 1:122:B:PHE:HB3 | 6        | 0.48          |
| (2,4)   | 1:127:B:ILE:HA   | 1:131:B:GLY:H   | 3        | 0.46          |
| (2,4)   | 1:127:B:ILE:HA   | 1:131:B:GLY:H   | 3        | 0.46          |
| (2,4)   | 1:127:B:ILE:HA   | 1:131:B:GLY:H   | 8        | 0.46          |
| (2,4)   | 1:127:B:ILE:HA   | 1:131:B:GLY:H   | 8        | 0.46          |
| (2,4)   | 1:127:B:ILE:HA   | 1:131:B:GLY:H   | 1        | 0.45          |
| (2,4)   | 1:127:B:ILE:HA   | 1:131:B:GLY:H   | 1        | 0.45          |
| (2,4)   | 1:127:B:ILE:HA   | 1:131:B:GLY:H   | 2        | 0.45          |
| (2,4)   | 1:127:B:ILE:HA   | 1:131:B:GLY:H   | 2        | 0.45          |
| (2,4)   | 1:127:B:ILE:HA   | 1:131:B:GLY:H   | 4        | 0.45          |
| (2,4)   | 1:127:B:ILE:HA   | 1:131:B:GLY:H   | 4        | 0.45          |
| (2,4)   | 1:127:B:ILE:HA   | 1:131:B:GLY:H   | 9        | 0.45          |
| (2,4)   | 1:127:B:ILE:HA   | 1:131:B:GLY:H   | 9        | 0.45          |
| (2,4)   | 1:127:B:ILE:HA   | 1:131:B:GLY:H   | 5        | 0.44          |
| (2,4)   | 1:127:B:ILE:HA   | 1:131:B:GLY:H   | 5        | 0.44          |
| (2,4)   | 1:127:B:ILE:HA   | 1:131:B:GLY:H   | 6        | 0.44          |
| (2,4)   | 1:127:B:ILE:HA   | 1:131:B:GLY:H   | 6        | 0.44          |
| (2,4)   | 1:127:B:ILE:HA   | 1:131:B:GLY:H   | 7        | 0.44          |
| (2,4)   | 1:127:B:ILE:HA   | 1:131:B:GLY:H   | 7        | 0.44          |
| (2,4)   | 1:127:B:ILE:HA   | 1:131:B:GLY:H   | 10       | 0.44          |
| (2,4)   | 1:127:B:ILE:HA   | 1:131:B:GLY:H   | 10       | 0.44          |
| (1,831) | 1:118:B:LEU:HD21 | 1:122:B:PHE:HB2 | 3        | 0.44          |
| (1,831) | 1:118:B:LEU:HD21 | 1:122:B:PHE:HB3 | 3        | 0.44          |
| (1,831) | 1:118:B:LEU:HD22 | 1:122:B:PHE:HB2 | 3        | 0.44          |
| (1,831) | 1:118:B:LEU:HD22 | 1:122:B:PHE:HB3 | 3        | 0.44          |
| (1,831) | 1:118:B:LEU:HD23 | 1:122:B:PHE:HB2 | 3        | 0.44          |
| (1,831) | 1:118:B:LEU:HD23 | 1:122:B:PHE:HB3 | 3        | 0.44          |
| (1,831) | 1:118:B:LEU:HD21 | 1:122:B:PHE:HB2 | 3        | 0.44          |
| (1,831) | 1:118:B:LEU:HD21 | 1:122:B:PHE:HB3 | 3        | 0.44          |
| (1,831) | 1:118:B:LEU:HD22 | 1:122:B:PHE:HB2 | 3        | 0.44          |
| (1,831) | 1:118:B:LEU:HD22 | 1:122:B:PHE:HB3 | 3        | 0.44          |
| (1,831) | 1:118:B:LEU:HD23 | 1:122:B:PHE:HB2 | 3        | 0.44          |
| (1,831) | 1:118:B:LEU:HD23 | 1:122:B:PHE:HB3 | 3        | 0.44          |
| (1,831) | 1:118:B:LEU:HD21 | 1:122:B:PHE:HB2 | 10       | 0.44          |
| (1,831) | 1:118:B:LEU:HD21 | 1:122:B:PHE:HB3 | 10       | 0.44          |
| (1,831) | 1:118:B:LEU:HD22 | 1:122:B:PHE:HB2 | 10       | 0.44          |
| (1,831) | 1:118:B:LEU:HD22 | 1:122:B:PHE:HB3 | 10       | 0.44          |
| (1,831) | 1:118:B:LEU:HD23 | 1:122:B:PHE:HB2 | 10       | 0.44          |
| (1,831) | 1:118:B:LEU:HD23 | 1:122:B:PHE:HB3 | 10       | 0.44          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,831) | 1:118:B:LEU:HD21 | 1:122:B:PHE:HB2  | 10       | 0.44          |
| (1,831) | 1:118:B:LEU:HD21 | 1:122:B:PHE:HB3  | 10       | 0.44          |
| (1,831) | 1:118:B:LEU:HD22 | 1:122:B:PHE:HB2  | 10       | 0.44          |
| (1,831) | 1:118:B:LEU:HD22 | 1:122:B:PHE:HB3  | 10       | 0.44          |
| (1,831) | 1:118:B:LEU:HD23 | 1:122:B:PHE:HB2  | 10       | 0.44          |
| (1,831) | 1:118:B:LEU:HD23 | 1:122:B:PHE:HB3  | 10       | 0.44          |
| (1,509) | 1:32:A:TRP:HA    | 1:33:A:ARG:H     | 8        | 0.44          |
| (1,74)  | 1:132:B:TRP:HA   | 1:133:B:ARG:H    | 8        | 0.44          |
| (1,73)  | 1:32:A:TRP:HA    | 1:33:A:ARG:H     | 8        | 0.44          |
| (1,799) | 1:124:B:VAL:HA   | 1:125:B:LEU:HD21 | 5        | 0.42          |
| (1,799) | 1:124:B:VAL:HA   | 1:125:B:LEU:HD22 | 5        | 0.42          |
| (1,799) | 1:124:B:VAL:HA   | 1:125:B:LEU:HD23 | 5        | 0.42          |
| (1,799) | 1:124:B:VAL:HA   | 1:125:B:LEU:HD21 | 5        | 0.42          |
| (1,799) | 1:124:B:VAL:HA   | 1:125:B:LEU:HD22 | 5        | 0.42          |
| (1,799) | 1:124:B:VAL:HA   | 1:125:B:LEU:HD23 | 5        | 0.42          |
| (3,4)   | 1:129:B:PHE:HA   | 1:132:B:TRP:H    | 1        | 0.4           |
| (3,4)   | 1:129:B:PHE:HA   | 1:132:B:TRP:H    | 1        | 0.4           |
| (3,4)   | 1:129:B:PHE:HA   | 1:132:B:TRP:H    | 2        | 0.4           |
| (3,4)   | 1:129:B:PHE:HA   | 1:132:B:TRP:H    | 2        | 0.4           |
| (3,4)   | 1:129:B:PHE:HA   | 1:132:B:TRP:H    | 3        | 0.4           |
| (3,4)   | 1:129:B:PHE:HA   | 1:132:B:TRP:H    | 3        | 0.4           |
| (3,4)   | 1:129:B:PHE:HA   | 1:132:B:TRP:H    | 4        | 0.4           |
| (3,4)   | 1:129:B:PHE:HA   | 1:132:B:TRP:H    | 4        | 0.4           |
| (3,4)   | 1:129:B:PHE:HA   | 1:132:B:TRP:H    | 5        | 0.4           |
| (3,4)   | 1:129:B:PHE:HA   | 1:132:B:TRP:H    | 5        | 0.4           |
| (3,4)   | 1:129:B:PHE:HA   | 1:132:B:TRP:H    | 6        | 0.4           |
| (3,4)   | 1:129:B:PHE:HA   | 1:132:B:TRP:H    | 6        | 0.4           |
| (3,4)   | 1:129:B:PHE:HA   | 1:132:B:TRP:H    | 7        | 0.4           |
| (3,4)   | 1:129:B:PHE:HA   | 1:132:B:TRP:H    | 7        | 0.4           |
| (3,4)   | 1:129:B:PHE:HA   | 1:132:B:TRP:H    | 8        | 0.4           |
| (3,4)   | 1:129:B:PHE:HA   | 1:132:B:TRP:H    | 8        | 0.4           |
| (3,4)   | 1:129:B:PHE:HA   | 1:132:B:TRP:H    | 9        | 0.4           |
| (3,4)   | 1:129:B:PHE:HA   | 1:132:B:TRP:H    | 9        | 0.4           |
| (3,4)   | 1:129:B:PHE:HA   | 1:132:B:TRP:H    | 10       | 0.39          |
| (3,4)   | 1:129:B:PHE:HA   | 1:132:B:TRP:H    | 10       | 0.39          |
| (1,831) | 1:118:B:LEU:HD21 | 1:122:B:PHE:HB2  | 1        | 0.35          |
| (1,831) | 1:118:B:LEU:HD21 | 1:122:B:PHE:HB3  | 1        | 0.35          |
| (1,831) | 1:118:B:LEU:HD22 | 1:122:B:PHE:HB2  | 1        | 0.35          |
| (1,831) | 1:118:B:LEU:HD22 | 1:122:B:PHE:HB3  | 1        | 0.35          |
| (1,831) | 1:118:B:LEU:HD23 | 1:122:B:PHE:HB2  | 1        | 0.35          |
| (1,831) | 1:118:B:LEU:HD23 | 1:122:B:PHE:HB3  | 1        | 0.35          |
| (1,831) | 1:118:B:LEU:HD21 | 1:122:B:PHE:HB2  | 1        | 0.35          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,831) | 1:118:B:LEU:HD21 | 1:122:B:PHE:HB3  | 1        | 0.35          |
| (1,831) | 1:118:B:LEU:HD22 | 1:122:B:PHE:HB2  | 1        | 0.35          |
| (1,831) | 1:118:B:LEU:HD22 | 1:122:B:PHE:HB3  | 1        | 0.35          |
| (1,831) | 1:118:B:LEU:HD23 | 1:122:B:PHE:HB2  | 1        | 0.35          |
| (1,831) | 1:118:B:LEU:HD23 | 1:122:B:PHE:HB3  | 1        | 0.35          |
| (1,831) | 1:118:B:LEU:HD21 | 1:122:B:PHE:HB2  | 5        | 0.34          |
| (1,831) | 1:118:B:LEU:HD21 | 1:122:B:PHE:HB3  | 5        | 0.34          |
| (1,831) | 1:118:B:LEU:HD22 | 1:122:B:PHE:HB2  | 5        | 0.34          |
| (1,831) | 1:118:B:LEU:HD22 | 1:122:B:PHE:HB3  | 5        | 0.34          |
| (1,831) | 1:118:B:LEU:HD23 | 1:122:B:PHE:HB2  | 5        | 0.34          |
| (1,831) | 1:118:B:LEU:HD23 | 1:122:B:PHE:HB3  | 5        | 0.34          |
| (1,831) | 1:118:B:LEU:HD21 | 1:122:B:PHE:HB2  | 5        | 0.34          |
| (1,831) | 1:118:B:LEU:HD21 | 1:122:B:PHE:HB3  | 5        | 0.34          |
| (1,831) | 1:118:B:LEU:HD22 | 1:122:B:PHE:HB2  | 5        | 0.34          |
| (1,831) | 1:118:B:LEU:HD22 | 1:122:B:PHE:HB3  | 5        | 0.34          |
| (1,831) | 1:118:B:LEU:HD23 | 1:122:B:PHE:HB2  | 5        | 0.34          |
| (1,831) | 1:118:B:LEU:HD23 | 1:122:B:PHE:HB3  | 5        | 0.34          |
| (1,831) | 1:118:B:LEU:HD21 | 1:122:B:PHE:HB2  | 7        | 0.33          |
| (1,831) | 1:118:B:LEU:HD21 | 1:122:B:PHE:HB3  | 7        | 0.33          |
| (1,831) | 1:118:B:LEU:HD22 | 1:122:B:PHE:HB2  | 7        | 0.33          |
| (1,831) | 1:118:B:LEU:HD22 | 1:122:B:PHE:HB3  | 7        | 0.33          |
| (1,831) | 1:118:B:LEU:HD23 | 1:122:B:PHE:HB2  | 7        | 0.33          |
| (1,831) | 1:118:B:LEU:HD23 | 1:122:B:PHE:HB3  | 7        | 0.33          |
| (1,831) | 1:118:B:LEU:HD21 | 1:122:B:PHE:HB2  | 7        | 0.33          |
| (1,831) | 1:118:B:LEU:HD21 | 1:122:B:PHE:HB3  | 7        | 0.33          |
| (1,831) | 1:118:B:LEU:HD22 | 1:122:B:PHE:HB2  | 7        | 0.33          |
| (1,831) | 1:118:B:LEU:HD22 | 1:122:B:PHE:HB3  | 7        | 0.33          |
| (1,831) | 1:118:B:LEU:HD23 | 1:122:B:PHE:HB2  | 7        | 0.33          |
| (1,831) | 1:118:B:LEU:HD23 | 1:122:B:PHE:HB3  | 7        | 0.33          |
| (1,831) | 1:118:B:LEU:HD21 | 1:122:B:PHE:HB2  | 8        | 0.32          |
| (1,831) | 1:118:B:LEU:HD21 | 1:122:B:PHE:HB3  | 8        | 0.32          |
| (1,831) | 1:118:B:LEU:HD22 | 1:122:B:PHE:HB2  | 8        | 0.32          |
| (1,831) | 1:118:B:LEU:HD22 | 1:122:B:PHE:HB3  | 8        | 0.32          |
| (1,831) | 1:118:B:LEU:HD23 | 1:122:B:PHE:HB2  | 8        | 0.32          |
| (1,831) | 1:118:B:LEU:HD23 | 1:122:B:PHE:HB3  | 8        | 0.32          |
| (1,831) | 1:118:B:LEU:HD21 | 1:122:B:PHE:HB2  | 8        | 0.32          |
| (1,831) | 1:118:B:LEU:HD21 | 1:122:B:PHE:HB3  | 8        | 0.32          |
| (1,831) | 1:118:B:LEU:HD22 | 1:122:B:PHE:HB2  | 8        | 0.32          |
| (1,831) | 1:118:B:LEU:HD22 | 1:122:B:PHE:HB3  | 8        | 0.32          |
| (1,831) | 1:118:B:LEU:HD23 | 1:122:B:PHE:HB2  | 8        | 0.32          |
| (1,831) | 1:118:B:LEU:HD23 | 1:122:B:PHE:HB3  | 8        | 0.32          |
| (1,799) | 1:124:B:VAL:HA   | 1:125:B:LEU:HD21 | 7        | 0.31          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,799) | 1:124:B:VAL:HA   | 1:125:B:LEU:HD22 | 7        | 0.31          |
| (1,799) | 1:124:B:VAL:HA   | 1:125:B:LEU:HD23 | 7        | 0.31          |
| (1,799) | 1:124:B:VAL:HA   | 1:125:B:LEU:HD21 | 7        | 0.31          |
| (1,799) | 1:124:B:VAL:HA   | 1:125:B:LEU:HD22 | 7        | 0.31          |
| (1,799) | 1:124:B:VAL:HA   | 1:125:B:LEU:HD23 | 7        | 0.31          |
| (1,190) | 1:132:B:TRP:HB2  | 1:133:B:ARG:H    | 4        | 0.31          |
| (1,190) | 1:132:B:TRP:HB3  | 1:133:B:ARG:H    | 4        | 0.31          |
| (1,831) | 1:118:B:LEU:HD21 | 1:122:B:PHE:HB2  | 2        | 0.3           |
| (1,831) | 1:118:B:LEU:HD21 | 1:122:B:PHE:HB3  | 2        | 0.3           |
| (1,831) | 1:118:B:LEU:HD22 | 1:122:B:PHE:HB2  | 2        | 0.3           |
| (1,831) | 1:118:B:LEU:HD22 | 1:122:B:PHE:HB3  | 2        | 0.3           |
| (1,831) | 1:118:B:LEU:HD23 | 1:122:B:PHE:HB2  | 2        | 0.3           |
| (1,831) | 1:118:B:LEU:HD23 | 1:122:B:PHE:HB3  | 2        | 0.3           |
| (1,831) | 1:118:B:LEU:HD21 | 1:122:B:PHE:HB2  | 2        | 0.3           |
| (1,831) | 1:118:B:LEU:HD21 | 1:122:B:PHE:HB3  | 2        | 0.3           |
| (1,831) | 1:118:B:LEU:HD22 | 1:122:B:PHE:HB2  | 2        | 0.3           |
| (1,831) | 1:118:B:LEU:HD22 | 1:122:B:PHE:HB3  | 2        | 0.3           |
| (1,831) | 1:118:B:LEU:HD23 | 1:122:B:PHE:HB2  | 2        | 0.3           |
| (1,831) | 1:118:B:LEU:HD23 | 1:122:B:PHE:HB3  | 2        | 0.3           |
| (1,799) | 1:124:B:VAL:HA   | 1:125:B:LEU:HD21 | 6        | 0.3           |
| (1,799) | 1:124:B:VAL:HA   | 1:125:B:LEU:HD22 | 6        | 0.3           |
| (1,799) | 1:124:B:VAL:HA   | 1:125:B:LEU:HD23 | 6        | 0.3           |
| (1,799) | 1:124:B:VAL:HA   | 1:125:B:LEU:HD21 | 6        | 0.3           |
| (1,799) | 1:124:B:VAL:HA   | 1:125:B:LEU:HD22 | 6        | 0.3           |
| (1,799) | 1:124:B:VAL:HA   | 1:125:B:LEU:HD23 | 6        | 0.3           |
| (1,436) | 1:18:A:LEU:HA    | 1:118:B:LEU:HD11 | 10       | 0.28          |
| (1,436) | 1:18:A:LEU:HA    | 1:118:B:LEU:HD12 | 10       | 0.28          |
| (1,436) | 1:18:A:LEU:HA    | 1:118:B:LEU:HD13 | 10       | 0.28          |
| (1,436) | 1:18:A:LEU:HA    | 1:118:B:LEU:HD21 | 10       | 0.28          |
| (1,436) | 1:18:A:LEU:HA    | 1:118:B:LEU:HD22 | 10       | 0.28          |
| (1,436) | 1:18:A:LEU:HA    | 1:118:B:LEU:HD23 | 10       | 0.28          |
| (1,435) | 1:18:A:LEU:HD11  | 1:118:B:LEU:HA   | 9        | 0.28          |
| (1,435) | 1:18:A:LEU:HD12  | 1:118:B:LEU:HA   | 9        | 0.28          |
| (1,435) | 1:18:A:LEU:HD13  | 1:118:B:LEU:HA   | 9        | 0.28          |
| (1,435) | 1:18:A:LEU:HD21  | 1:118:B:LEU:HA   | 9        | 0.28          |
| (1,435) | 1:18:A:LEU:HD22  | 1:118:B:LEU:HA   | 9        | 0.28          |
| (1,435) | 1:18:A:LEU:HD23  | 1:118:B:LEU:HA   | 9        | 0.28          |
| (1,804) | 1:20:A:PHE:HA    | 1:23:A:ILE:HD11  | 7        | 0.27          |
| (1,804) | 1:20:A:PHE:HA    | 1:23:A:ILE:HD12  | 7        | 0.27          |
| (1,804) | 1:20:A:PHE:HA    | 1:23:A:ILE:HD13  | 7        | 0.27          |
| (1,628) | 1:32:A:TRP:HB2   | 1:33:A:ARG:H     | 2        | 0.27          |
| (1,628) | 1:32:A:TRP:HB3   | 1:33:A:ARG:H     | 2        | 0.27          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,628) | 1:32:A:TRP:HB2   | 1:33:A:ARG:H     | 9        | 0.27          |
| (1,628) | 1:32:A:TRP:HB3   | 1:33:A:ARG:H     | 9        | 0.27          |
| (1,369) | 1:20:A:PHE:HA    | 1:23:A:ILE:HD11  | 7        | 0.27          |
| (1,369) | 1:20:A:PHE:HA    | 1:23:A:ILE:HD12  | 7        | 0.27          |
| (1,369) | 1:20:A:PHE:HA    | 1:23:A:ILE:HD13  | 7        | 0.27          |
| (1,190) | 1:132:B:TRP:HB2  | 1:133:B:ARG:H    | 2        | 0.27          |
| (1,190) | 1:132:B:TRP:HB3  | 1:133:B:ARG:H    | 2        | 0.27          |
| (1,190) | 1:132:B:TRP:HB2  | 1:133:B:ARG:H    | 9        | 0.27          |
| (1,190) | 1:132:B:TRP:HB3  | 1:133:B:ARG:H    | 9        | 0.27          |
| (1,189) | 1:32:A:TRP:HB2   | 1:33:A:ARG:H     | 2        | 0.27          |
| (1,189) | 1:32:A:TRP:HB3   | 1:33:A:ARG:H     | 2        | 0.27          |
| (1,189) | 1:32:A:TRP:HB2   | 1:33:A:ARG:H     | 9        | 0.27          |
| (1,189) | 1:32:A:TRP:HB3   | 1:33:A:ARG:H     | 9        | 0.27          |
| (1,436) | 1:18:A:LEU:HA    | 1:118:B:LEU:HD11 | 8        | 0.26          |
| (1,436) | 1:18:A:LEU:HA    | 1:118:B:LEU:HD12 | 8        | 0.26          |
| (1,436) | 1:18:A:LEU:HA    | 1:118:B:LEU:HD13 | 8        | 0.26          |
| (1,436) | 1:18:A:LEU:HA    | 1:118:B:LEU:HD21 | 8        | 0.26          |
| (1,436) | 1:18:A:LEU:HA    | 1:118:B:LEU:HD22 | 8        | 0.26          |
| (1,436) | 1:18:A:LEU:HA    | 1:118:B:LEU:HD23 | 8        | 0.26          |
| (1,628) | 1:32:A:TRP:HB2   | 1:33:A:ARG:H     | 6        | 0.25          |
| (1,628) | 1:32:A:TRP:HB3   | 1:33:A:ARG:H     | 6        | 0.25          |
| (1,436) | 1:18:A:LEU:HA    | 1:118:B:LEU:HD11 | 5        | 0.25          |
| (1,436) | 1:18:A:LEU:HA    | 1:118:B:LEU:HD12 | 5        | 0.25          |
| (1,436) | 1:18:A:LEU:HA    | 1:118:B:LEU:HD13 | 5        | 0.25          |
| (1,436) | 1:18:A:LEU:HA    | 1:118:B:LEU:HD21 | 5        | 0.25          |
| (1,436) | 1:18:A:LEU:HA    | 1:118:B:LEU:HD22 | 5        | 0.25          |
| (1,436) | 1:18:A:LEU:HA    | 1:118:B:LEU:HD23 | 5        | 0.25          |
| (1,435) | 1:18:A:LEU:HD11  | 1:118:B:LEU:HA   | 10       | 0.25          |
| (1,435) | 1:18:A:LEU:HD12  | 1:118:B:LEU:HA   | 10       | 0.25          |
| (1,435) | 1:18:A:LEU:HD13  | 1:118:B:LEU:HA   | 10       | 0.25          |
| (1,435) | 1:18:A:LEU:HD21  | 1:118:B:LEU:HA   | 10       | 0.25          |
| (1,435) | 1:18:A:LEU:HD22  | 1:118:B:LEU:HA   | 10       | 0.25          |
| (1,435) | 1:18:A:LEU:HD23  | 1:118:B:LEU:HA   | 10       | 0.25          |
| (1,416) | 1:121:B:ILE:HG21 | 1:122:B:PHE:HB2  | 9        | 0.25          |
| (1,416) | 1:121:B:ILE:HG21 | 1:122:B:PHE:HB3  | 9        | 0.25          |
| (1,416) | 1:121:B:ILE:HG22 | 1:122:B:PHE:HB2  | 9        | 0.25          |
| (1,416) | 1:121:B:ILE:HG22 | 1:122:B:PHE:HB3  | 9        | 0.25          |
| (1,416) | 1:121:B:ILE:HG23 | 1:122:B:PHE:HB2  | 9        | 0.25          |
| (1,416) | 1:121:B:ILE:HG23 | 1:122:B:PHE:HB3  | 9        | 0.25          |
| (1,190) | 1:132:B:TRP:HB2  | 1:133:B:ARG:H    | 6        | 0.25          |
| (1,190) | 1:132:B:TRP:HB3  | 1:133:B:ARG:H    | 6        | 0.25          |
| (1,189) | 1:32:A:TRP:HB2   | 1:33:A:ARG:H     | 6        | 0.25          |

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| Key     | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (1,189) | 1:32:A:TRP:HB3  | 1:33:A:ARG:H     | 6        | 0.25          |
| (1,799) | 1:124:B:VAL:HA  | 1:125:B:LEU:HD21 | 4        | 0.24          |
| (1,799) | 1:124:B:VAL:HA  | 1:125:B:LEU:HD22 | 4        | 0.24          |
| (1,799) | 1:124:B:VAL:HA  | 1:125:B:LEU:HD23 | 4        | 0.24          |
| (1,799) | 1:124:B:VAL:HA  | 1:125:B:LEU:HD21 | 4        | 0.24          |
| (1,799) | 1:124:B:VAL:HA  | 1:125:B:LEU:HD22 | 4        | 0.24          |
| (1,799) | 1:124:B:VAL:HA  | 1:125:B:LEU:HD23 | 4        | 0.24          |
| (1,436) | 1:18:A:LEU:HA   | 1:118:B:LEU:HD11 | 1        | 0.24          |
| (1,436) | 1:18:A:LEU:HA   | 1:118:B:LEU:HD12 | 1        | 0.24          |
| (1,436) | 1:18:A:LEU:HA   | 1:118:B:LEU:HD13 | 1        | 0.24          |
| (1,436) | 1:18:A:LEU:HA   | 1:118:B:LEU:HD21 | 1        | 0.24          |
| (1,436) | 1:18:A:LEU:HA   | 1:118:B:LEU:HD22 | 1        | 0.24          |
| (1,436) | 1:18:A:LEU:HA   | 1:118:B:LEU:HD23 | 1        | 0.24          |
| (1,436) | 1:18:A:LEU:HA   | 1:118:B:LEU:HD11 | 6        | 0.24          |
| (1,436) | 1:18:A:LEU:HA   | 1:118:B:LEU:HD12 | 6        | 0.24          |
| (1,436) | 1:18:A:LEU:HA   | 1:118:B:LEU:HD13 | 6        | 0.24          |
| (1,436) | 1:18:A:LEU:HA   | 1:118:B:LEU:HD21 | 6        | 0.24          |
| (1,436) | 1:18:A:LEU:HA   | 1:118:B:LEU:HD22 | 6        | 0.24          |
| (1,436) | 1:18:A:LEU:HA   | 1:118:B:LEU:HD23 | 6        | 0.24          |
| (1,436) | 1:18:A:LEU:HA   | 1:118:B:LEU:HD11 | 7        | 0.24          |
| (1,436) | 1:18:A:LEU:HA   | 1:118:B:LEU:HD12 | 7        | 0.24          |
| (1,436) | 1:18:A:LEU:HA   | 1:118:B:LEU:HD13 | 7        | 0.24          |
| (1,436) | 1:18:A:LEU:HA   | 1:118:B:LEU:HD21 | 7        | 0.24          |
| (1,436) | 1:18:A:LEU:HA   | 1:118:B:LEU:HD22 | 7        | 0.24          |
| (1,436) | 1:18:A:LEU:HA   | 1:118:B:LEU:HD23 | 7        | 0.24          |
| (1,435) | 1:18:A:LEU:HD11 | 1:118:B:LEU:HA   | 1        | 0.24          |
| (1,435) | 1:18:A:LEU:HD12 | 1:118:B:LEU:HA   | 1        | 0.24          |
| (1,435) | 1:18:A:LEU:HD13 | 1:118:B:LEU:HA   | 1        | 0.24          |
| (1,435) | 1:18:A:LEU:HD21 | 1:118:B:LEU:HA   | 1        | 0.24          |
| (1,435) | 1:18:A:LEU:HD22 | 1:118:B:LEU:HA   | 1        | 0.24          |
| (1,435) | 1:18:A:LEU:HD23 | 1:118:B:LEU:HA   | 1        | 0.24          |
| (1,435) | 1:18:A:LEU:HD11 | 1:118:B:LEU:HA   | 4        | 0.24          |
| (1,435) | 1:18:A:LEU:HD12 | 1:118:B:LEU:HA   | 4        | 0.24          |
| (1,435) | 1:18:A:LEU:HD13 | 1:118:B:LEU:HA   | 4        | 0.24          |
| (1,435) | 1:18:A:LEU:HD21 | 1:118:B:LEU:HA   | 4        | 0.24          |
| (1,435) | 1:18:A:LEU:HD22 | 1:118:B:LEU:HA   | 4        | 0.24          |
| (1,435) | 1:18:A:LEU:HD23 | 1:118:B:LEU:HA   | 4        | 0.24          |
| (1,435) | 1:18:A:LEU:HD11 | 1:118:B:LEU:HA   | 8        | 0.24          |
| (1,435) | 1:18:A:LEU:HD12 | 1:118:B:LEU:HA   | 8        | 0.24          |
| (1,435) | 1:18:A:LEU:HD13 | 1:118:B:LEU:HA   | 8        | 0.24          |
| (1,435) | 1:18:A:LEU:HD21 | 1:118:B:LEU:HA   | 8        | 0.24          |
| (1,435) | 1:18:A:LEU:HD22 | 1:118:B:LEU:HA   | 8        | 0.24          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,435) | 1:18:A:LEU:HD23  | 1:118:B:LEU:HA   | 8        | 0.24          |
| (1,852) | 1:21:A:ILE:HG21  | 1:22:A:PHE:HB2   | 4        | 0.23          |
| (1,852) | 1:21:A:ILE:HG21  | 1:22:A:PHE:HB3   | 4        | 0.23          |
| (1,852) | 1:21:A:ILE:HG22  | 1:22:A:PHE:HB2   | 4        | 0.23          |
| (1,852) | 1:21:A:ILE:HG22  | 1:22:A:PHE:HB3   | 4        | 0.23          |
| (1,852) | 1:21:A:ILE:HG23  | 1:22:A:PHE:HB2   | 4        | 0.23          |
| (1,852) | 1:21:A:ILE:HG23  | 1:22:A:PHE:HB3   | 4        | 0.23          |
| (1,831) | 1:118:B:LEU:HD21 | 1:122:B:PHE:HB2  | 4        | 0.23          |
| (1,831) | 1:118:B:LEU:HD21 | 1:122:B:PHE:HB3  | 4        | 0.23          |
| (1,831) | 1:118:B:LEU:HD22 | 1:122:B:PHE:HB2  | 4        | 0.23          |
| (1,831) | 1:118:B:LEU:HD22 | 1:122:B:PHE:HB3  | 4        | 0.23          |
| (1,831) | 1:118:B:LEU:HD23 | 1:122:B:PHE:HB2  | 4        | 0.23          |
| (1,831) | 1:118:B:LEU:HD23 | 1:122:B:PHE:HB3  | 4        | 0.23          |
| (1,831) | 1:118:B:LEU:HD21 | 1:122:B:PHE:HB2  | 4        | 0.23          |
| (1,831) | 1:118:B:LEU:HD21 | 1:122:B:PHE:HB3  | 4        | 0.23          |
| (1,831) | 1:118:B:LEU:HD22 | 1:122:B:PHE:HB2  | 4        | 0.23          |
| (1,831) | 1:118:B:LEU:HD22 | 1:122:B:PHE:HB3  | 4        | 0.23          |
| (1,831) | 1:118:B:LEU:HD23 | 1:122:B:PHE:HB2  | 4        | 0.23          |
| (1,831) | 1:118:B:LEU:HD23 | 1:122:B:PHE:HB3  | 4        | 0.23          |
| (1,436) | 1:18:A:LEU:HA    | 1:118:B:LEU:HD11 | 9        | 0.23          |
| (1,436) | 1:18:A:LEU:HA    | 1:118:B:LEU:HD12 | 9        | 0.23          |
| (1,436) | 1:18:A:LEU:HA    | 1:118:B:LEU:HD13 | 9        | 0.23          |
| (1,436) | 1:18:A:LEU:HA    | 1:118:B:LEU:HD21 | 9        | 0.23          |
| (1,436) | 1:18:A:LEU:HA    | 1:118:B:LEU:HD22 | 9        | 0.23          |
| (1,436) | 1:18:A:LEU:HA    | 1:118:B:LEU:HD23 | 9        | 0.23          |
| (1,415) | 1:21:A:ILE:HG21  | 1:22:A:PHE:HB2   | 4        | 0.23          |
| (1,415) | 1:21:A:ILE:HG21  | 1:22:A:PHE:HB3   | 4        | 0.23          |
| (1,415) | 1:21:A:ILE:HG22  | 1:22:A:PHE:HB2   | 4        | 0.23          |
| (1,415) | 1:21:A:ILE:HG22  | 1:22:A:PHE:HB3   | 4        | 0.23          |
| (1,415) | 1:21:A:ILE:HG23  | 1:22:A:PHE:HB2   | 4        | 0.23          |
| (1,415) | 1:21:A:ILE:HG23  | 1:22:A:PHE:HB3   | 4        | 0.23          |
| (1,852) | 1:21:A:ILE:HG21  | 1:22:A:PHE:HB2   | 9        | 0.22          |
| (1,852) | 1:21:A:ILE:HG21  | 1:22:A:PHE:HB3   | 9        | 0.22          |
| (1,852) | 1:21:A:ILE:HG22  | 1:22:A:PHE:HB2   | 9        | 0.22          |
| (1,852) | 1:21:A:ILE:HG22  | 1:22:A:PHE:HB3   | 9        | 0.22          |
| (1,852) | 1:21:A:ILE:HG23  | 1:22:A:PHE:HB2   | 9        | 0.22          |
| (1,852) | 1:21:A:ILE:HG23  | 1:22:A:PHE:HB3   | 9        | 0.22          |
| (1,799) | 1:124:B:VAL:HA   | 1:125:B:LEU:HD21 | 10       | 0.22          |
| (1,799) | 1:124:B:VAL:HA   | 1:125:B:LEU:HD22 | 10       | 0.22          |
| (1,799) | 1:124:B:VAL:HA   | 1:125:B:LEU:HD23 | 10       | 0.22          |
| (1,799) | 1:124:B:VAL:HA   | 1:125:B:LEU:HD21 | 10       | 0.22          |
| (1,799) | 1:124:B:VAL:HA   | 1:125:B:LEU:HD22 | 10       | 0.22          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,799) | 1:124:B:VAL:HA   | 1:125:B:LEU:HD23 | 10       | 0.22          |
| (1,436) | 1:18:A:LEU:HA    | 1:118:B:LEU:HD11 | 2        | 0.22          |
| (1,436) | 1:18:A:LEU:HA    | 1:118:B:LEU:HD12 | 2        | 0.22          |
| (1,436) | 1:18:A:LEU:HA    | 1:118:B:LEU:HD13 | 2        | 0.22          |
| (1,436) | 1:18:A:LEU:HA    | 1:118:B:LEU:HD21 | 2        | 0.22          |
| (1,436) | 1:18:A:LEU:HA    | 1:118:B:LEU:HD22 | 2        | 0.22          |
| (1,436) | 1:18:A:LEU:HA    | 1:118:B:LEU:HD23 | 2        | 0.22          |
| (1,436) | 1:18:A:LEU:HA    | 1:118:B:LEU:HD11 | 3        | 0.22          |
| (1,436) | 1:18:A:LEU:HA    | 1:118:B:LEU:HD12 | 3        | 0.22          |
| (1,436) | 1:18:A:LEU:HA    | 1:118:B:LEU:HD13 | 3        | 0.22          |
| (1,436) | 1:18:A:LEU:HA    | 1:118:B:LEU:HD21 | 3        | 0.22          |
| (1,436) | 1:18:A:LEU:HA    | 1:118:B:LEU:HD22 | 3        | 0.22          |
| (1,436) | 1:18:A:LEU:HA    | 1:118:B:LEU:HD23 | 3        | 0.22          |
| (1,435) | 1:18:A:LEU:HD11  | 1:118:B:LEU:HA   | 5        | 0.22          |
| (1,435) | 1:18:A:LEU:HD12  | 1:118:B:LEU:HA   | 5        | 0.22          |
| (1,435) | 1:18:A:LEU:HD13  | 1:118:B:LEU:HA   | 5        | 0.22          |
| (1,435) | 1:18:A:LEU:HD21  | 1:118:B:LEU:HA   | 5        | 0.22          |
| (1,435) | 1:18:A:LEU:HD22  | 1:118:B:LEU:HA   | 5        | 0.22          |
| (1,435) | 1:18:A:LEU:HD23  | 1:118:B:LEU:HA   | 5        | 0.22          |
| (1,435) | 1:18:A:LEU:HD11  | 1:118:B:LEU:HA   | 6        | 0.22          |
| (1,435) | 1:18:A:LEU:HD12  | 1:118:B:LEU:HA   | 6        | 0.22          |
| (1,435) | 1:18:A:LEU:HD13  | 1:118:B:LEU:HA   | 6        | 0.22          |
| (1,435) | 1:18:A:LEU:HD21  | 1:118:B:LEU:HA   | 6        | 0.22          |
| (1,435) | 1:18:A:LEU:HD22  | 1:118:B:LEU:HA   | 6        | 0.22          |
| (1,435) | 1:18:A:LEU:HD23  | 1:118:B:LEU:HA   | 6        | 0.22          |
| (1,435) | 1:18:A:LEU:HD11  | 1:118:B:LEU:HA   | 7        | 0.22          |
| (1,435) | 1:18:A:LEU:HD12  | 1:118:B:LEU:HA   | 7        | 0.22          |
| (1,435) | 1:18:A:LEU:HD13  | 1:118:B:LEU:HA   | 7        | 0.22          |
| (1,435) | 1:18:A:LEU:HD21  | 1:118:B:LEU:HA   | 7        | 0.22          |
| (1,435) | 1:18:A:LEU:HD22  | 1:118:B:LEU:HA   | 7        | 0.22          |
| (1,435) | 1:18:A:LEU:HD23  | 1:118:B:LEU:HA   | 7        | 0.22          |
| (1,416) | 1:121:B:ILE:HG21 | 1:122:B:PHE:HB2  | 4        | 0.22          |
| (1,416) | 1:121:B:ILE:HG21 | 1:122:B:PHE:HB3  | 4        | 0.22          |
| (1,416) | 1:121:B:ILE:HG22 | 1:122:B:PHE:HB2  | 4        | 0.22          |
| (1,416) | 1:121:B:ILE:HG22 | 1:122:B:PHE:HB3  | 4        | 0.22          |
| (1,416) | 1:121:B:ILE:HG23 | 1:122:B:PHE:HB2  | 4        | 0.22          |
| (1,416) | 1:121:B:ILE:HG23 | 1:122:B:PHE:HB3  | 4        | 0.22          |
| (1,415) | 1:21:A:ILE:HG21  | 1:22:A:PHE:HB2   | 9        | 0.22          |
| (1,415) | 1:21:A:ILE:HG21  | 1:22:A:PHE:HB3   | 9        | 0.22          |
| (1,415) | 1:21:A:ILE:HG22  | 1:22:A:PHE:HB2   | 9        | 0.22          |
| (1,415) | 1:21:A:ILE:HG22  | 1:22:A:PHE:HB3   | 9        | 0.22          |
| (1,415) | 1:21:A:ILE:HG23  | 1:22:A:PHE:HB2   | 9        | 0.22          |

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| Key     | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (1,415) | 1:21:A:ILE:HG23 | 1:22:A:PHE:HB3   | 9        | 0.22          |
| (1,804) | 1:20:A:PHE:HA   | 1:23:A:ILE:HD11  | 6        | 0.21          |
| (1,804) | 1:20:A:PHE:HA   | 1:23:A:ILE:HD12  | 6        | 0.21          |
| (1,804) | 1:20:A:PHE:HA   | 1:23:A:ILE:HD13  | 6        | 0.21          |
| (1,436) | 1:18:A:LEU:HA   | 1:118:B:LEU:HD11 | 4        | 0.21          |
| (1,436) | 1:18:A:LEU:HA   | 1:118:B:LEU:HD12 | 4        | 0.21          |
| (1,436) | 1:18:A:LEU:HA   | 1:118:B:LEU:HD13 | 4        | 0.21          |
| (1,436) | 1:18:A:LEU:HA   | 1:118:B:LEU:HD21 | 4        | 0.21          |
| (1,436) | 1:18:A:LEU:HA   | 1:118:B:LEU:HD22 | 4        | 0.21          |
| (1,436) | 1:18:A:LEU:HA   | 1:118:B:LEU:HD23 | 4        | 0.21          |
| (1,435) | 1:18:A:LEU:HD11 | 1:118:B:LEU:HA   | 2        | 0.21          |
| (1,435) | 1:18:A:LEU:HD12 | 1:118:B:LEU:HA   | 2        | 0.21          |
| (1,435) | 1:18:A:LEU:HD13 | 1:118:B:LEU:HA   | 2        | 0.21          |
| (1,435) | 1:18:A:LEU:HD21 | 1:118:B:LEU:HA   | 2        | 0.21          |
| (1,435) | 1:18:A:LEU:HD22 | 1:118:B:LEU:HA   | 2        | 0.21          |
| (1,435) | 1:18:A:LEU:HD23 | 1:118:B:LEU:HA   | 2        | 0.21          |
| (1,435) | 1:18:A:LEU:HD11 | 1:118:B:LEU:HA   | 3        | 0.21          |
| (1,435) | 1:18:A:LEU:HD12 | 1:118:B:LEU:HA   | 3        | 0.21          |
| (1,435) | 1:18:A:LEU:HD13 | 1:118:B:LEU:HA   | 3        | 0.21          |
| (1,435) | 1:18:A:LEU:HD21 | 1:118:B:LEU:HA   | 3        | 0.21          |
| (1,435) | 1:18:A:LEU:HD22 | 1:118:B:LEU:HA   | 3        | 0.21          |
| (1,435) | 1:18:A:LEU:HD23 | 1:118:B:LEU:HA   | 3        | 0.21          |
| (1,369) | 1:20:A:PHE:HA   | 1:23:A:ILE:HD11  | 6        | 0.21          |
| (1,369) | 1:20:A:PHE:HA   | 1:23:A:ILE:HD12  | 6        | 0.21          |
| (1,369) | 1:20:A:PHE:HA   | 1:23:A:ILE:HD13  | 6        | 0.21          |
| (1,370) | 1:120:B:PHE:HA  | 1:123:B:ILE:HD11 | 6        | 0.2           |
| (1,370) | 1:120:B:PHE:HA  | 1:123:B:ILE:HD12 | 6        | 0.2           |
| (1,370) | 1:120:B:PHE:HA  | 1:123:B:ILE:HD13 | 6        | 0.2           |
| (1,370) | 1:120:B:PHE:HA  | 1:123:B:ILE:HD11 | 7        | 0.2           |
| (1,370) | 1:120:B:PHE:HA  | 1:123:B:ILE:HD12 | 7        | 0.2           |
| (1,370) | 1:120:B:PHE:HA  | 1:123:B:ILE:HD13 | 7        | 0.2           |
| (1,370) | 1:120:B:PHE:HA  | 1:123:B:ILE:HD11 | 9        | 0.2           |
| (1,370) | 1:120:B:PHE:HA  | 1:123:B:ILE:HD12 | 9        | 0.2           |
| (1,370) | 1:120:B:PHE:HA  | 1:123:B:ILE:HD13 | 9        | 0.2           |
| (1,852) | 1:21:A:ILE:HG21 | 1:22:A:PHE:HB2   | 1        | 0.19          |
| (1,852) | 1:21:A:ILE:HG21 | 1:22:A:PHE:HB3   | 1        | 0.19          |
| (1,852) | 1:21:A:ILE:HG22 | 1:22:A:PHE:HB2   | 1        | 0.19          |
| (1,852) | 1:21:A:ILE:HG22 | 1:22:A:PHE:HB3   | 1        | 0.19          |
| (1,852) | 1:21:A:ILE:HG23 | 1:22:A:PHE:HB2   | 1        | 0.19          |
| (1,852) | 1:21:A:ILE:HG23 | 1:22:A:PHE:HB3   | 1        | 0.19          |
| (1,852) | 1:21:A:ILE:HG21 | 1:22:A:PHE:HB2   | 3        | 0.19          |
| (1,852) | 1:21:A:ILE:HG21 | 1:22:A:PHE:HB3   | 3        | 0.19          |

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| Key     | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|---------|------------------|-----------------|----------|---------------|
| (1,852) | 1:21:A:ILE:HG22  | 1:22:A:PHE:HB2  | 3        | 0.19          |
| (1,852) | 1:21:A:ILE:HG22  | 1:22:A:PHE:HB3  | 3        | 0.19          |
| (1,852) | 1:21:A:ILE:HG23  | 1:22:A:PHE:HB2  | 3        | 0.19          |
| (1,852) | 1:21:A:ILE:HG23  | 1:22:A:PHE:HB3  | 3        | 0.19          |
| (1,416) | 1:121:B:ILE:HG21 | 1:122:B:PHE:HB2 | 3        | 0.19          |
| (1,416) | 1:121:B:ILE:HG21 | 1:122:B:PHE:HB3 | 3        | 0.19          |
| (1,416) | 1:121:B:ILE:HG22 | 1:122:B:PHE:HB2 | 3        | 0.19          |
| (1,416) | 1:121:B:ILE:HG22 | 1:122:B:PHE:HB3 | 3        | 0.19          |
| (1,416) | 1:121:B:ILE:HG23 | 1:122:B:PHE:HB2 | 3        | 0.19          |
| (1,416) | 1:121:B:ILE:HG23 | 1:122:B:PHE:HB3 | 3        | 0.19          |
| (1,416) | 1:121:B:ILE:HG21 | 1:122:B:PHE:HB2 | 5        | 0.19          |
| (1,416) | 1:121:B:ILE:HG21 | 1:122:B:PHE:HB3 | 5        | 0.19          |
| (1,416) | 1:121:B:ILE:HG22 | 1:122:B:PHE:HB2 | 5        | 0.19          |
| (1,416) | 1:121:B:ILE:HG22 | 1:122:B:PHE:HB3 | 5        | 0.19          |
| (1,416) | 1:121:B:ILE:HG23 | 1:122:B:PHE:HB2 | 5        | 0.19          |
| (1,416) | 1:121:B:ILE:HG23 | 1:122:B:PHE:HB3 | 5        | 0.19          |
| (1,416) | 1:121:B:ILE:HG21 | 1:122:B:PHE:HB2 | 10       | 0.19          |
| (1,416) | 1:121:B:ILE:HG21 | 1:122:B:PHE:HB3 | 10       | 0.19          |
| (1,416) | 1:121:B:ILE:HG22 | 1:122:B:PHE:HB2 | 10       | 0.19          |
| (1,416) | 1:121:B:ILE:HG22 | 1:122:B:PHE:HB3 | 10       | 0.19          |
| (1,416) | 1:121:B:ILE:HG23 | 1:122:B:PHE:HB2 | 10       | 0.19          |
| (1,416) | 1:121:B:ILE:HG23 | 1:122:B:PHE:HB3 | 10       | 0.19          |
| (1,415) | 1:21:A:ILE:HG21  | 1:22:A:PHE:HB2  | 1        | 0.19          |
| (1,415) | 1:21:A:ILE:HG21  | 1:22:A:PHE:HB3  | 1        | 0.19          |
| (1,415) | 1:21:A:ILE:HG22  | 1:22:A:PHE:HB2  | 1        | 0.19          |
| (1,415) | 1:21:A:ILE:HG22  | 1:22:A:PHE:HB3  | 1        | 0.19          |
| (1,415) | 1:21:A:ILE:HG23  | 1:22:A:PHE:HB2  | 1        | 0.19          |
| (1,415) | 1:21:A:ILE:HG23  | 1:22:A:PHE:HB3  | 1        | 0.19          |
| (1,415) | 1:21:A:ILE:HG21  | 1:22:A:PHE:HB2  | 3        | 0.19          |
| (1,415) | 1:21:A:ILE:HG21  | 1:22:A:PHE:HB3  | 3        | 0.19          |
| (1,415) | 1:21:A:ILE:HG22  | 1:22:A:PHE:HB2  | 3        | 0.19          |
| (1,415) | 1:21:A:ILE:HG22  | 1:22:A:PHE:HB3  | 3        | 0.19          |
| (1,415) | 1:21:A:ILE:HG23  | 1:22:A:PHE:HB2  | 3        | 0.19          |
| (1,415) | 1:21:A:ILE:HG23  | 1:22:A:PHE:HB3  | 3        | 0.19          |
| (1,254) | 1:117:B:LEU:HA   | 1:120:B:PHE:HB2 | 7        | 0.19          |
| (1,254) | 1:117:B:LEU:HA   | 1:120:B:PHE:HB3 | 7        | 0.19          |
| (1,852) | 1:21:A:ILE:HG21  | 1:22:A:PHE:HB2  | 2        | 0.18          |
| (1,852) | 1:21:A:ILE:HG21  | 1:22:A:PHE:HB3  | 2        | 0.18          |
| (1,852) | 1:21:A:ILE:HG22  | 1:22:A:PHE:HB2  | 2        | 0.18          |
| (1,852) | 1:21:A:ILE:HG22  | 1:22:A:PHE:HB3  | 2        | 0.18          |
| (1,852) | 1:21:A:ILE:HG23  | 1:22:A:PHE:HB2  | 2        | 0.18          |
| (1,852) | 1:21:A:ILE:HG23  | 1:22:A:PHE:HB3  | 2        | 0.18          |

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| Key     | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|---------|------------------|-----------------|----------|---------------|
| (1,852) | 1:21:A:ILE:HG21  | 1:22:A:PHE:HB2  | 5        | 0.18          |
| (1,852) | 1:21:A:ILE:HG21  | 1:22:A:PHE:HB3  | 5        | 0.18          |
| (1,852) | 1:21:A:ILE:HG22  | 1:22:A:PHE:HB2  | 5        | 0.18          |
| (1,852) | 1:21:A:ILE:HG22  | 1:22:A:PHE:HB3  | 5        | 0.18          |
| (1,852) | 1:21:A:ILE:HG23  | 1:22:A:PHE:HB2  | 5        | 0.18          |
| (1,852) | 1:21:A:ILE:HG23  | 1:22:A:PHE:HB3  | 5        | 0.18          |
| (1,852) | 1:21:A:ILE:HG21  | 1:22:A:PHE:HB2  | 8        | 0.18          |
| (1,852) | 1:21:A:ILE:HG21  | 1:22:A:PHE:HB3  | 8        | 0.18          |
| (1,852) | 1:21:A:ILE:HG22  | 1:22:A:PHE:HB2  | 8        | 0.18          |
| (1,852) | 1:21:A:ILE:HG22  | 1:22:A:PHE:HB3  | 8        | 0.18          |
| (1,852) | 1:21:A:ILE:HG23  | 1:22:A:PHE:HB2  | 8        | 0.18          |
| (1,852) | 1:21:A:ILE:HG23  | 1:22:A:PHE:HB3  | 8        | 0.18          |
| (1,804) | 1:20:A:PHE:HA    | 1:23:A:ILE:HD11 | 2        | 0.18          |
| (1,804) | 1:20:A:PHE:HA    | 1:23:A:ILE:HD12 | 2        | 0.18          |
| (1,804) | 1:20:A:PHE:HA    | 1:23:A:ILE:HD13 | 2        | 0.18          |
| (1,804) | 1:20:A:PHE:HA    | 1:23:A:ILE:HD11 | 10       | 0.18          |
| (1,804) | 1:20:A:PHE:HA    | 1:23:A:ILE:HD12 | 10       | 0.18          |
| (1,804) | 1:20:A:PHE:HA    | 1:23:A:ILE:HD13 | 10       | 0.18          |
| (1,790) | 1:27:A:ILE:HG21  | 1:28:A:HIS:HB2  | 3        | 0.18          |
| (1,790) | 1:27:A:ILE:HG22  | 1:28:A:HIS:HB2  | 3        | 0.18          |
| (1,790) | 1:27:A:ILE:HG23  | 1:28:A:HIS:HB2  | 3        | 0.18          |
| (1,692) | 1:17:A:LEU:HA    | 1:20:A:PHE:HB2  | 6        | 0.18          |
| (1,692) | 1:17:A:LEU:HA    | 1:20:A:PHE:HB3  | 6        | 0.18          |
| (1,692) | 1:17:A:LEU:HA    | 1:20:A:PHE:HB2  | 10       | 0.18          |
| (1,692) | 1:17:A:LEU:HA    | 1:20:A:PHE:HB3  | 10       | 0.18          |
| (1,680) | 1:19:A:ILE:HA    | 1:22:A:PHE:H    | 9        | 0.18          |
| (1,416) | 1:121:B:ILE:HG21 | 1:122:B:PHE:HB2 | 1        | 0.18          |
| (1,416) | 1:121:B:ILE:HG21 | 1:122:B:PHE:HB3 | 1        | 0.18          |
| (1,416) | 1:121:B:ILE:HG22 | 1:122:B:PHE:HB2 | 1        | 0.18          |
| (1,416) | 1:121:B:ILE:HG22 | 1:122:B:PHE:HB3 | 1        | 0.18          |
| (1,416) | 1:121:B:ILE:HG23 | 1:122:B:PHE:HB2 | 1        | 0.18          |
| (1,416) | 1:121:B:ILE:HG23 | 1:122:B:PHE:HB3 | 1        | 0.18          |
| (1,416) | 1:121:B:ILE:HG21 | 1:122:B:PHE:HB2 | 2        | 0.18          |
| (1,416) | 1:121:B:ILE:HG21 | 1:122:B:PHE:HB3 | 2        | 0.18          |
| (1,416) | 1:121:B:ILE:HG22 | 1:122:B:PHE:HB2 | 2        | 0.18          |
| (1,416) | 1:121:B:ILE:HG22 | 1:122:B:PHE:HB3 | 2        | 0.18          |
| (1,416) | 1:121:B:ILE:HG23 | 1:122:B:PHE:HB2 | 2        | 0.18          |
| (1,416) | 1:121:B:ILE:HG23 | 1:122:B:PHE:HB3 | 2        | 0.18          |
| (1,416) | 1:121:B:ILE:HG21 | 1:122:B:PHE:HB2 | 6        | 0.18          |
| (1,416) | 1:121:B:ILE:HG21 | 1:122:B:PHE:HB3 | 6        | 0.18          |
| (1,416) | 1:121:B:ILE:HG22 | 1:122:B:PHE:HB2 | 6        | 0.18          |
| (1,416) | 1:121:B:ILE:HG22 | 1:122:B:PHE:HB3 | 6        | 0.18          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,416) | 1:121:B:ILE:HG23 | 1:122:B:PHE:HB2  | 6        | 0.18          |
| (1,416) | 1:121:B:ILE:HG23 | 1:122:B:PHE:HB3  | 6        | 0.18          |
| (1,416) | 1:121:B:ILE:HG21 | 1:122:B:PHE:HB2  | 8        | 0.18          |
| (1,416) | 1:121:B:ILE:HG21 | 1:122:B:PHE:HB3  | 8        | 0.18          |
| (1,416) | 1:121:B:ILE:HG22 | 1:122:B:PHE:HB2  | 8        | 0.18          |
| (1,416) | 1:121:B:ILE:HG22 | 1:122:B:PHE:HB3  | 8        | 0.18          |
| (1,416) | 1:121:B:ILE:HG23 | 1:122:B:PHE:HB2  | 8        | 0.18          |
| (1,416) | 1:121:B:ILE:HG23 | 1:122:B:PHE:HB3  | 8        | 0.18          |
| (1,415) | 1:21:A:ILE:HG21  | 1:22:A:PHE:HB2   | 2        | 0.18          |
| (1,415) | 1:21:A:ILE:HG21  | 1:22:A:PHE:HB3   | 2        | 0.18          |
| (1,415) | 1:21:A:ILE:HG22  | 1:22:A:PHE:HB2   | 2        | 0.18          |
| (1,415) | 1:21:A:ILE:HG22  | 1:22:A:PHE:HB3   | 2        | 0.18          |
| (1,415) | 1:21:A:ILE:HG23  | 1:22:A:PHE:HB2   | 2        | 0.18          |
| (1,415) | 1:21:A:ILE:HG23  | 1:22:A:PHE:HB3   | 2        | 0.18          |
| (1,415) | 1:21:A:ILE:HG21  | 1:22:A:PHE:HB2   | 5        | 0.18          |
| (1,415) | 1:21:A:ILE:HG21  | 1:22:A:PHE:HB3   | 5        | 0.18          |
| (1,415) | 1:21:A:ILE:HG22  | 1:22:A:PHE:HB2   | 5        | 0.18          |
| (1,415) | 1:21:A:ILE:HG22  | 1:22:A:PHE:HB3   | 5        | 0.18          |
| (1,415) | 1:21:A:ILE:HG23  | 1:22:A:PHE:HB2   | 5        | 0.18          |
| (1,415) | 1:21:A:ILE:HG23  | 1:22:A:PHE:HB3   | 5        | 0.18          |
| (1,415) | 1:21:A:ILE:HG21  | 1:22:A:PHE:HB2   | 8        | 0.18          |
| (1,415) | 1:21:A:ILE:HG21  | 1:22:A:PHE:HB3   | 8        | 0.18          |
| (1,415) | 1:21:A:ILE:HG22  | 1:22:A:PHE:HB2   | 8        | 0.18          |
| (1,415) | 1:21:A:ILE:HG22  | 1:22:A:PHE:HB3   | 8        | 0.18          |
| (1,415) | 1:21:A:ILE:HG23  | 1:22:A:PHE:HB2   | 8        | 0.18          |
| (1,415) | 1:21:A:ILE:HG23  | 1:22:A:PHE:HB3   | 8        | 0.18          |
| (1,370) | 1:120:B:PHE:HA   | 1:123:B:ILE:HD11 | 2        | 0.18          |
| (1,370) | 1:120:B:PHE:HA   | 1:123:B:ILE:HD12 | 2        | 0.18          |
| (1,370) | 1:120:B:PHE:HA   | 1:123:B:ILE:HD13 | 2        | 0.18          |
| (1,370) | 1:120:B:PHE:HA   | 1:123:B:ILE:HD11 | 10       | 0.18          |
| (1,370) | 1:120:B:PHE:HA   | 1:123:B:ILE:HD12 | 10       | 0.18          |
| (1,370) | 1:120:B:PHE:HA   | 1:123:B:ILE:HD13 | 10       | 0.18          |
| (1,369) | 1:20:A:PHE:HA    | 1:23:A:ILE:HD11  | 2        | 0.18          |
| (1,369) | 1:20:A:PHE:HA    | 1:23:A:ILE:HD12  | 2        | 0.18          |
| (1,369) | 1:20:A:PHE:HA    | 1:23:A:ILE:HD13  | 2        | 0.18          |
| (1,369) | 1:20:A:PHE:HA    | 1:23:A:ILE:HD11  | 10       | 0.18          |
| (1,369) | 1:20:A:PHE:HA    | 1:23:A:ILE:HD12  | 10       | 0.18          |
| (1,369) | 1:20:A:PHE:HA    | 1:23:A:ILE:HD13  | 10       | 0.18          |
| (1,355) | 1:27:A:ILE:HG21  | 1:28:A:HIS:HB2   | 3        | 0.18          |
| (1,355) | 1:27:A:ILE:HG22  | 1:28:A:HIS:HB2   | 3        | 0.18          |
| (1,355) | 1:27:A:ILE:HG23  | 1:28:A:HIS:HB2   | 3        | 0.18          |
| (1,253) | 1:17:A:LEU:HA    | 1:20:A:PHE:HB2   | 6        | 0.18          |

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| Key     | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|---------|------------------|-----------------|----------|---------------|
| (1,253) | 1:17:A:LEU:HA    | 1:20:A:PHE:HB3  | 6        | 0.18          |
| (1,253) | 1:17:A:LEU:HA    | 1:20:A:PHE:HB2  | 10       | 0.18          |
| (1,253) | 1:17:A:LEU:HA    | 1:20:A:PHE:HB3  | 10       | 0.18          |
| (1,242) | 1:119:B:ILE:HA   | 1:122:B:PHE:H   | 7        | 0.18          |
| (1,241) | 1:19:A:ILE:HA    | 1:22:A:PHE:H    | 9        | 0.18          |
| (1,852) | 1:21:A:ILE:HG21  | 1:22:A:PHE:HB2  | 6        | 0.17          |
| (1,852) | 1:21:A:ILE:HG21  | 1:22:A:PHE:HB3  | 6        | 0.17          |
| (1,852) | 1:21:A:ILE:HG22  | 1:22:A:PHE:HB2  | 6        | 0.17          |
| (1,852) | 1:21:A:ILE:HG22  | 1:22:A:PHE:HB3  | 6        | 0.17          |
| (1,852) | 1:21:A:ILE:HG23  | 1:22:A:PHE:HB2  | 6        | 0.17          |
| (1,852) | 1:21:A:ILE:HG23  | 1:22:A:PHE:HB3  | 6        | 0.17          |
| (1,852) | 1:21:A:ILE:HG21  | 1:22:A:PHE:HB2  | 7        | 0.17          |
| (1,852) | 1:21:A:ILE:HG21  | 1:22:A:PHE:HB3  | 7        | 0.17          |
| (1,852) | 1:21:A:ILE:HG22  | 1:22:A:PHE:HB2  | 7        | 0.17          |
| (1,852) | 1:21:A:ILE:HG22  | 1:22:A:PHE:HB3  | 7        | 0.17          |
| (1,852) | 1:21:A:ILE:HG23  | 1:22:A:PHE:HB2  | 7        | 0.17          |
| (1,852) | 1:21:A:ILE:HG23  | 1:22:A:PHE:HB3  | 7        | 0.17          |
| (1,692) | 1:17:A:LEU:HA    | 1:20:A:PHE:HB2  | 9        | 0.17          |
| (1,692) | 1:17:A:LEU:HA    | 1:20:A:PHE:HB3  | 9        | 0.17          |
| (1,680) | 1:19:A:ILE:HA    | 1:22:A:PHE:H    | 7        | 0.17          |
| (1,664) | 1:34:A:ILE:H     | 1:34:A:ILE:HA   | 8        | 0.17          |
| (1,628) | 1:32:A:TRP:HB2   | 1:33:A:ARG:H    | 4        | 0.17          |
| (1,628) | 1:32:A:TRP:HB3   | 1:33:A:ARG:H    | 4        | 0.17          |
| (1,415) | 1:21:A:ILE:HG21  | 1:22:A:PHE:HB2  | 6        | 0.17          |
| (1,415) | 1:21:A:ILE:HG21  | 1:22:A:PHE:HB3  | 6        | 0.17          |
| (1,415) | 1:21:A:ILE:HG22  | 1:22:A:PHE:HB2  | 6        | 0.17          |
| (1,415) | 1:21:A:ILE:HG22  | 1:22:A:PHE:HB3  | 6        | 0.17          |
| (1,415) | 1:21:A:ILE:HG23  | 1:22:A:PHE:HB2  | 6        | 0.17          |
| (1,415) | 1:21:A:ILE:HG23  | 1:22:A:PHE:HB3  | 6        | 0.17          |
| (1,415) | 1:21:A:ILE:HG21  | 1:22:A:PHE:HB2  | 7        | 0.17          |
| (1,415) | 1:21:A:ILE:HG21  | 1:22:A:PHE:HB3  | 7        | 0.17          |
| (1,415) | 1:21:A:ILE:HG22  | 1:22:A:PHE:HB2  | 7        | 0.17          |
| (1,415) | 1:21:A:ILE:HG22  | 1:22:A:PHE:HB3  | 7        | 0.17          |
| (1,415) | 1:21:A:ILE:HG23  | 1:22:A:PHE:HB2  | 7        | 0.17          |
| (1,415) | 1:21:A:ILE:HG23  | 1:22:A:PHE:HB3  | 7        | 0.17          |
| (1,356) | 1:127:B:ILE:HG21 | 1:128:B:HIS:HB2 | 3        | 0.17          |
| (1,356) | 1:127:B:ILE:HG22 | 1:128:B:HIS:HB2 | 3        | 0.17          |
| (1,356) | 1:127:B:ILE:HG23 | 1:128:B:HIS:HB2 | 3        | 0.17          |
| (1,254) | 1:117:B:LEU:HA   | 1:120:B:PHE:HB2 | 4        | 0.17          |
| (1,254) | 1:117:B:LEU:HA   | 1:120:B:PHE:HB3 | 4        | 0.17          |
| (1,253) | 1:17:A:LEU:HA    | 1:20:A:PHE:HB2  | 9        | 0.17          |
| (1,253) | 1:17:A:LEU:HA    | 1:20:A:PHE:HB3  | 9        | 0.17          |

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| Key     | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|---------|------------------|-----------------|----------|---------------|
| (1,242) | 1:119:B:ILE:HA   | 1:122:B:PHE:H   | 9        | 0.17          |
| (1,241) | 1:19:A:ILE:HA    | 1:22:A:PHE:H    | 7        | 0.17          |
| (1,226) | 1:134:B:ILE:H    | 1:134:B:ILE:HA  | 8        | 0.17          |
| (1,225) | 1:34:A:ILE:H     | 1:34:A:ILE:HA   | 8        | 0.17          |
| (1,189) | 1:32:A:TRP:HB2   | 1:33:A:ARG:H    | 4        | 0.17          |
| (1,189) | 1:32:A:TRP:HB3   | 1:33:A:ARG:H    | 4        | 0.17          |
| (1,852) | 1:21:A:ILE:HG21  | 1:22:A:PHE:HB2  | 10       | 0.16          |
| (1,852) | 1:21:A:ILE:HG21  | 1:22:A:PHE:HB3  | 10       | 0.16          |
| (1,852) | 1:21:A:ILE:HG22  | 1:22:A:PHE:HB2  | 10       | 0.16          |
| (1,852) | 1:21:A:ILE:HG22  | 1:22:A:PHE:HB3  | 10       | 0.16          |
| (1,852) | 1:21:A:ILE:HG23  | 1:22:A:PHE:HB2  | 10       | 0.16          |
| (1,852) | 1:21:A:ILE:HG23  | 1:22:A:PHE:HB3  | 10       | 0.16          |
| (1,790) | 1:27:A:ILE:HG21  | 1:28:A:HIS:HB2  | 1        | 0.16          |
| (1,790) | 1:27:A:ILE:HG22  | 1:28:A:HIS:HB2  | 1        | 0.16          |
| (1,790) | 1:27:A:ILE:HG23  | 1:28:A:HIS:HB2  | 1        | 0.16          |
| (1,790) | 1:27:A:ILE:HG21  | 1:28:A:HIS:HB2  | 8        | 0.16          |
| (1,790) | 1:27:A:ILE:HG22  | 1:28:A:HIS:HB2  | 8        | 0.16          |
| (1,790) | 1:27:A:ILE:HG23  | 1:28:A:HIS:HB2  | 8        | 0.16          |
| (1,790) | 1:27:A:ILE:HG21  | 1:28:A:HIS:HB2  | 10       | 0.16          |
| (1,790) | 1:27:A:ILE:HG22  | 1:28:A:HIS:HB2  | 10       | 0.16          |
| (1,790) | 1:27:A:ILE:HG23  | 1:28:A:HIS:HB2  | 10       | 0.16          |
| (1,692) | 1:17:A:LEU:HA    | 1:20:A:PHE:HB2  | 4        | 0.16          |
| (1,692) | 1:17:A:LEU:HA    | 1:20:A:PHE:HB3  | 4        | 0.16          |
| (1,680) | 1:19:A:ILE:HA    | 1:22:A:PHE:H    | 8        | 0.16          |
| (1,416) | 1:121:B:ILE:HG21 | 1:122:B:PHE:HB2 | 7        | 0.16          |
| (1,416) | 1:121:B:ILE:HG21 | 1:122:B:PHE:HB3 | 7        | 0.16          |
| (1,416) | 1:121:B:ILE:HG22 | 1:122:B:PHE:HB2 | 7        | 0.16          |
| (1,416) | 1:121:B:ILE:HG22 | 1:122:B:PHE:HB3 | 7        | 0.16          |
| (1,416) | 1:121:B:ILE:HG23 | 1:122:B:PHE:HB2 | 7        | 0.16          |
| (1,416) | 1:121:B:ILE:HG23 | 1:122:B:PHE:HB3 | 7        | 0.16          |
| (1,415) | 1:21:A:ILE:HG21  | 1:22:A:PHE:HB2  | 10       | 0.16          |
| (1,415) | 1:21:A:ILE:HG21  | 1:22:A:PHE:HB3  | 10       | 0.16          |
| (1,415) | 1:21:A:ILE:HG22  | 1:22:A:PHE:HB2  | 10       | 0.16          |
| (1,415) | 1:21:A:ILE:HG22  | 1:22:A:PHE:HB3  | 10       | 0.16          |
| (1,415) | 1:21:A:ILE:HG23  | 1:22:A:PHE:HB2  | 10       | 0.16          |
| (1,415) | 1:21:A:ILE:HG23  | 1:22:A:PHE:HB3  | 10       | 0.16          |
| (1,356) | 1:127:B:ILE:HG21 | 1:128:B:HIS:HB2 | 1        | 0.16          |
| (1,356) | 1:127:B:ILE:HG22 | 1:128:B:HIS:HB2 | 1        | 0.16          |
| (1,356) | 1:127:B:ILE:HG23 | 1:128:B:HIS:HB2 | 1        | 0.16          |
| (1,356) | 1:127:B:ILE:HG21 | 1:128:B:HIS:HB2 | 8        | 0.16          |
| (1,356) | 1:127:B:ILE:HG22 | 1:128:B:HIS:HB2 | 8        | 0.16          |
| (1,356) | 1:127:B:ILE:HG23 | 1:128:B:HIS:HB2 | 8        | 0.16          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,355) | 1:27:A:ILE:HG21 | 1:28:A:HIS:HB2  | 1        | 0.16          |
| (1,355) | 1:27:A:ILE:HG22 | 1:28:A:HIS:HB2  | 1        | 0.16          |
| (1,355) | 1:27:A:ILE:HG23 | 1:28:A:HIS:HB2  | 1        | 0.16          |
| (1,355) | 1:27:A:ILE:HG21 | 1:28:A:HIS:HB2  | 8        | 0.16          |
| (1,355) | 1:27:A:ILE:HG22 | 1:28:A:HIS:HB2  | 8        | 0.16          |
| (1,355) | 1:27:A:ILE:HG23 | 1:28:A:HIS:HB2  | 8        | 0.16          |
| (1,355) | 1:27:A:ILE:HG21 | 1:28:A:HIS:HB2  | 10       | 0.16          |
| (1,355) | 1:27:A:ILE:HG22 | 1:28:A:HIS:HB2  | 10       | 0.16          |
| (1,355) | 1:27:A:ILE:HG23 | 1:28:A:HIS:HB2  | 10       | 0.16          |
| (1,254) | 1:117:B:LEU:HA  | 1:120:B:PHE:HB2 | 5        | 0.16          |
| (1,254) | 1:117:B:LEU:HA  | 1:120:B:PHE:HB3 | 5        | 0.16          |
| (1,253) | 1:17:A:LEU:HA   | 1:20:A:PHE:HB2  | 4        | 0.16          |
| (1,253) | 1:17:A:LEU:HA   | 1:20:A:PHE:HB3  | 4        | 0.16          |
| (1,242) | 1:119:B:ILE:HA  | 1:122:B:PHE:H   | 2        | 0.16          |
| (1,241) | 1:19:A:ILE:HA   | 1:22:A:PHE:H    | 8        | 0.16          |
| (1,810) | 1:20:A:PHE:HD1  | 1:23:A:ILE:HG21 | 6        | 0.15          |
| (1,810) | 1:20:A:PHE:HD1  | 1:23:A:ILE:HG22 | 6        | 0.15          |
| (1,810) | 1:20:A:PHE:HD1  | 1:23:A:ILE:HG23 | 6        | 0.15          |
| (1,810) | 1:20:A:PHE:HD2  | 1:23:A:ILE:HG21 | 6        | 0.15          |
| (1,810) | 1:20:A:PHE:HD2  | 1:23:A:ILE:HG22 | 6        | 0.15          |
| (1,810) | 1:20:A:PHE:HD2  | 1:23:A:ILE:HG23 | 6        | 0.15          |
| (1,810) | 1:20:A:PHE:HD1  | 1:23:A:ILE:HG21 | 10       | 0.15          |
| (1,810) | 1:20:A:PHE:HD1  | 1:23:A:ILE:HG22 | 10       | 0.15          |
| (1,810) | 1:20:A:PHE:HD1  | 1:23:A:ILE:HG23 | 10       | 0.15          |
| (1,810) | 1:20:A:PHE:HD2  | 1:23:A:ILE:HG21 | 10       | 0.15          |
| (1,810) | 1:20:A:PHE:HD2  | 1:23:A:ILE:HG22 | 10       | 0.15          |
| (1,810) | 1:20:A:PHE:HD2  | 1:23:A:ILE:HG23 | 10       | 0.15          |
| (1,804) | 1:20:A:PHE:HA   | 1:23:A:ILE:HD11 | 3        | 0.15          |
| (1,804) | 1:20:A:PHE:HA   | 1:23:A:ILE:HD12 | 3        | 0.15          |
| (1,804) | 1:20:A:PHE:HA   | 1:23:A:ILE:HD13 | 3        | 0.15          |
| (1,804) | 1:20:A:PHE:HA   | 1:23:A:ILE:HD11 | 9        | 0.15          |
| (1,804) | 1:20:A:PHE:HA   | 1:23:A:ILE:HD12 | 9        | 0.15          |
| (1,804) | 1:20:A:PHE:HA   | 1:23:A:ILE:HD13 | 9        | 0.15          |
| (1,692) | 1:17:A:LEU:HA   | 1:20:A:PHE:HB2  | 5        | 0.15          |
| (1,692) | 1:17:A:LEU:HA   | 1:20:A:PHE:HB3  | 5        | 0.15          |
| (1,680) | 1:19:A:ILE:HA   | 1:22:A:PHE:H    | 1        | 0.15          |
| (1,680) | 1:19:A:ILE:HA   | 1:22:A:PHE:H    | 2        | 0.15          |
| (1,680) | 1:19:A:ILE:HA   | 1:22:A:PHE:H    | 3        | 0.15          |
| (1,664) | 1:34:A:ILE:H    | 1:34:A:ILE:HA   | 9        | 0.15          |
| (1,375) | 1:20:A:PHE:HD1  | 1:23:A:ILE:HG21 | 6        | 0.15          |
| (1,375) | 1:20:A:PHE:HD1  | 1:23:A:ILE:HG22 | 6        | 0.15          |
| (1,375) | 1:20:A:PHE:HD1  | 1:23:A:ILE:HG23 | 6        | 0.15          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,375) | 1:20:A:PHE:HD2   | 1:23:A:ILE:HG21  | 6        | 0.15          |
| (1,375) | 1:20:A:PHE:HD2   | 1:23:A:ILE:HG22  | 6        | 0.15          |
| (1,375) | 1:20:A:PHE:HD2   | 1:23:A:ILE:HG23  | 6        | 0.15          |
| (1,375) | 1:20:A:PHE:HD1   | 1:23:A:ILE:HG21  | 10       | 0.15          |
| (1,375) | 1:20:A:PHE:HD1   | 1:23:A:ILE:HG22  | 10       | 0.15          |
| (1,375) | 1:20:A:PHE:HD1   | 1:23:A:ILE:HG23  | 10       | 0.15          |
| (1,375) | 1:20:A:PHE:HD2   | 1:23:A:ILE:HG21  | 10       | 0.15          |
| (1,375) | 1:20:A:PHE:HD2   | 1:23:A:ILE:HG22  | 10       | 0.15          |
| (1,375) | 1:20:A:PHE:HD2   | 1:23:A:ILE:HG23  | 10       | 0.15          |
| (1,370) | 1:120:B:PHE:HA   | 1:123:B:ILE:HD11 | 3        | 0.15          |
| (1,370) | 1:120:B:PHE:HA   | 1:123:B:ILE:HD12 | 3        | 0.15          |
| (1,370) | 1:120:B:PHE:HA   | 1:123:B:ILE:HD13 | 3        | 0.15          |
| (1,369) | 1:20:A:PHE:HA    | 1:23:A:ILE:HD11  | 3        | 0.15          |
| (1,369) | 1:20:A:PHE:HA    | 1:23:A:ILE:HD12  | 3        | 0.15          |
| (1,369) | 1:20:A:PHE:HA    | 1:23:A:ILE:HD13  | 3        | 0.15          |
| (1,369) | 1:20:A:PHE:HA    | 1:23:A:ILE:HD11  | 9        | 0.15          |
| (1,369) | 1:20:A:PHE:HA    | 1:23:A:ILE:HD12  | 9        | 0.15          |
| (1,369) | 1:20:A:PHE:HA    | 1:23:A:ILE:HD13  | 9        | 0.15          |
| (1,356) | 1:127:B:ILE:HG21 | 1:128:B:HIS:HB2  | 10       | 0.15          |
| (1,356) | 1:127:B:ILE:HG22 | 1:128:B:HIS:HB2  | 10       | 0.15          |
| (1,356) | 1:127:B:ILE:HG23 | 1:128:B:HIS:HB2  | 10       | 0.15          |
| (1,253) | 1:17:A:LEU:HA    | 1:20:A:PHE:HB2   | 5        | 0.15          |
| (1,253) | 1:17:A:LEU:HA    | 1:20:A:PHE:HB3   | 5        | 0.15          |
| (1,242) | 1:119:B:ILE:HA   | 1:122:B:PHE:H    | 1        | 0.15          |
| (1,242) | 1:119:B:ILE:HA   | 1:122:B:PHE:H    | 3        | 0.15          |
| (1,242) | 1:119:B:ILE:HA   | 1:122:B:PHE:H    | 8        | 0.15          |
| (1,241) | 1:19:A:ILE:HA    | 1:22:A:PHE:H     | 1        | 0.15          |
| (1,241) | 1:19:A:ILE:HA    | 1:22:A:PHE:H     | 2        | 0.15          |
| (1,241) | 1:19:A:ILE:HA    | 1:22:A:PHE:H     | 3        | 0.15          |
| (1,225) | 1:34:A:ILE:H     | 1:34:A:ILE:HA    | 9        | 0.15          |
| (1,778) | 1:25:A:LEU:HD11  | 1:29:A:PHE:HD1   | 3        | 0.14          |
| (1,778) | 1:25:A:LEU:HD11  | 1:29:A:PHE:HD2   | 3        | 0.14          |
| (1,778) | 1:25:A:LEU:HD12  | 1:29:A:PHE:HD1   | 3        | 0.14          |
| (1,778) | 1:25:A:LEU:HD12  | 1:29:A:PHE:HD2   | 3        | 0.14          |
| (1,778) | 1:25:A:LEU:HD13  | 1:29:A:PHE:HD1   | 3        | 0.14          |
| (1,778) | 1:25:A:LEU:HD13  | 1:29:A:PHE:HD2   | 3        | 0.14          |
| (1,712) | 1:26:A:LEU:HA    | 1:30:A:GLU:H     | 10       | 0.14          |
| (1,552) | 1:26:A:LEU:HA    | 1:29:A:PHE:H     | 8        | 0.14          |
| (1,370) | 1:120:B:PHE:HA   | 1:123:B:ILE:HD11 | 1        | 0.14          |
| (1,370) | 1:120:B:PHE:HA   | 1:123:B:ILE:HD12 | 1        | 0.14          |
| (1,370) | 1:120:B:PHE:HA   | 1:123:B:ILE:HD13 | 1        | 0.14          |
| (1,343) | 1:25:A:LEU:HD11  | 1:29:A:PHE:HD1   | 3        | 0.14          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,343) | 1:25:A:LEU:HD11 | 1:29:A:PHE:HD2  | 3        | 0.14          |
| (1,343) | 1:25:A:LEU:HD12 | 1:29:A:PHE:HD1  | 3        | 0.14          |
| (1,343) | 1:25:A:LEU:HD12 | 1:29:A:PHE:HD2  | 3        | 0.14          |
| (1,343) | 1:25:A:LEU:HD13 | 1:29:A:PHE:HD1  | 3        | 0.14          |
| (1,343) | 1:25:A:LEU:HD13 | 1:29:A:PHE:HD2  | 3        | 0.14          |
| (1,274) | 1:126:B:LEU:HA  | 1:130:B:GLU:H   | 10       | 0.14          |
| (1,273) | 1:26:A:LEU:HA   | 1:30:A:GLU:H    | 10       | 0.14          |
| (1,114) | 1:126:B:LEU:HA  | 1:129:B:PHE:H   | 4        | 0.14          |
| (1,113) | 1:26:A:LEU:HA   | 1:29:A:PHE:H    | 8        | 0.14          |
| (1,814) | 1:20:A:PHE:HE1  | 1:24:A:VAL:HG11 | 9        | 0.13          |
| (1,814) | 1:20:A:PHE:HE1  | 1:24:A:VAL:HG12 | 9        | 0.13          |
| (1,814) | 1:20:A:PHE:HE1  | 1:24:A:VAL:HG13 | 9        | 0.13          |
| (1,814) | 1:20:A:PHE:HE2  | 1:24:A:VAL:HG11 | 9        | 0.13          |
| (1,814) | 1:20:A:PHE:HE2  | 1:24:A:VAL:HG12 | 9        | 0.13          |
| (1,814) | 1:20:A:PHE:HE2  | 1:24:A:VAL:HG13 | 9        | 0.13          |
| (1,804) | 1:20:A:PHE:HA   | 1:23:A:ILE:HD11 | 1        | 0.13          |
| (1,804) | 1:20:A:PHE:HA   | 1:23:A:ILE:HD12 | 1        | 0.13          |
| (1,804) | 1:20:A:PHE:HA   | 1:23:A:ILE:HD13 | 1        | 0.13          |
| (1,804) | 1:20:A:PHE:HA   | 1:23:A:ILE:HD11 | 8        | 0.13          |
| (1,804) | 1:20:A:PHE:HA   | 1:23:A:ILE:HD12 | 8        | 0.13          |
| (1,804) | 1:20:A:PHE:HA   | 1:23:A:ILE:HD13 | 8        | 0.13          |
| (1,778) | 1:25:A:LEU:HD11 | 1:29:A:PHE:HD1  | 10       | 0.13          |
| (1,778) | 1:25:A:LEU:HD11 | 1:29:A:PHE:HD2  | 10       | 0.13          |
| (1,778) | 1:25:A:LEU:HD12 | 1:29:A:PHE:HD1  | 10       | 0.13          |
| (1,778) | 1:25:A:LEU:HD12 | 1:29:A:PHE:HD2  | 10       | 0.13          |
| (1,778) | 1:25:A:LEU:HD13 | 1:29:A:PHE:HD1  | 10       | 0.13          |
| (1,778) | 1:25:A:LEU:HD13 | 1:29:A:PHE:HD2  | 10       | 0.13          |
| (1,732) | 1:12:A:ILE:HA   | 1:12:A:ILE:HD11 | 10       | 0.13          |
| (1,732) | 1:12:A:ILE:HA   | 1:12:A:ILE:HD12 | 10       | 0.13          |
| (1,732) | 1:12:A:ILE:HA   | 1:12:A:ILE:HD13 | 10       | 0.13          |
| (1,692) | 1:17:A:LEU:HA   | 1:20:A:PHE:HB2  | 2        | 0.13          |
| (1,692) | 1:17:A:LEU:HA   | 1:20:A:PHE:HB3  | 2        | 0.13          |
| (1,644) | 1:30:A:GLU:H    | 1:30:A:GLU:HG2  | 3        | 0.13          |
| (1,644) | 1:30:A:GLU:H    | 1:30:A:GLU:HG3  | 3        | 0.13          |
| (1,552) | 1:26:A:LEU:HA   | 1:29:A:PHE:H    | 6        | 0.13          |
| (1,531) | 1:20:A:PHE:HB2  | 1:21:A:ILE:H    | 9        | 0.13          |
| (1,531) | 1:20:A:PHE:HB3  | 1:21:A:ILE:H    | 9        | 0.13          |
| (1,379) | 1:20:A:PHE:HE1  | 1:24:A:VAL:HG11 | 9        | 0.13          |
| (1,379) | 1:20:A:PHE:HE1  | 1:24:A:VAL:HG12 | 9        | 0.13          |
| (1,379) | 1:20:A:PHE:HE1  | 1:24:A:VAL:HG13 | 9        | 0.13          |
| (1,379) | 1:20:A:PHE:HE2  | 1:24:A:VAL:HG11 | 9        | 0.13          |
| (1,379) | 1:20:A:PHE:HE2  | 1:24:A:VAL:HG12 | 9        | 0.13          |

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| Key     | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|---------|------------------|-----------------|----------|---------------|
| (1,379) | 1:20:A:PHE:HE2   | 1:24:A:VAL:HG13 | 9        | 0.13          |
| (1,369) | 1:20:A:PHE:HA    | 1:23:A:ILE:HD11 | 1        | 0.13          |
| (1,369) | 1:20:A:PHE:HA    | 1:23:A:ILE:HD12 | 1        | 0.13          |
| (1,369) | 1:20:A:PHE:HA    | 1:23:A:ILE:HD13 | 1        | 0.13          |
| (1,369) | 1:20:A:PHE:HA    | 1:23:A:ILE:HD11 | 8        | 0.13          |
| (1,369) | 1:20:A:PHE:HA    | 1:23:A:ILE:HD12 | 8        | 0.13          |
| (1,369) | 1:20:A:PHE:HA    | 1:23:A:ILE:HD13 | 8        | 0.13          |
| (1,344) | 1:125:B:LEU:HD11 | 1:129:B:PHE:HD1 | 3        | 0.13          |
| (1,344) | 1:125:B:LEU:HD11 | 1:129:B:PHE:HD2 | 3        | 0.13          |
| (1,344) | 1:125:B:LEU:HD12 | 1:129:B:PHE:HD1 | 3        | 0.13          |
| (1,344) | 1:125:B:LEU:HD12 | 1:129:B:PHE:HD2 | 3        | 0.13          |
| (1,344) | 1:125:B:LEU:HD13 | 1:129:B:PHE:HD1 | 3        | 0.13          |
| (1,344) | 1:125:B:LEU:HD13 | 1:129:B:PHE:HD2 | 3        | 0.13          |
| (1,343) | 1:25:A:LEU:HD11  | 1:29:A:PHE:HD1  | 10       | 0.13          |
| (1,343) | 1:25:A:LEU:HD11  | 1:29:A:PHE:HD2  | 10       | 0.13          |
| (1,343) | 1:25:A:LEU:HD12  | 1:29:A:PHE:HD1  | 10       | 0.13          |
| (1,343) | 1:25:A:LEU:HD12  | 1:29:A:PHE:HD2  | 10       | 0.13          |
| (1,343) | 1:25:A:LEU:HD13  | 1:29:A:PHE:HD1  | 10       | 0.13          |
| (1,343) | 1:25:A:LEU:HD13  | 1:29:A:PHE:HD2  | 10       | 0.13          |
| (1,293) | 1:12:A:ILE:HA    | 1:12:A:ILE:HD11 | 10       | 0.13          |
| (1,293) | 1:12:A:ILE:HA    | 1:12:A:ILE:HD12 | 10       | 0.13          |
| (1,293) | 1:12:A:ILE:HA    | 1:12:A:ILE:HD13 | 10       | 0.13          |
| (1,254) | 1:117:B:LEU:HA   | 1:120:B:PHE:HB2 | 2        | 0.13          |
| (1,254) | 1:117:B:LEU:HA   | 1:120:B:PHE:HB3 | 2        | 0.13          |
| (1,254) | 1:117:B:LEU:HA   | 1:120:B:PHE:HB2 | 6        | 0.13          |
| (1,254) | 1:117:B:LEU:HA   | 1:120:B:PHE:HB3 | 6        | 0.13          |
| (1,254) | 1:117:B:LEU:HA   | 1:120:B:PHE:HB2 | 9        | 0.13          |
| (1,254) | 1:117:B:LEU:HA   | 1:120:B:PHE:HB3 | 9        | 0.13          |
| (1,254) | 1:117:B:LEU:HA   | 1:120:B:PHE:HB2 | 10       | 0.13          |
| (1,254) | 1:117:B:LEU:HA   | 1:120:B:PHE:HB3 | 10       | 0.13          |
| (1,253) | 1:17:A:LEU:HA    | 1:20:A:PHE:HB2  | 2        | 0.13          |
| (1,253) | 1:17:A:LEU:HA    | 1:20:A:PHE:HB3  | 2        | 0.13          |
| (1,205) | 1:30:A:GLU:H     | 1:30:A:GLU:HG2  | 3        | 0.13          |
| (1,205) | 1:30:A:GLU:H     | 1:30:A:GLU:HG3  | 3        | 0.13          |
| (1,114) | 1:126:B:LEU:HA   | 1:129:B:PHE:H   | 6        | 0.13          |
| (1,114) | 1:126:B:LEU:HA   | 1:129:B:PHE:H   | 8        | 0.13          |
| (1,113) | 1:26:A:LEU:HA    | 1:29:A:PHE:H    | 6        | 0.13          |
| (1,95)  | 1:20:A:PHE:HB2   | 1:21:A:ILE:H    | 9        | 0.13          |
| (1,95)  | 1:20:A:PHE:HB3   | 1:21:A:ILE:H    | 9        | 0.13          |
| (1,834) | 1:14:A:THR:HA    | 1:18:A:LEU:HD21 | 7        | 0.12          |
| (1,834) | 1:14:A:THR:HA    | 1:18:A:LEU:HD22 | 7        | 0.12          |
| (1,834) | 1:14:A:THR:HA    | 1:18:A:LEU:HD23 | 7        | 0.12          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,790) | 1:27:A:ILE:HG21  | 1:28:A:HIS:HB2   | 7        | 0.12          |
| (1,790) | 1:27:A:ILE:HG22  | 1:28:A:HIS:HB2   | 7        | 0.12          |
| (1,790) | 1:27:A:ILE:HG23  | 1:28:A:HIS:HB2   | 7        | 0.12          |
| (1,778) | 1:25:A:LEU:HD11  | 1:29:A:PHE:HD1   | 1        | 0.12          |
| (1,778) | 1:25:A:LEU:HD11  | 1:29:A:PHE:HD2   | 1        | 0.12          |
| (1,778) | 1:25:A:LEU:HD12  | 1:29:A:PHE:HD1   | 1        | 0.12          |
| (1,778) | 1:25:A:LEU:HD12  | 1:29:A:PHE:HD2   | 1        | 0.12          |
| (1,778) | 1:25:A:LEU:HD13  | 1:29:A:PHE:HD1   | 1        | 0.12          |
| (1,778) | 1:25:A:LEU:HD13  | 1:29:A:PHE:HD2   | 1        | 0.12          |
| (1,692) | 1:17:A:LEU:HA    | 1:20:A:PHE:HB2   | 1        | 0.12          |
| (1,692) | 1:17:A:LEU:HA    | 1:20:A:PHE:HB3   | 1        | 0.12          |
| (1,692) | 1:17:A:LEU:HA    | 1:20:A:PHE:HB2   | 8        | 0.12          |
| (1,692) | 1:17:A:LEU:HA    | 1:20:A:PHE:HB3   | 8        | 0.12          |
| (1,628) | 1:32:A:TRP:HB2   | 1:33:A:ARG:H     | 7        | 0.12          |
| (1,628) | 1:32:A:TRP:HB3   | 1:33:A:ARG:H     | 7        | 0.12          |
| (1,594) | 1:31:A:GLY:HA3   | 1:32:A:TRP:H     | 4        | 0.12          |
| (1,594) | 1:31:A:GLY:HA3   | 1:32:A:TRP:H     | 8        | 0.12          |
| (1,552) | 1:26:A:LEU:HA    | 1:29:A:PHE:H     | 2        | 0.12          |
| (1,552) | 1:26:A:LEU:HA    | 1:29:A:PHE:H     | 4        | 0.12          |
| (1,552) | 1:26:A:LEU:HA    | 1:29:A:PHE:H     | 5        | 0.12          |
| (1,552) | 1:26:A:LEU:HA    | 1:29:A:PHE:H     | 9        | 0.12          |
| (1,398) | 1:114:B:THR:HA   | 1:118:B:LEU:HD21 | 7        | 0.12          |
| (1,398) | 1:114:B:THR:HA   | 1:118:B:LEU:HD22 | 7        | 0.12          |
| (1,398) | 1:114:B:THR:HA   | 1:118:B:LEU:HD23 | 7        | 0.12          |
| (1,397) | 1:14:A:THR:HA    | 1:18:A:LEU:HD21  | 7        | 0.12          |
| (1,397) | 1:14:A:THR:HA    | 1:18:A:LEU:HD22  | 7        | 0.12          |
| (1,397) | 1:14:A:THR:HA    | 1:18:A:LEU:HD23  | 7        | 0.12          |
| (1,370) | 1:120:B:PHE:HA   | 1:123:B:ILE:HD11 | 5        | 0.12          |
| (1,370) | 1:120:B:PHE:HA   | 1:123:B:ILE:HD12 | 5        | 0.12          |
| (1,370) | 1:120:B:PHE:HA   | 1:123:B:ILE:HD13 | 5        | 0.12          |
| (1,370) | 1:120:B:PHE:HA   | 1:123:B:ILE:HD11 | 8        | 0.12          |
| (1,370) | 1:120:B:PHE:HA   | 1:123:B:ILE:HD12 | 8        | 0.12          |
| (1,370) | 1:120:B:PHE:HA   | 1:123:B:ILE:HD13 | 8        | 0.12          |
| (1,356) | 1:127:B:ILE:HG21 | 1:128:B:HIS:HB2  | 7        | 0.12          |
| (1,356) | 1:127:B:ILE:HG22 | 1:128:B:HIS:HB2  | 7        | 0.12          |
| (1,356) | 1:127:B:ILE:HG23 | 1:128:B:HIS:HB2  | 7        | 0.12          |
| (1,355) | 1:27:A:ILE:HG21  | 1:28:A:HIS:HB2   | 7        | 0.12          |
| (1,355) | 1:27:A:ILE:HG22  | 1:28:A:HIS:HB2   | 7        | 0.12          |
| (1,355) | 1:27:A:ILE:HG23  | 1:28:A:HIS:HB2   | 7        | 0.12          |
| (1,343) | 1:25:A:LEU:HD11  | 1:29:A:PHE:HD1   | 1        | 0.12          |
| (1,343) | 1:25:A:LEU:HD11  | 1:29:A:PHE:HD2   | 1        | 0.12          |
| (1,343) | 1:25:A:LEU:HD12  | 1:29:A:PHE:HD1   | 1        | 0.12          |

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| Key     | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (1,343) | 1:25:A:LEU:HD12 | 1:29:A:PHE:HD2   | 1        | 0.12          |
| (1,343) | 1:25:A:LEU:HD13 | 1:29:A:PHE:HD1   | 1        | 0.12          |
| (1,343) | 1:25:A:LEU:HD13 | 1:29:A:PHE:HD2   | 1        | 0.12          |
| (1,294) | 1:112:B:ILE:HA  | 1:112:B:ILE:HD11 | 10       | 0.12          |
| (1,294) | 1:112:B:ILE:HA  | 1:112:B:ILE:HD12 | 10       | 0.12          |
| (1,294) | 1:112:B:ILE:HA  | 1:112:B:ILE:HD13 | 10       | 0.12          |
| (1,253) | 1:17:A:LEU:HA   | 1:20:A:PHE:HB2   | 1        | 0.12          |
| (1,253) | 1:17:A:LEU:HA   | 1:20:A:PHE:HB3   | 1        | 0.12          |
| (1,253) | 1:17:A:LEU:HA   | 1:20:A:PHE:HB2   | 8        | 0.12          |
| (1,253) | 1:17:A:LEU:HA   | 1:20:A:PHE:HB3   | 8        | 0.12          |
| (1,190) | 1:132:B:TRP:HB2 | 1:133:B:ARG:H    | 7        | 0.12          |
| (1,190) | 1:132:B:TRP:HB3 | 1:133:B:ARG:H    | 7        | 0.12          |
| (1,189) | 1:32:A:TRP:HB2  | 1:33:A:ARG:H     | 7        | 0.12          |
| (1,189) | 1:32:A:TRP:HB3  | 1:33:A:ARG:H     | 7        | 0.12          |
| (1,156) | 1:131:B:GLY:HA3 | 1:132:B:TRP:H    | 8        | 0.12          |
| (1,155) | 1:31:A:GLY:HA3  | 1:32:A:TRP:H     | 4        | 0.12          |
| (1,155) | 1:31:A:GLY:HA3  | 1:32:A:TRP:H     | 8        | 0.12          |
| (1,114) | 1:126:B:LEU:HA  | 1:129:B:PHE:H    | 2        | 0.12          |
| (1,114) | 1:126:B:LEU:HA  | 1:129:B:PHE:H    | 5        | 0.12          |
| (1,113) | 1:26:A:LEU:HA   | 1:29:A:PHE:H     | 2        | 0.12          |
| (1,113) | 1:26:A:LEU:HA   | 1:29:A:PHE:H     | 4        | 0.12          |
| (1,113) | 1:26:A:LEU:HA   | 1:29:A:PHE:H     | 5        | 0.12          |
| (1,113) | 1:26:A:LEU:HA   | 1:29:A:PHE:H     | 9        | 0.12          |
| (1,96)  | 1:120:B:PHE:HB2 | 1:121:B:ILE:H    | 9        | 0.12          |
| (1,96)  | 1:120:B:PHE:HB3 | 1:121:B:ILE:H    | 9        | 0.12          |
| (1,804) | 1:20:A:PHE:HA   | 1:23:A:ILE:HD11  | 5        | 0.11          |
| (1,804) | 1:20:A:PHE:HA   | 1:23:A:ILE:HD12  | 5        | 0.11          |
| (1,804) | 1:20:A:PHE:HA   | 1:23:A:ILE:HD13  | 5        | 0.11          |
| (1,790) | 1:27:A:ILE:HG21 | 1:28:A:HIS:HB2   | 4        | 0.11          |
| (1,790) | 1:27:A:ILE:HG22 | 1:28:A:HIS:HB2   | 4        | 0.11          |
| (1,790) | 1:27:A:ILE:HG23 | 1:28:A:HIS:HB2   | 4        | 0.11          |
| (1,716) | 1:4:A:ALA:HA    | 1:5:A:PRO:HD2    | 1        | 0.11          |
| (1,716) | 1:4:A:ALA:HA    | 1:5:A:PRO:HD3    | 1        | 0.11          |
| (1,716) | 1:4:A:ALA:HA    | 1:5:A:PRO:HD2    | 2        | 0.11          |
| (1,716) | 1:4:A:ALA:HA    | 1:5:A:PRO:HD3    | 2        | 0.11          |
| (1,716) | 1:4:A:ALA:HA    | 1:5:A:PRO:HD2    | 3        | 0.11          |
| (1,716) | 1:4:A:ALA:HA    | 1:5:A:PRO:HD3    | 3        | 0.11          |
| (1,716) | 1:4:A:ALA:HA    | 1:5:A:PRO:HD2    | 4        | 0.11          |
| (1,716) | 1:4:A:ALA:HA    | 1:5:A:PRO:HD3    | 4        | 0.11          |
| (1,716) | 1:4:A:ALA:HA    | 1:5:A:PRO:HD2    | 5        | 0.11          |
| (1,716) | 1:4:A:ALA:HA    | 1:5:A:PRO:HD3    | 5        | 0.11          |
| (1,716) | 1:4:A:ALA:HA    | 1:5:A:PRO:HD2    | 6        | 0.11          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,716) | 1:4:A:ALA:HA     | 1:5:A:PRO:HD3    | 6        | 0.11          |
| (1,716) | 1:4:A:ALA:HA     | 1:5:A:PRO:HD2    | 7        | 0.11          |
| (1,716) | 1:4:A:ALA:HA     | 1:5:A:PRO:HD3    | 7        | 0.11          |
| (1,716) | 1:4:A:ALA:HA     | 1:5:A:PRO:HD2    | 8        | 0.11          |
| (1,716) | 1:4:A:ALA:HA     | 1:5:A:PRO:HD3    | 8        | 0.11          |
| (1,716) | 1:4:A:ALA:HA     | 1:5:A:PRO:HD2    | 9        | 0.11          |
| (1,716) | 1:4:A:ALA:HA     | 1:5:A:PRO:HD3    | 9        | 0.11          |
| (1,716) | 1:4:A:ALA:HA     | 1:5:A:PRO:HD2    | 10       | 0.11          |
| (1,716) | 1:4:A:ALA:HA     | 1:5:A:PRO:HD3    | 10       | 0.11          |
| (1,712) | 1:26:A:LEU:HA    | 1:30:A:GLU:H     | 1        | 0.11          |
| (1,692) | 1:17:A:LEU:HA    | 1:20:A:PHE:HB2   | 7        | 0.11          |
| (1,692) | 1:17:A:LEU:HA    | 1:20:A:PHE:HB3   | 7        | 0.11          |
| (1,680) | 1:19:A:ILE:HA    | 1:22:A:PHE:H     | 4        | 0.11          |
| (1,594) | 1:31:A:GLY:HA3   | 1:32:A:TRP:H     | 2        | 0.11          |
| (1,594) | 1:31:A:GLY:HA3   | 1:32:A:TRP:H     | 3        | 0.11          |
| (1,594) | 1:31:A:GLY:HA3   | 1:32:A:TRP:H     | 5        | 0.11          |
| (1,594) | 1:31:A:GLY:HA3   | 1:32:A:TRP:H     | 6        | 0.11          |
| (1,594) | 1:31:A:GLY:HA3   | 1:32:A:TRP:H     | 7        | 0.11          |
| (1,594) | 1:31:A:GLY:HA3   | 1:32:A:TRP:H     | 9        | 0.11          |
| (1,594) | 1:31:A:GLY:HA3   | 1:32:A:TRP:H     | 10       | 0.11          |
| (1,592) | 1:32:A:TRP:H     | 1:33:A:ARG:H     | 6        | 0.11          |
| (1,552) | 1:26:A:LEU:HA    | 1:29:A:PHE:H     | 7        | 0.11          |
| (1,380) | 1:120:B:PHE:HE1  | 1:124:B:VAL:HG11 | 9        | 0.11          |
| (1,380) | 1:120:B:PHE:HE1  | 1:124:B:VAL:HG12 | 9        | 0.11          |
| (1,380) | 1:120:B:PHE:HE1  | 1:124:B:VAL:HG13 | 9        | 0.11          |
| (1,380) | 1:120:B:PHE:HE2  | 1:124:B:VAL:HG11 | 9        | 0.11          |
| (1,380) | 1:120:B:PHE:HE2  | 1:124:B:VAL:HG12 | 9        | 0.11          |
| (1,380) | 1:120:B:PHE:HE2  | 1:124:B:VAL:HG13 | 9        | 0.11          |
| (1,376) | 1:120:B:PHE:HD1  | 1:123:B:ILE:HG21 | 7        | 0.11          |
| (1,376) | 1:120:B:PHE:HD1  | 1:123:B:ILE:HG22 | 7        | 0.11          |
| (1,376) | 1:120:B:PHE:HD1  | 1:123:B:ILE:HG23 | 7        | 0.11          |
| (1,376) | 1:120:B:PHE:HD2  | 1:123:B:ILE:HG21 | 7        | 0.11          |
| (1,376) | 1:120:B:PHE:HD2  | 1:123:B:ILE:HG22 | 7        | 0.11          |
| (1,376) | 1:120:B:PHE:HD2  | 1:123:B:ILE:HG23 | 7        | 0.11          |
| (1,369) | 1:20:A:PHE:HA    | 1:23:A:ILE:HD11  | 5        | 0.11          |
| (1,369) | 1:20:A:PHE:HA    | 1:23:A:ILE:HD12  | 5        | 0.11          |
| (1,369) | 1:20:A:PHE:HA    | 1:23:A:ILE:HD13  | 5        | 0.11          |
| (1,355) | 1:27:A:ILE:HG21  | 1:28:A:HIS:HB2   | 4        | 0.11          |
| (1,355) | 1:27:A:ILE:HG22  | 1:28:A:HIS:HB2   | 4        | 0.11          |
| (1,355) | 1:27:A:ILE:HG23  | 1:28:A:HIS:HB2   | 4        | 0.11          |
| (1,344) | 1:125:B:LEU:HD11 | 1:129:B:PHE:HD1  | 1        | 0.11          |
| (1,344) | 1:125:B:LEU:HD11 | 1:129:B:PHE:HD2  | 1        | 0.11          |

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| Key     | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|---------|------------------|-----------------|----------|---------------|
| (1,344) | 1:125:B:LEU:HD12 | 1:129:B:PHE:HD1 | 1        | 0.11          |
| (1,344) | 1:125:B:LEU:HD12 | 1:129:B:PHE:HD2 | 1        | 0.11          |
| (1,344) | 1:125:B:LEU:HD13 | 1:129:B:PHE:HD1 | 1        | 0.11          |
| (1,344) | 1:125:B:LEU:HD13 | 1:129:B:PHE:HD2 | 1        | 0.11          |
| (1,278) | 1:104:B:ALA:HA   | 1:105:B:PRO:HD2 | 1        | 0.11          |
| (1,278) | 1:104:B:ALA:HA   | 1:105:B:PRO:HD3 | 1        | 0.11          |
| (1,278) | 1:104:B:ALA:HA   | 1:105:B:PRO:HD2 | 2        | 0.11          |
| (1,278) | 1:104:B:ALA:HA   | 1:105:B:PRO:HD3 | 2        | 0.11          |
| (1,278) | 1:104:B:ALA:HA   | 1:105:B:PRO:HD2 | 3        | 0.11          |
| (1,278) | 1:104:B:ALA:HA   | 1:105:B:PRO:HD3 | 3        | 0.11          |
| (1,278) | 1:104:B:ALA:HA   | 1:105:B:PRO:HD2 | 4        | 0.11          |
| (1,278) | 1:104:B:ALA:HA   | 1:105:B:PRO:HD3 | 4        | 0.11          |
| (1,278) | 1:104:B:ALA:HA   | 1:105:B:PRO:HD2 | 5        | 0.11          |
| (1,278) | 1:104:B:ALA:HA   | 1:105:B:PRO:HD3 | 5        | 0.11          |
| (1,278) | 1:104:B:ALA:HA   | 1:105:B:PRO:HD2 | 6        | 0.11          |
| (1,278) | 1:104:B:ALA:HA   | 1:105:B:PRO:HD3 | 6        | 0.11          |
| (1,278) | 1:104:B:ALA:HA   | 1:105:B:PRO:HD2 | 7        | 0.11          |
| (1,278) | 1:104:B:ALA:HA   | 1:105:B:PRO:HD3 | 7        | 0.11          |
| (1,278) | 1:104:B:ALA:HA   | 1:105:B:PRO:HD2 | 8        | 0.11          |
| (1,278) | 1:104:B:ALA:HA   | 1:105:B:PRO:HD3 | 8        | 0.11          |
| (1,278) | 1:104:B:ALA:HA   | 1:105:B:PRO:HD2 | 9        | 0.11          |
| (1,278) | 1:104:B:ALA:HA   | 1:105:B:PRO:HD3 | 9        | 0.11          |
| (1,278) | 1:104:B:ALA:HA   | 1:105:B:PRO:HD2 | 10       | 0.11          |
| (1,278) | 1:104:B:ALA:HA   | 1:105:B:PRO:HD3 | 10       | 0.11          |
| (1,277) | 1:4:A:ALA:HA     | 1:5:A:PRO:HD2   | 1        | 0.11          |
| (1,277) | 1:4:A:ALA:HA     | 1:5:A:PRO:HD3   | 1        | 0.11          |
| (1,277) | 1:4:A:ALA:HA     | 1:5:A:PRO:HD2   | 2        | 0.11          |
| (1,277) | 1:4:A:ALA:HA     | 1:5:A:PRO:HD3   | 2        | 0.11          |
| (1,277) | 1:4:A:ALA:HA     | 1:5:A:PRO:HD2   | 3        | 0.11          |
| (1,277) | 1:4:A:ALA:HA     | 1:5:A:PRO:HD3   | 3        | 0.11          |
| (1,277) | 1:4:A:ALA:HA     | 1:5:A:PRO:HD2   | 4        | 0.11          |
| (1,277) | 1:4:A:ALA:HA     | 1:5:A:PRO:HD3   | 4        | 0.11          |
| (1,277) | 1:4:A:ALA:HA     | 1:5:A:PRO:HD2   | 5        | 0.11          |
| (1,277) | 1:4:A:ALA:HA     | 1:5:A:PRO:HD3   | 5        | 0.11          |
| (1,277) | 1:4:A:ALA:HA     | 1:5:A:PRO:HD2   | 6        | 0.11          |
| (1,277) | 1:4:A:ALA:HA     | 1:5:A:PRO:HD3   | 6        | 0.11          |
| (1,277) | 1:4:A:ALA:HA     | 1:5:A:PRO:HD2   | 7        | 0.11          |
| (1,277) | 1:4:A:ALA:HA     | 1:5:A:PRO:HD3   | 7        | 0.11          |
| (1,277) | 1:4:A:ALA:HA     | 1:5:A:PRO:HD2   | 8        | 0.11          |
| (1,277) | 1:4:A:ALA:HA     | 1:5:A:PRO:HD3   | 8        | 0.11          |
| (1,277) | 1:4:A:ALA:HA     | 1:5:A:PRO:HD2   | 9        | 0.11          |
| (1,277) | 1:4:A:ALA:HA     | 1:5:A:PRO:HD3   | 9        | 0.11          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,277) | 1:4:A:ALA:HA    | 1:5:A:PRO:HD2   | 10       | 0.11          |
| (1,277) | 1:4:A:ALA:HA    | 1:5:A:PRO:HD3   | 10       | 0.11          |
| (1,274) | 1:126:B:LEU:HA  | 1:130:B:GLU:H   | 1        | 0.11          |
| (1,273) | 1:26:A:LEU:HA   | 1:30:A:GLU:H    | 1        | 0.11          |
| (1,254) | 1:117:B:LEU:HA  | 1:120:B:PHE:HB2 | 1        | 0.11          |
| (1,254) | 1:117:B:LEU:HA  | 1:120:B:PHE:HB3 | 1        | 0.11          |
| (1,254) | 1:117:B:LEU:HA  | 1:120:B:PHE:HB2 | 8        | 0.11          |
| (1,254) | 1:117:B:LEU:HA  | 1:120:B:PHE:HB3 | 8        | 0.11          |
| (1,253) | 1:17:A:LEU:HA   | 1:20:A:PHE:HB2  | 7        | 0.11          |
| (1,253) | 1:17:A:LEU:HA   | 1:20:A:PHE:HB3  | 7        | 0.11          |
| (1,242) | 1:119:B:ILE:HA  | 1:122:B:PHE:H   | 4        | 0.11          |
| (1,241) | 1:19:A:ILE:HA   | 1:22:A:PHE:H    | 4        | 0.11          |
| (1,226) | 1:134:B:ILE:H   | 1:134:B:ILE:HA  | 9        | 0.11          |
| (1,156) | 1:131:B:GLY:HA3 | 1:132:B:TRP:H   | 2        | 0.11          |
| (1,156) | 1:131:B:GLY:HA3 | 1:132:B:TRP:H   | 3        | 0.11          |
| (1,156) | 1:131:B:GLY:HA3 | 1:132:B:TRP:H   | 4        | 0.11          |
| (1,156) | 1:131:B:GLY:HA3 | 1:132:B:TRP:H   | 5        | 0.11          |
| (1,156) | 1:131:B:GLY:HA3 | 1:132:B:TRP:H   | 6        | 0.11          |
| (1,156) | 1:131:B:GLY:HA3 | 1:132:B:TRP:H   | 7        | 0.11          |
| (1,156) | 1:131:B:GLY:HA3 | 1:132:B:TRP:H   | 9        | 0.11          |
| (1,155) | 1:31:A:GLY:HA3  | 1:32:A:TRP:H    | 2        | 0.11          |
| (1,155) | 1:31:A:GLY:HA3  | 1:32:A:TRP:H    | 3        | 0.11          |
| (1,155) | 1:31:A:GLY:HA3  | 1:32:A:TRP:H    | 5        | 0.11          |
| (1,155) | 1:31:A:GLY:HA3  | 1:32:A:TRP:H    | 6        | 0.11          |
| (1,155) | 1:31:A:GLY:HA3  | 1:32:A:TRP:H    | 7        | 0.11          |
| (1,155) | 1:31:A:GLY:HA3  | 1:32:A:TRP:H    | 9        | 0.11          |
| (1,155) | 1:31:A:GLY:HA3  | 1:32:A:TRP:H    | 10       | 0.11          |
| (1,153) | 1:32:A:TRP:H    | 1:33:A:ARG:H    | 6        | 0.11          |
| (1,114) | 1:126:B:LEU:HA  | 1:129:B:PHE:H   | 7        | 0.11          |
| (1,114) | 1:126:B:LEU:HA  | 1:129:B:PHE:H   | 9        | 0.11          |
| (1,113) | 1:26:A:LEU:HA   | 1:29:A:PHE:H    | 7        | 0.11          |
| (1,790) | 1:27:A:ILE:HG21 | 1:28:A:HIS:HB2  | 5        | 0.1           |
| (1,790) | 1:27:A:ILE:HG22 | 1:28:A:HIS:HB2  | 5        | 0.1           |
| (1,790) | 1:27:A:ILE:HG23 | 1:28:A:HIS:HB2  | 5        | 0.1           |
| (1,696) | 1:23:A:ILE:HA   | 1:26:A:LEU:HB2  | 9        | 0.1           |
| (1,696) | 1:23:A:ILE:HA   | 1:26:A:LEU:HB3  | 9        | 0.1           |
| (1,692) | 1:17:A:LEU:HA   | 1:20:A:PHE:HB2  | 3        | 0.1           |
| (1,692) | 1:17:A:LEU:HA   | 1:20:A:PHE:HB3  | 3        | 0.1           |
| (1,594) | 1:31:A:GLY:HA3  | 1:32:A:TRP:H    | 1        | 0.1           |
| (1,355) | 1:27:A:ILE:HG21 | 1:28:A:HIS:HB2  | 5        | 0.1           |
| (1,355) | 1:27:A:ILE:HG22 | 1:28:A:HIS:HB2  | 5        | 0.1           |
| (1,355) | 1:27:A:ILE:HG23 | 1:28:A:HIS:HB2  | 5        | 0.1           |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,257) | 1:23:A:ILE:HA   | 1:26:A:LEU:HB2  | 9        | 0.1           |
| (1,257) | 1:23:A:ILE:HA   | 1:26:A:LEU:HB3  | 9        | 0.1           |
| (1,253) | 1:17:A:LEU:HA   | 1:20:A:PHE:HB2  | 3        | 0.1           |
| (1,253) | 1:17:A:LEU:HA   | 1:20:A:PHE:HB3  | 3        | 0.1           |
| (1,206) | 1:130:B:GLU:H   | 1:130:B:GLU:HG2 | 3        | 0.1           |
| (1,206) | 1:130:B:GLU:H   | 1:130:B:GLU:HG3 | 3        | 0.1           |
| (1,190) | 1:132:B:TRP:HB2 | 1:133:B:ARG:H   | 5        | 0.1           |
| (1,190) | 1:132:B:TRP:HB3 | 1:133:B:ARG:H   | 5        | 0.1           |
| (1,156) | 1:131:B:GLY:HA3 | 1:132:B:TRP:H   | 1        | 0.1           |
| (1,156) | 1:131:B:GLY:HA3 | 1:132:B:TRP:H   | 10       | 0.1           |
| (1,155) | 1:31:A:GLY:HA3  | 1:32:A:TRP:H    | 1        | 0.1           |

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

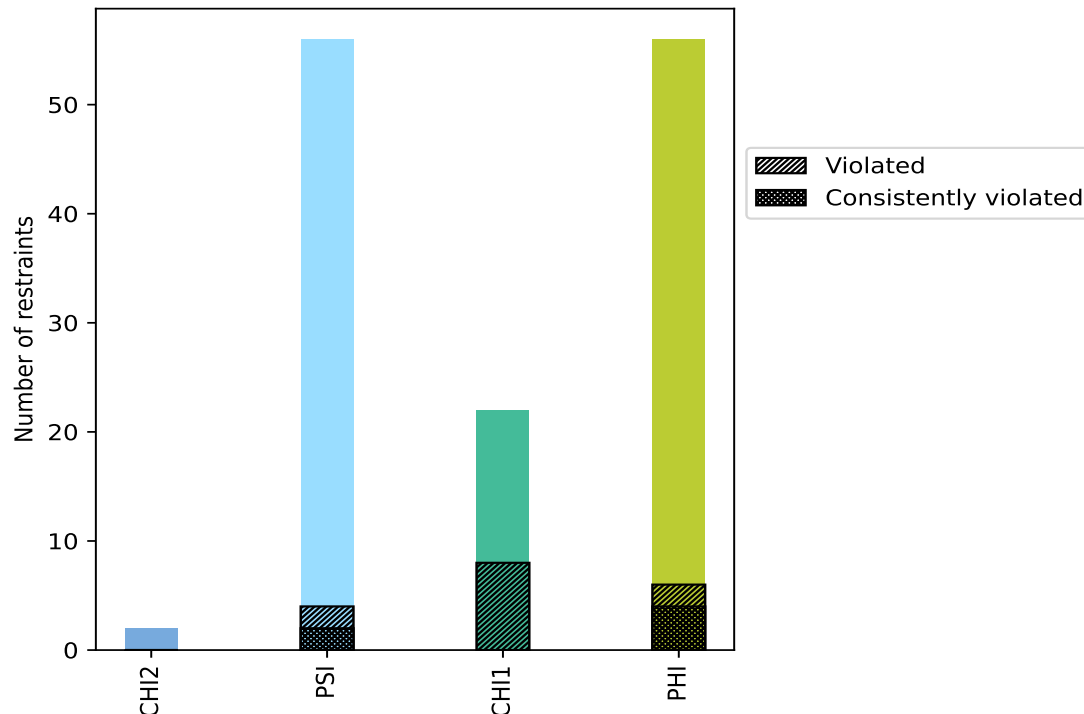
### 10.1 Summary of dihedral-angle violations [i](#)

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

| Angle type | Count | % <sup>1</sup> | Violated <sup>3</sup> |                |                | Consistently Violated <sup>4</sup> |                |                |
|------------|-------|----------------|-----------------------|----------------|----------------|------------------------------------|----------------|----------------|
|            |       |                | Count                 | % <sup>2</sup> | % <sup>1</sup> | Count                              | % <sup>2</sup> | % <sup>1</sup> |
| CHI2       | 2     | 1.5            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| PSI        | 56    | 41.2           | 4                     | 7.1            | 2.9            | 2                                  | 3.6            | 1.5            |
| CHI1       | 22    | 16.2           | 8                     | 36.4           | 5.9            | 0                                  | 0.0            | 0.0            |
| PHI        | 56    | 41.2           | 6                     | 10.7           | 4.4            | 4                                  | 7.1            | 2.9            |
| Total      | 136   | 100.0          | 18                    | 13.2           | 13.2           | 6                                  | 4.4            | 4.4            |

<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](#)



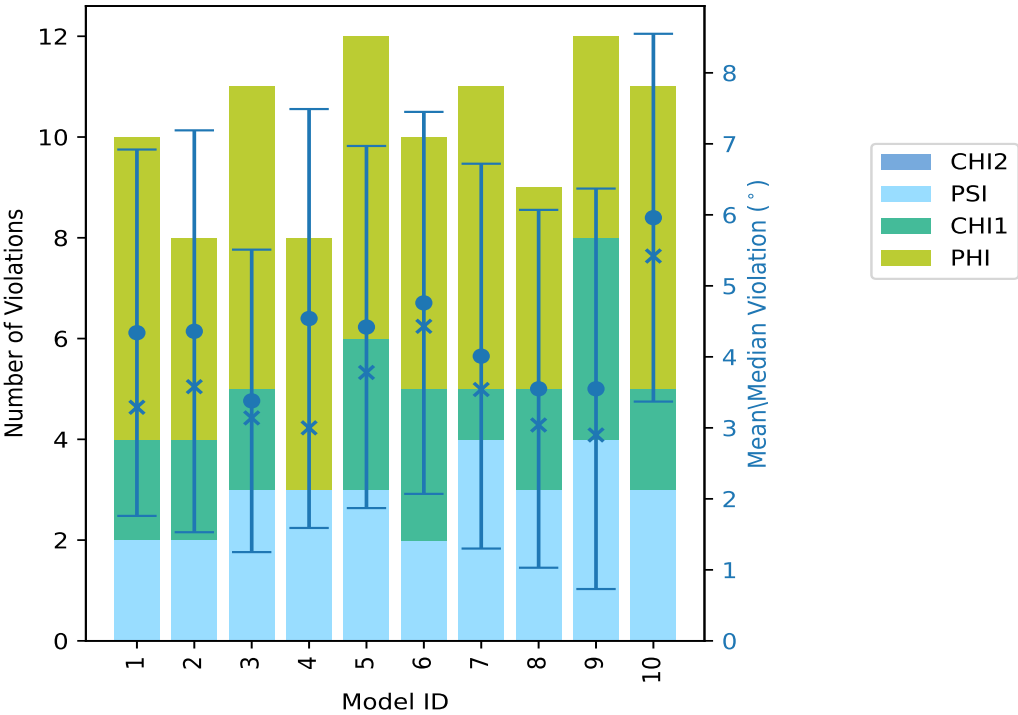
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

# 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 (°) |
|----------|----------------------|-----|------|-----|-------|----------|---------|--------|------------|
|          | CHI2                 | PSI | CHI1 | PHI | Total |          |         |        |            |
| 1        | 0                    | 2   | 2    | 6   | 10    | 4.34     | 9.12    | 2.58   | 3.29       |
| 2        | 0                    | 2   | 2    | 4   | 8     | 4.36     | 9.2     | 2.83   | 3.58       |
| 3        | 0                    | 3   | 2    | 6   | 11    | 3.38     | 7.2     | 2.13   | 3.14       |
| 4        | 0                    | 3   | 0    | 5   | 8     | 4.54     | 9.36    | 2.95   | 3.0        |
| 5        | 0                    | 3   | 3    | 6   | 12    | 4.42     | 9.42    | 2.55   | 3.78       |
| 6        | 0                    | 2   | 3    | 5   | 10    | 4.76     | 9.52    | 2.69   | 4.43       |
| 7        | 0                    | 4   | 1    | 6   | 11    | 4.01     | 9.29    | 2.71   | 3.54       |
| 8        | 0                    | 3   | 2    | 4   | 9     | 3.55     | 8.04    | 2.52   | 3.04       |
| 9        | 0                    | 4   | 4    | 4   | 12    | 3.55     | 9.63    | 2.82   | 2.9        |
| 10       | 0                    | 3   | 2    | 6   | 11    | 5.96     | 10.65   | 2.59   | 5.42       |

## 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

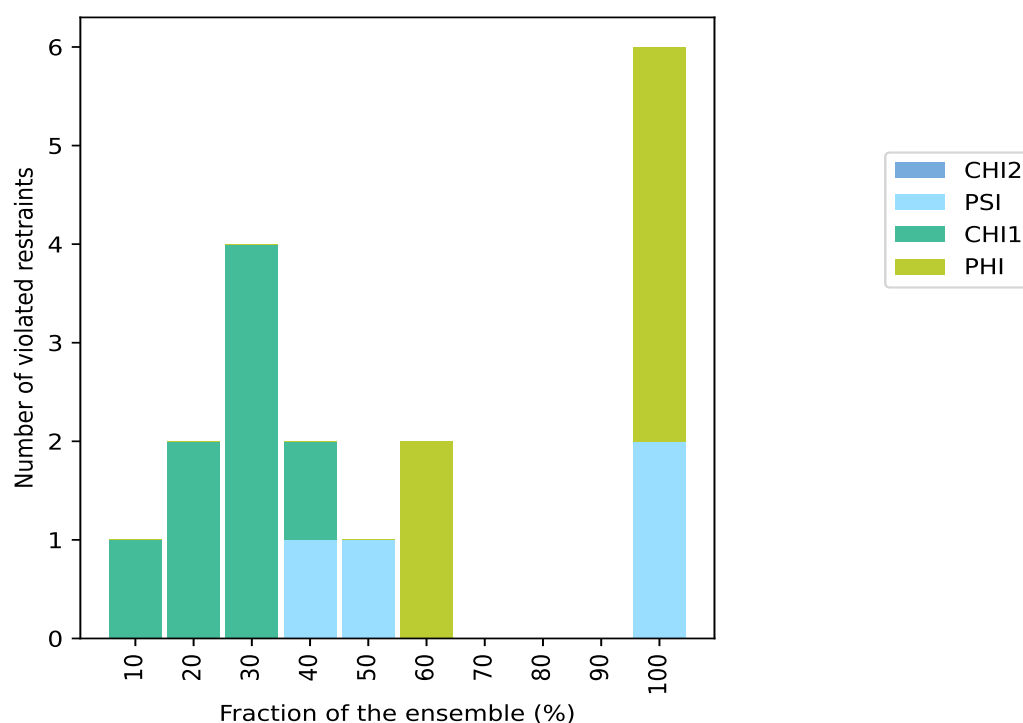
### 10.3 Dihedral-angle violation statistics for the ensemble [i](#)

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 |       |
|-------------------------------|-----|------|-----|-------|--------------------------|-------|
| CHI2                          | PSI | CHI1 | PHI | Total | Count <sup>1</sup>       | %     |
| 0                             | 0   | 1    | 0   | 1     | 1                        | 10.0  |
| 0                             | 0   | 2    | 0   | 2     | 2                        | 20.0  |
| 0                             | 0   | 4    | 0   | 4     | 3                        | 30.0  |
| 0                             | 1   | 1    | 0   | 2     | 4                        | 40.0  |
| 0                             | 1   | 0    | 0   | 1     | 5                        | 50.0  |
| 0                             | 0   | 0    | 2   | 2     | 6                        | 60.0  |
| 0                             | 0   | 0    | 0   | 0     | 7                        | 70.0  |
| 0                             | 0   | 0    | 0   | 0     | 8                        | 80.0  |
| 0                             | 0   | 0    | 0   | 0     | 9                        | 90.0  |
| 0                             | 2   | 0    | 4   | 6     | 10                       | 100.0 |

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

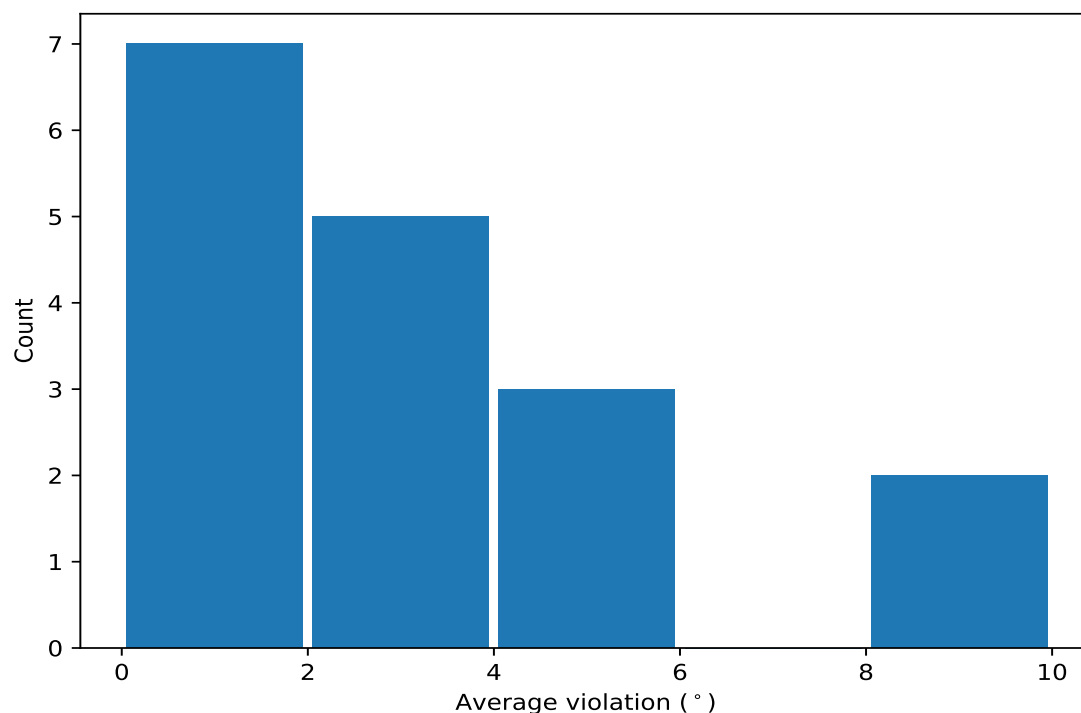
#### 10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



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

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

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



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

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

| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4          | Models <sup>1</sup> | Mean | SD <sup>2</sup> | Median |
|---------|---------------|----------------|----------------|-----------------|---------------------|------|-----------------|--------|
| (1,134) | 1:130:B:GLU:C | 1:131:B:GLY:N  | 1:131:B:GLY:CA | 1:131:B:GLY:C   | 10                  | 9.1  | 0.88            | 9.25   |
| (1,133) | 1:30:A:GLU:C  | 1:31:A:GLY:N   | 1:31:A:GLY:CA  | 1:31:A:GLY:C    | 10                  | 8.9  | 0.91            | 8.94   |
| (1,125) | 1:28:A:HIS:C  | 1:29:A:PHE:N   | 1:29:A:PHE:CA  | 1:29:A:PHE:C    | 10                  | 4.6  | 1.14            | 5.02   |
| (1,126) | 1:128:B:HIS:C | 1:129:B:PHE:N  | 1:129:B:PHE:CA | 1:129:B:PHE:C   | 10                  | 4.23 | 1.19            | 3.88   |
| (1,87)  | 1:19:A:ILE:N  | 1:19:A:ILE:CA  | 1:19:A:ILE:C   | 1:20:A:PHE:N    | 10                  | 3.83 | 0.87            | 3.58   |
| (1,88)  | 1:119:B:ILE:N | 1:119:B:ILE:CA | 1:119:B:ILE:C  | 1:120:B:PHE:N   | 10                  | 3.72 | 0.75            | 3.54   |
| (1,129) | 1:29:A:PHE:C  | 1:30:A:GLU:N   | 1:30:A:GLU:CA  | 1:30:A:GLU:C    | 6                   | 3.33 | 1.02            | 3.07   |
| (1,130) | 1:129:B:PHE:C | 1:130:B:GLU:N  | 1:130:B:GLU:CA | 1:130:B:GLU:C   | 6                   | 2.69 | 1.51            | 2.47   |
| (1,71)  | 1:15:A:SER:N  | 1:15:A:SER:CA  | 1:15:A:SER:C   | 1:16:A:ILE:N    | 5                   | 1.26 | 0.08            | 1.2    |
| (1,10)  | 1:123:B:ILE:N | 1:123:B:ILE:CA | 1:123:B:ILE:CB | 1:123:B:ILE:CG1 | 4                   | 3.03 | 0.85            | 3.26   |
| (1,72)  | 1:115:B:SER:N | 1:115:B:SER:CA | 1:115:B:SER:C  | 1:116:B:ILE:N   | 4                   | 1.33 | 0.17            | 1.36   |
| (1,9)   | 1:23:A:ILE:N  | 1:23:A:ILE:CA  | 1:23:A:ILE:CB  | 1:23:A:ILE:CG1  | 3                   | 4.55 | 1.12            | 5.26   |
| (1,15)  | 1:11:A:MET:N  | 1:11:A:MET:CA  | 1:11:A:MET:CB  | 1:11:A:MET:CG   | 3                   | 1.7  | 0.67            | 1.25   |

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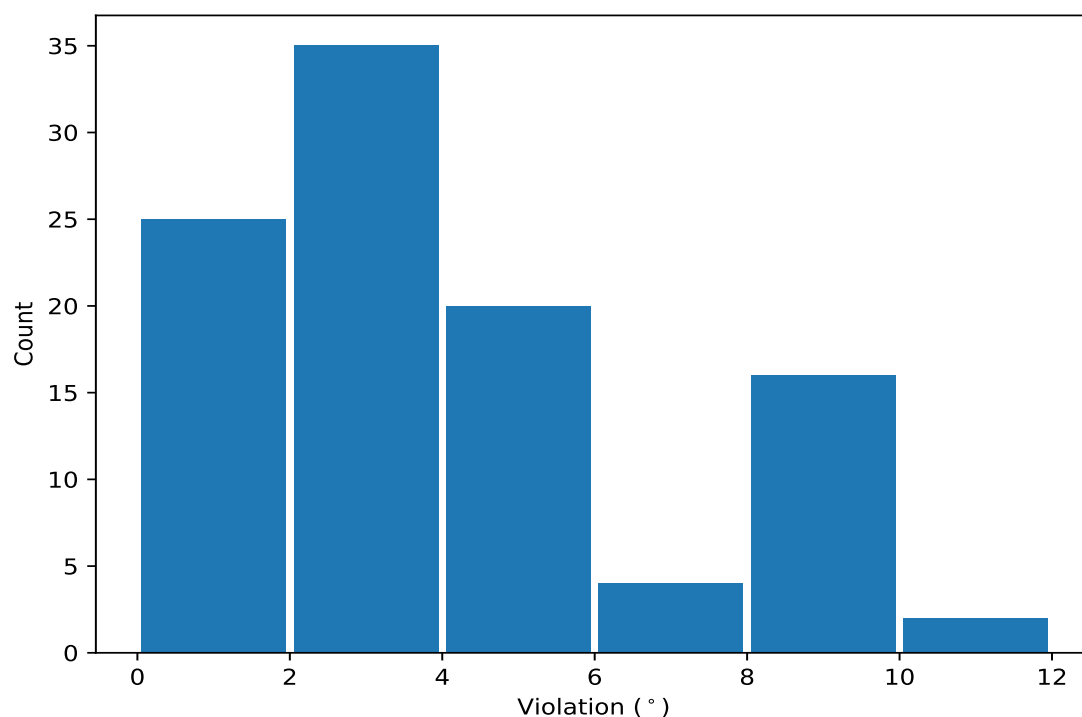
| Key    | Atom-1        | Atom-2         | Atom-3         | Atom-4          | Models <sup>1</sup> | Mean | SD <sup>2</sup> | Median |
|--------|---------------|----------------|----------------|-----------------|---------------------|------|-----------------|--------|
| (1,20) | 1:125:B:LEU:N | 1:125:B:LEU:CA | 1:125:B:LEU:CB | 1:125:B:LEU:CG  | 3                   | 1.16 | 0.17            | 1.06   |
| (1,12) | 1:127:B:ILE:N | 1:127:B:ILE:CA | 1:127:B:ILE:CB | 1:127:B:ILE:CG1 | 3                   | 1.16 | 0.17            | 1.06   |
| (1,16) | 1:111:B:MET:N | 1:111:B:MET:CA | 1:111:B:MET:CB | 1:111:B:MET:CG  | 2                   | 1.88 | 0.62            | 1.88   |
| (1,19) | 1:25:A:LEU:N  | 1:25:A:LEU:CA  | 1:25:A:LEU:CB  | 1:25:A:LEU:CG   | 2                   | 1.24 | 0.08            | 1.24   |

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

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

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

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



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

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

| Key     | Atom-1        | Atom-2        | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|---------------|----------------|---------------|----------|---------------|
| (1,134) | 1:130:B:GLU:C | 1:131:B:GLY:N | 1:131:B:GLY:CA | 1:131:B:GLY:C | 10       | 10.65         |
| (1,133) | 1:30:A:GLU:C  | 1:31:A:GLY:N  | 1:31:A:GLY:CA  | 1:31:A:GLY:C  | 10       | 10.55         |
| (1,134) | 1:130:B:GLU:C | 1:131:B:GLY:N | 1:131:B:GLY:CA | 1:131:B:GLY:C | 9        | 9.63          |

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| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4          | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|-----------------|----------|---------------|
| (1,133) | 1:30:A:GLU:C  | 1:31:A:GLY:N   | 1:31:A:GLY:CA  | 1:31:A:GLY:C    | 6        | 9.52          |
| (1,133) | 1:30:A:GLU:C  | 1:31:A:GLY:N   | 1:31:A:GLY:CA  | 1:31:A:GLY:C    | 9        | 9.5           |
| (1,134) | 1:130:B:GLU:C | 1:131:B:GLY:N  | 1:131:B:GLY:CA | 1:131:B:GLY:C   | 5        | 9.42          |
| (1,133) | 1:30:A:GLU:C  | 1:31:A:GLY:N   | 1:31:A:GLY:CA  | 1:31:A:GLY:C    | 4        | 9.36          |
| (1,134) | 1:130:B:GLU:C | 1:131:B:GLY:N  | 1:131:B:GLY:CA | 1:131:B:GLY:C   | 7        | 9.29          |
| (1,134) | 1:130:B:GLU:C | 1:131:B:GLY:N  | 1:131:B:GLY:CA | 1:131:B:GLY:C   | 4        | 9.25          |
| (1,134) | 1:130:B:GLU:C | 1:131:B:GLY:N  | 1:131:B:GLY:CA | 1:131:B:GLY:C   | 6        | 9.25          |
| (1,134) | 1:130:B:GLU:C | 1:131:B:GLY:N  | 1:131:B:GLY:CA | 1:131:B:GLY:C   | 2        | 9.2           |
| (1,133) | 1:30:A:GLU:C  | 1:31:A:GLY:N   | 1:31:A:GLY:CA  | 1:31:A:GLY:C    | 5        | 9.13          |
| (1,134) | 1:130:B:GLU:C | 1:131:B:GLY:N  | 1:131:B:GLY:CA | 1:131:B:GLY:C   | 1        | 9.12          |
| (1,133) | 1:30:A:GLU:C  | 1:31:A:GLY:N   | 1:31:A:GLY:CA  | 1:31:A:GLY:C    | 1        | 8.75          |
| (1,133) | 1:30:A:GLU:C  | 1:31:A:GLY:N   | 1:31:A:GLY:CA  | 1:31:A:GLY:C    | 2        | 8.67          |
| (1,133) | 1:30:A:GLU:C  | 1:31:A:GLY:N   | 1:31:A:GLY:CA  | 1:31:A:GLY:C    | 7        | 8.45          |
| (1,133) | 1:30:A:GLU:C  | 1:31:A:GLY:N   | 1:31:A:GLY:CA  | 1:31:A:GLY:C    | 8        | 8.04          |
| (1,134) | 1:130:B:GLU:C | 1:131:B:GLY:N  | 1:131:B:GLY:CA | 1:131:B:GLY:C   | 8        | 8.0           |
| (1,134) | 1:130:B:GLU:C | 1:131:B:GLY:N  | 1:131:B:GLY:CA | 1:131:B:GLY:C   | 3        | 7.2           |
| (1,133) | 1:30:A:GLU:C  | 1:31:A:GLY:N   | 1:31:A:GLY:CA  | 1:31:A:GLY:C    | 3        | 7.0           |
| (1,126) | 1:128:B:HIS:C | 1:129:B:PHE:N  | 1:129:B:PHE:CA | 1:129:B:PHE:C   | 10       | 6.8           |
| (1,125) | 1:28:A:HIS:C  | 1:29:A:PHE:N   | 1:29:A:PHE:CA  | 1:29:A:PHE:C    | 10       | 6.2           |
| (1,125) | 1:28:A:HIS:C  | 1:29:A:PHE:N   | 1:29:A:PHE:CA  | 1:29:A:PHE:C    | 5        | 5.89          |
| (1,130) | 1:129:B:PHE:C | 1:130:B:GLU:N  | 1:130:B:GLU:CA | 1:130:B:GLU:C   | 10       | 5.55          |
| (1,129) | 1:29:A:PHE:C  | 1:30:A:GLU:N   | 1:30:A:GLU:CA  | 1:30:A:GLU:C    | 10       | 5.42          |
| (1,9)   | 1:23:A:ILE:N  | 1:23:A:ILE:CA  | 1:23:A:ILE:CB  | 1:23:A:ILE:CG1  | 10       | 5.41          |
| (1,125) | 1:28:A:HIS:C  | 1:29:A:PHE:N   | 1:29:A:PHE:CA  | 1:29:A:PHE:C    | 7        | 5.36          |
| (1,125) | 1:28:A:HIS:C  | 1:29:A:PHE:N   | 1:29:A:PHE:CA  | 1:29:A:PHE:C    | 1        | 5.35          |
| (1,125) | 1:28:A:HIS:C  | 1:29:A:PHE:N   | 1:29:A:PHE:CA  | 1:29:A:PHE:C    | 4        | 5.29          |
| (1,126) | 1:128:B:HIS:C | 1:129:B:PHE:N  | 1:129:B:PHE:CA | 1:129:B:PHE:C   | 7        | 5.27          |
| (1,9)   | 1:23:A:ILE:N  | 1:23:A:ILE:CA  | 1:23:A:ILE:CB  | 1:23:A:ILE:CG1  | 6        | 5.26          |
| (1,87)  | 1:19:A:ILE:N  | 1:19:A:ILE:CA  | 1:19:A:ILE:C   | 1:20:A:PHE:N    | 6        | 5.25          |
| (1,87)  | 1:19:A:ILE:N  | 1:19:A:ILE:CA  | 1:19:A:ILE:C   | 1:20:A:PHE:N    | 10       | 5.18          |
| (1,126) | 1:128:B:HIS:C | 1:129:B:PHE:N  | 1:129:B:PHE:CA | 1:129:B:PHE:C   | 5        | 5.11          |
| (1,88)  | 1:119:B:ILE:N | 1:119:B:ILE:CA | 1:119:B:ILE:C  | 1:120:B:PHE:N   | 6        | 4.98          |
| (1,88)  | 1:119:B:ILE:N | 1:119:B:ILE:CA | 1:119:B:ILE:C  | 1:120:B:PHE:N   | 10       | 4.95          |
| (1,126) | 1:128:B:HIS:C | 1:129:B:PHE:N  | 1:129:B:PHE:CA | 1:129:B:PHE:C   | 1        | 4.74          |
| (1,125) | 1:28:A:HIS:C  | 1:29:A:PHE:N   | 1:29:A:PHE:CA  | 1:29:A:PHE:C    | 3        | 4.74          |
| (1,87)  | 1:19:A:ILE:N  | 1:19:A:ILE:CA  | 1:19:A:ILE:C   | 1:20:A:PHE:N    | 5        | 4.5           |
| (1,126) | 1:128:B:HIS:C | 1:129:B:PHE:N  | 1:129:B:PHE:CA | 1:129:B:PHE:C   | 3        | 4.42          |
| (1,88)  | 1:119:B:ILE:N | 1:119:B:ILE:CA | 1:119:B:ILE:C  | 1:120:B:PHE:N   | 5        | 4.2           |
| (1,87)  | 1:19:A:ILE:N  | 1:19:A:ILE:CA  | 1:19:A:ILE:C   | 1:20:A:PHE:N    | 2        | 4.13          |
| (1,88)  | 1:119:B:ILE:N | 1:119:B:ILE:CA | 1:119:B:ILE:C  | 1:120:B:PHE:N   | 2        | 3.93          |
| (1,87)  | 1:19:A:ILE:N  | 1:19:A:ILE:CA  | 1:19:A:ILE:C   | 1:20:A:PHE:N    | 7        | 3.89          |
| (1,10)  | 1:123:B:ILE:N | 1:123:B:ILE:CA | 1:123:B:ILE:CB | 1:123:B:ILE:CG1 | 6        | 3.88          |
| (1,125) | 1:28:A:HIS:C  | 1:29:A:PHE:N   | 1:29:A:PHE:CA  | 1:29:A:PHE:C    | 6        | 3.68          |
| (1,10)  | 1:123:B:ILE:N | 1:123:B:ILE:CA | 1:123:B:ILE:CB | 1:123:B:ILE:CG1 | 10       | 3.64          |
| (1,88)  | 1:119:B:ILE:N | 1:119:B:ILE:CA | 1:119:B:ILE:C  | 1:120:B:PHE:N   | 9        | 3.55          |
| (1,88)  | 1:119:B:ILE:N | 1:119:B:ILE:CA | 1:119:B:ILE:C  | 1:120:B:PHE:N   | 7        | 3.54          |
| (1,129) | 1:29:A:PHE:C  | 1:30:A:GLU:N   | 1:30:A:GLU:CA  | 1:30:A:GLU:C    | 1        | 3.47          |
| (1,129) | 1:29:A:PHE:C  | 1:30:A:GLU:N   | 1:30:A:GLU:CA  | 1:30:A:GLU:C    | 5        | 3.35          |
| (1,126) | 1:128:B:HIS:C | 1:129:B:PHE:N  | 1:129:B:PHE:CA | 1:129:B:PHE:C   | 6        | 3.33          |
| (1,125) | 1:28:A:HIS:C  | 1:29:A:PHE:N   | 1:29:A:PHE:CA  | 1:29:A:PHE:C    | 9        | 3.33          |
| (1,87)  | 1:19:A:ILE:N  | 1:19:A:ILE:CA  | 1:19:A:ILE:C   | 1:20:A:PHE:N    | 3        | 3.26          |

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| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4          | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|-----------------|----------|---------------|
| (1,87)  | 1:19:A:ILE:N  | 1:19:A:ILE:CA  | 1:19:A:ILE:C   | 1:20:A:PHE:N    | 9        | 3.25          |
| (1,126) | 1:128:B:HIS:C | 1:129:B:PHE:N  | 1:129:B:PHE:CA | 1:129:B:PHE:C   | 4        | 3.23          |
| (1,125) | 1:28:A:HIS:C  | 1:29:A:PHE:N   | 1:29:A:PHE:CA  | 1:29:A:PHE:C    | 2        | 3.23          |
| (1,130) | 1:129:B:PHE:C | 1:130:B:GLU:N  | 1:130:B:GLU:CA | 1:130:B:GLU:C   | 5        | 3.22          |
| (1,126) | 1:128:B:HIS:C | 1:129:B:PHE:N  | 1:129:B:PHE:CA | 1:129:B:PHE:C   | 2        | 3.18          |
| (1,126) | 1:128:B:HIS:C | 1:129:B:PHE:N  | 1:129:B:PHE:CA | 1:129:B:PHE:C   | 9        | 3.16          |
| (1,88)  | 1:119:B:ILE:N | 1:119:B:ILE:CA | 1:119:B:ILE:C  | 1:120:B:PHE:N   | 3        | 3.14          |
| (1,87)  | 1:19:A:ILE:N  | 1:19:A:ILE:CA  | 1:19:A:ILE:C   | 1:20:A:PHE:N    | 8        | 3.13          |
| (1,130) | 1:129:B:PHE:C | 1:130:B:GLU:N  | 1:130:B:GLU:CA | 1:130:B:GLU:C   | 1        | 3.11          |
| (1,87)  | 1:19:A:ILE:N  | 1:19:A:ILE:CA  | 1:19:A:ILE:C   | 1:20:A:PHE:N    | 1        | 3.08          |
| (1,126) | 1:128:B:HIS:C | 1:129:B:PHE:N  | 1:129:B:PHE:CA | 1:129:B:PHE:C   | 8        | 3.06          |
| (1,88)  | 1:119:B:ILE:N | 1:119:B:ILE:CA | 1:119:B:ILE:C  | 1:120:B:PHE:N   | 1        | 3.06          |
| (1,88)  | 1:119:B:ILE:N | 1:119:B:ILE:CA | 1:119:B:ILE:C  | 1:120:B:PHE:N   | 8        | 3.04          |
| (1,9)   | 1:23:A:ILE:N  | 1:23:A:ILE:CA  | 1:23:A:ILE:CB  | 1:23:A:ILE:CG1  | 5        | 2.97          |
| (1,125) | 1:28:A:HIS:C  | 1:29:A:PHE:N   | 1:29:A:PHE:CA  | 1:29:A:PHE:C    | 8        | 2.93          |
| (1,10)  | 1:123:B:ILE:N | 1:123:B:ILE:CA | 1:123:B:ILE:CB | 1:123:B:ILE:CG1 | 5        | 2.87          |
| (1,129) | 1:29:A:PHE:C  | 1:30:A:GLU:N   | 1:30:A:GLU:CA  | 1:30:A:GLU:C    | 7        | 2.79          |
| (1,88)  | 1:119:B:ILE:N | 1:119:B:ILE:CA | 1:119:B:ILE:C  | 1:120:B:PHE:N   | 4        | 2.76          |
| (1,129) | 1:29:A:PHE:C  | 1:30:A:GLU:N   | 1:30:A:GLU:CA  | 1:30:A:GLU:C    | 4        | 2.71          |
| (1,15)  | 1:11:A:MET:N  | 1:11:A:MET:CA  | 1:11:A:MET:CB  | 1:11:A:MET:CG   | 9        | 2.64          |
| (1,87)  | 1:19:A:ILE:N  | 1:19:A:ILE:CA  | 1:19:A:ILE:C   | 1:20:A:PHE:N    | 4        | 2.61          |
| (1,16)  | 1:111:B:MET:N | 1:111:B:MET:CA | 1:111:B:MET:CB | 1:111:B:MET:CG  | 9        | 2.5           |
| (1,129) | 1:29:A:PHE:C  | 1:30:A:GLU:N   | 1:30:A:GLU:CA  | 1:30:A:GLU:C    | 3        | 2.25          |
| (1,130) | 1:129:B:PHE:C | 1:130:B:GLU:N  | 1:130:B:GLU:CA | 1:130:B:GLU:C   | 3        | 1.83          |
| (1,10)  | 1:123:B:ILE:N | 1:123:B:ILE:CA | 1:123:B:ILE:CB | 1:123:B:ILE:CG1 | 7        | 1.71          |
| (1,72)  | 1:115:B:SER:N | 1:115:B:SER:CA | 1:115:B:SER:C  | 1:116:B:ILE:N   | 9        | 1.5           |
| (1,72)  | 1:115:B:SER:N | 1:115:B:SER:CA | 1:115:B:SER:C  | 1:116:B:ILE:N   | 7        | 1.47          |
| (1,20)  | 1:125:B:LEU:N | 1:125:B:LEU:CA | 1:125:B:LEU:CB | 1:125:B:LEU:CG  | 1        | 1.4           |
| (1,12)  | 1:127:B:ILE:N | 1:127:B:ILE:CA | 1:127:B:ILE:CB | 1:127:B:ILE:CG1 | 8        | 1.4           |
| (1,71)  | 1:15:A:SER:N  | 1:15:A:SER:CA  | 1:15:A:SER:C   | 1:16:A:ILE:N    | 9        | 1.37          |
| (1,71)  | 1:15:A:SER:N  | 1:15:A:SER:CA  | 1:15:A:SER:C   | 1:16:A:ILE:N    | 5        | 1.35          |
| (1,19)  | 1:25:A:LEU:N  | 1:25:A:LEU:CA  | 1:25:A:LEU:CB  | 1:25:A:LEU:CG   | 1        | 1.32          |
| (1,130) | 1:129:B:PHE:C | 1:130:B:GLU:N  | 1:130:B:GLU:CA | 1:130:B:GLU:C   | 6        | 1.28          |
| (1,16)  | 1:111:B:MET:N | 1:111:B:MET:CA | 1:111:B:MET:CB | 1:111:B:MET:CG  | 2        | 1.26          |
| (1,15)  | 1:11:A:MET:N  | 1:11:A:MET:CA  | 1:11:A:MET:CB  | 1:11:A:MET:CG   | 2        | 1.25          |
| (1,72)  | 1:115:B:SER:N | 1:115:B:SER:CA | 1:115:B:SER:C  | 1:116:B:ILE:N   | 10       | 1.24          |
| (1,71)  | 1:15:A:SER:N  | 1:15:A:SER:CA  | 1:15:A:SER:C   | 1:16:A:ILE:N    | 3        | 1.2           |
| (1,15)  | 1:11:A:MET:N  | 1:11:A:MET:CA  | 1:11:A:MET:CB  | 1:11:A:MET:CG   | 6        | 1.2           |
| (1,71)  | 1:15:A:SER:N  | 1:15:A:SER:CA  | 1:15:A:SER:C   | 1:16:A:ILE:N    | 7        | 1.19          |
| (1,71)  | 1:15:A:SER:N  | 1:15:A:SER:CA  | 1:15:A:SER:C   | 1:16:A:ILE:N    | 8        | 1.19          |
| (1,19)  | 1:25:A:LEU:N  | 1:25:A:LEU:CA  | 1:25:A:LEU:CB  | 1:25:A:LEU:CG   | 9        | 1.16          |
| (1,130) | 1:129:B:PHE:C | 1:130:B:GLU:N  | 1:130:B:GLU:CA | 1:130:B:GLU:C   | 7        | 1.14          |
| (1,11)  | 1:27:A:ILE:N  | 1:27:A:ILE:CA  | 1:27:A:ILE:CB  | 1:27:A:ILE:CG1  | 8        | 1.14          |
| (1,72)  | 1:115:B:SER:N | 1:115:B:SER:CA | 1:115:B:SER:C  | 1:116:B:ILE:N   | 4        | 1.1           |
| (1,20)  | 1:125:B:LEU:N | 1:125:B:LEU:CA | 1:125:B:LEU:CB | 1:125:B:LEU:CG  | 9        | 1.06          |
| (1,12)  | 1:127:B:ILE:N | 1:127:B:ILE:CA | 1:127:B:ILE:CB | 1:127:B:ILE:CG1 | 3        | 1.06          |
| (1,20)  | 1:125:B:LEU:N | 1:125:B:LEU:CA | 1:125:B:LEU:CB | 1:125:B:LEU:CG  | 3        | 1.03          |
| (1,12)  | 1:127:B:ILE:N | 1:127:B:ILE:CA | 1:127:B:ILE:CB | 1:127:B:ILE:CG1 | 5        | 1.02          |