



# Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2026 – 04:47 PM UTC

PDB ID : 2X8N / pdb\_00002x8n  
BMRB ID : 16790  
Title : Solution NMR structure of uncharacterized protein CV0863 from *Chromobacterium violaceum*. NORTHEAST STRUCTURAL GENOMICS TARGET (NESG) target CvT3. OSCP target CV0863.  
Authors : Gutmanas, A.; Fares, C.; Yee, A.; Lemak, A.; Semesi, A.; Arrowsmith, C.H.; Ontario Centre for Structural Proteomics (OCSF); Northeast Structural Genomics Consortium (NESG)  
Deposited on : 2010-03-10

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

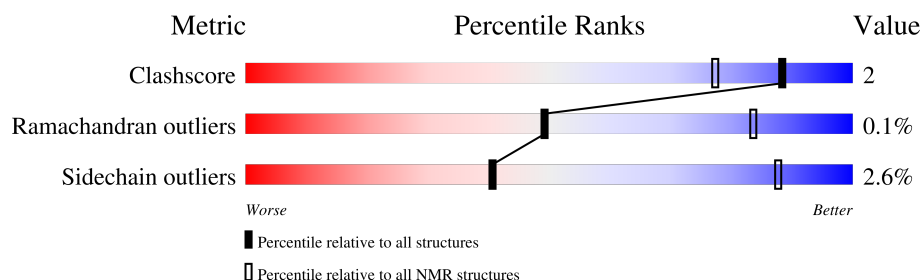
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 91%.

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     | 111    |                  |

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 7 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative.

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:15-A:102 (88)       | 0.57              | 7            |

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

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

The models can be grouped into 3 clusters. No single-model clusters were found.

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

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1710 atoms, of which 846 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called CV0863.

| Mol | Chain | Residues | Atoms |     |     |     |     |   | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|-------|
| 1   | A     | 109      | Total | C   | H   | N   | O   | S | 0     |
|     |       |          | 1710  | 538 | 846 | 147 | 175 | 4 |       |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | -1      | GLN      | -      | expression tag | UNP Q7NZQ8 |
| A     | 0       | GLY      | -      | expression tag | UNP Q7NZQ8 |

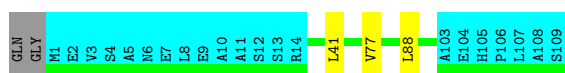
## 4 Residue-property plots [i](#)

### 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: CV0863

Chain A: 



### 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: CV0863

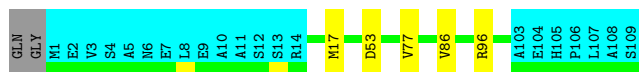
Chain A: 



#### 4.2.2 Score per residue for model 2

- Molecule 1: CV0863

Chain A: 



### 4.2.3 Score per residue for model 3

- Molecule 1: CV0863

Chain A:  77% 19%



### 4.2.4 Score per residue for model 4

- Molecule 1: CV0863

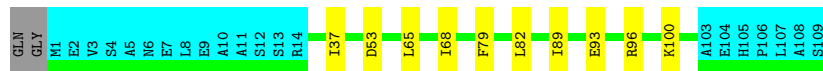
Chain A:  72% 7% 19%



### 4.2.5 Score per residue for model 5

- Molecule 1: CV0863

Chain A:  70% 9% 19%



### 4.2.6 Score per residue for model 6

- Molecule 1: CV0863

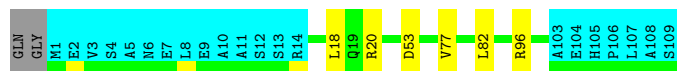
Chain A:  71% 8% 19%



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

- Molecule 1: CV0863

Chain A:  74% 5% 19%



### 4.2.8 Score per residue for model 8

- Molecule 1: CV0863

Chain A:  73% 5% 19%



### 4.2.9 Score per residue for model 9

- Molecule 1: CV0863

Chain A:  73% 6% 19%



### 4.2.10 Score per residue for model 10

- Molecule 1: CV0863

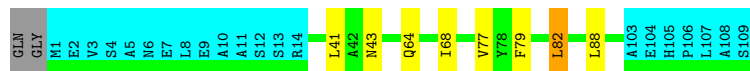
Chain A:  73% 6% 19%



### 4.2.11 Score per residue for model 11

- Molecule 1: CV0863

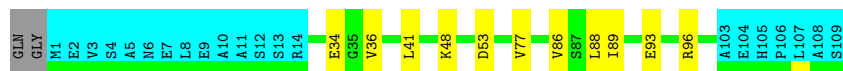
Chain A:  72% 6% 19%



### 4.2.12 Score per residue for model 12

- Molecule 1: CV0863

Chain A:  69% 10% 19%



### 4.2.13 Score per residue for model 13

- Molecule 1: CV0863

Chain A:  73% 6% 19% .



### 4.2.14 Score per residue for model 14

- Molecule 1: CV0863

Chain A:  72% 7% 19% .



### 4.2.15 Score per residue for model 15

- Molecule 1: CV0863

Chain A:  69% 10% 19% .



### 4.2.16 Score per residue for model 16

- Molecule 1: CV0863

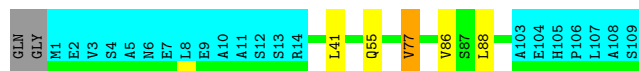
Chain A:  75% 5% 19% .



### 4.2.17 Score per residue for model 17

- Molecule 1: CV0863

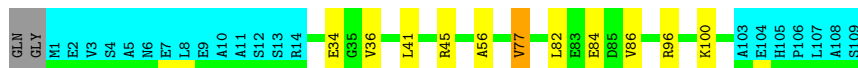
Chain A:  75% 19% .



### 4.2.18 Score per residue for model 18

- Molecule 1: CV0863

Chain A:  69% 9% 19%



### 4.2.19 Score per residue for model 19

- Molecule 1: CV0863

Chain A:  68% 11% 19%



### 4.2.20 Score per residue for model 20

- Molecule 1: CV0863

Chain A:  77% 19%



## 5 Refinement protocol and experimental data overview

The models were refined using the following method: *TORSION ANGLE DYNAMICS*, *RESTRAINED MOLECULAR DYNAMICS*.

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *LOWEST ENERGY*.

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

| Software name   | Classification     | Version |
|-----------------|--------------------|---------|
| CNS             | refinement         |         |
| NMRPipe         | structure solution |         |
| MddNMR          | structure solution |         |
| MDDGUI          | structure solution |         |
| ABACUS          | structure solution |         |
| CcpNmr Analysis | structure solution | ANAYSIS |
| CYANA           | structure solution |         |
| CNS             | structure solution |         |

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                       | 1353           |
| Number of shifts mapped to atoms             | 1353           |
| Number of unparsed shifts                    | 0              |
| Number of shifts with mapping errors         | 0              |
| Number of shifts with mapping warnings       | 0              |
| Assignment completeness (well-defined parts) | 91%            |

## 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     | 711   | 702      | 702      | 3±1     |
| All | All   | 14220 | 14040    | 14040    | 54      |

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 2.

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

| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:41:LEU:HD21 | 1:A:88:LEU:HD11 | 0.63     | 1.69        | 4      | 12    |
| 1:A:53:ASP:HB3  | 1:A:96:ARG:HD3  | 0.53     | 1.80        | 12     | 5     |
| 1:A:39:PHE:HB2  | 1:A:47:LEU:HB2  | 0.47     | 1.86        | 14     | 2     |
| 1:A:77:VAL:HG12 | 1:A:86:VAL:HB   | 0.46     | 1.88        | 1      | 9     |
| 1:A:89:ILE:O    | 1:A:93:GLU:HG2  | 0.44     | 2.13        | 15     | 5     |
| 1:A:76:GLY:HA2  | 1:A:88:LEU:HB2  | 0.43     | 1.91        | 19     | 4     |
| 1:A:56:ALA:HA   | 1:A:84:GLU:HB3  | 0.43     | 1.90        | 18     | 1     |
| 1:A:53:ASP:HB3  | 1:A:96:ARG:HD2  | 0.42     | 1.92        | 7      | 1     |
| 1:A:37:ILE:HD11 | 1:A:65:LEU:HD13 | 0.42     | 1.90        | 5      | 1     |
| 1:A:68:ILE:HG12 | 1:A:79:PHE:CD1  | 0.42     | 2.50        | 5      | 5     |
| 1:A:34:GLU:HB2  | 1:A:36:VAL:HG22 | 0.42     | 1.91        | 12     | 3     |
| 1:A:93:GLU:HB3  | 1:A:95:ARG:NH2  | 0.42     | 2.29        | 8      | 1     |
| 1:A:53:ASP:HB3  | 1:A:96:ARG:HE   | 0.41     | 1.75        | 13     | 1     |
| 1:A:56:ALA:HA   | 1:A:84:GLU:HG2  | 0.41     | 1.92        | 15     | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:41:LEU:HD12 | 1:A:45:ARG:HB3  | 0.41     | 1.92        | 18     | 1     |
| 1:A:64:GLN:HB3  | 1:A:82:LEU:HD22 | 0.41     | 1.93        | 11     | 1     |
| 1:A:36:VAL:HG21 | 1:A:48:LYS:HG3  | 0.41     | 1.92        | 12     | 1     |

## 6.3 Torsion angles [i](#)

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

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

| Mol | Chain | Analysed        | Favoured     | Allowed    | Outliers   | Percentiles |    |
|-----|-------|-----------------|--------------|------------|------------|-------------|----|
| 1   | A     | 88/111 (79%)    | 84±1 (95±1%) | 4±1 (5±1%) | 0±0 (0±0%) | 49          | 83 |
| All | All   | 1760/2220 (79%) | 1671 (95%)   | 87 (5%)    | 2 (0%)     | 49          | 83 |

All 2 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 23  | SER  | 1              |
| 1   | A     | 75  | LEU  | 1              |

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

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

| Mol | Chain | Analysed        | Rotameric    | Outliers   | Percentiles |    |
|-----|-------|-----------------|--------------|------------|-------------|----|
| 1   | A     | 77/94 (82%)     | 75±1 (97±1%) | 2±1 (3±1%) | 41          | 88 |
| All | All   | 1540/1880 (82%) | 1500 (97%)   | 40 (3%)    | 41          | 88 |

All 15 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     | 77  | VAL  | 10             |
| 1   | A     | 82  | LEU  | 8              |
| 1   | A     | 15  | MET  | 4              |
| 1   | A     | 33  | GLU  | 3              |
| 1   | A     | 100 | LYS  | 2              |
| 1   | A     | 20  | ARG  | 2              |
| 1   | A     | 96  | ARG  | 2              |
| 1   | A     | 81  | THR  | 2              |
| 1   | A     | 50  | ARG  | 1              |
| 1   | A     | 95  | ARG  | 1              |
| 1   | A     | 63  | GLU  | 1              |
| 1   | A     | 43  | ASN  | 1              |
| 1   | A     | 48  | LYS  | 1              |
| 1   | A     | 55  | GLN  | 1              |
| 1   | A     | 102 | MET  | 1              |

### 6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 6.7 Other polymers [i](#)

There are no such molecules in this entry.

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

There are no chain breaks in this entry.

## 7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 91% for the well-defined parts and 91% 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                  | 1353 |
| Number of shifts mapped to atoms        | 1353 |
| Number of unparsed shifts               | 0    |
| Number of shifts with mapping errors    | 0    |
| Number of shifts with mapping warnings  | 0    |
| Number of shift outliers (ShiftChecker) | 7    |

#### 7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

| Nucleus                | # values | Correction $\pm$ precision, ppm | Suggested action           |
|------------------------|----------|---------------------------------|----------------------------|
| $^{13}\text{C}_\alpha$ | 109      | $-0.03 \pm 0.33$                | None needed ( $< 0.5$ ppm) |
| $^{13}\text{C}_\beta$  | 102      | $0.16 \pm 0.23$                 | None needed ( $< 0.5$ ppm) |
| $^{13}\text{C}'$       | 101      | $0.20 \pm 0.26$                 | None needed ( $< 0.5$ ppm) |
| $^{15}\text{N}$        | 102      | $0.35 \pm 0.37$                 | None needed ( $< 0.5$ ppm) |

#### 7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 91%, i.e. 1121 atoms were assigned a chemical shift out of a possible 1236. 0 out of 16 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total         | $^1\text{H}$  | $^{13}\text{C}$ | $^{15}\text{N}$ |
|-----------|---------------|---------------|-----------------|-----------------|
| Backbone  | 431/441 (98%) | 178/180 (99%) | 170/176 (97%)   | 83/85 (98%)     |
| Sidechain | 616/717 (86%) | 419/464 (90%) | 192/222 (86%)   | 5/31 (16%)      |

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|          | Total           | <sup>1</sup> H | <sup>13</sup> C | <sup>15</sup> N |
|----------|-----------------|----------------|-----------------|-----------------|
| Aromatic | 74/78 (95%)     | 37/37 (100%)   | 36/40 (90%)     | 1/1 (100%)      |
| Overall  | 1121/1236 (91%) | 634/681 (93%)  | 398/438 (91%)   | 89/117 (76%)    |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 91%, i.e. 1353 atoms were assigned a chemical shift out of a possible 1490. 0 out of 19 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total           | <sup>1</sup> H | <sup>13</sup> C | <sup>15</sup> N |
|-----------|-----------------|----------------|-----------------|-----------------|
| Backbone  | 530/544 (97%)   | 218/221 (99%)  | 210/218 (96%)   | 102/105 (97%)   |
| Sidechain | 745/860 (87%)   | 508/558 (91%)  | 231/267 (87%)   | 6/35 (17%)      |
| Aromatic  | 78/86 (91%)     | 39/41 (95%)    | 38/42 (90%)     | 1/3 (33%)       |
| Overall   | 1353/1490 (91%) | 765/820 (93%)  | 479/527 (91%)   | 109/143 (76%)   |

#### 7.1.4 Statistically unusual chemical shifts ⓘ

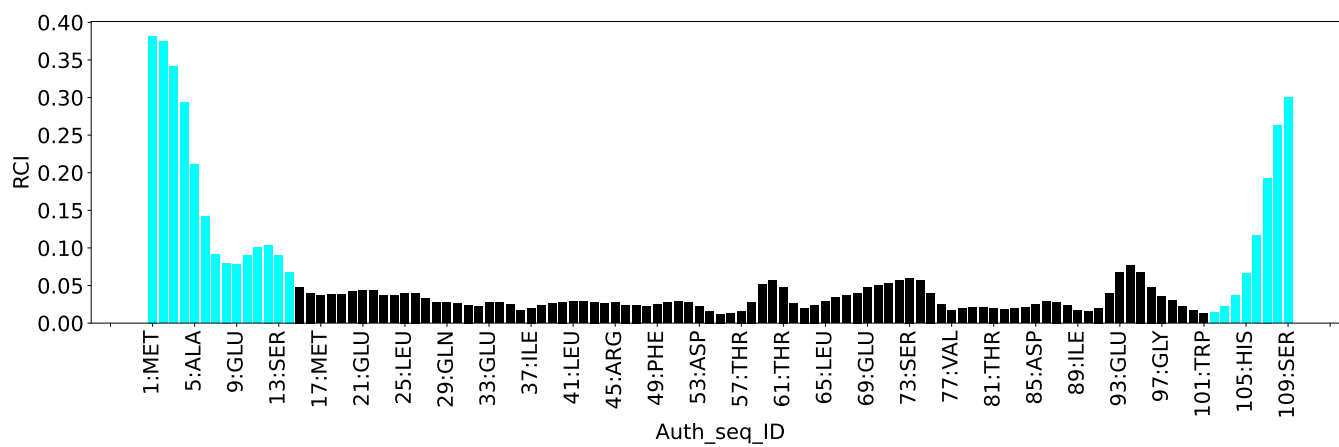
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

| List Id | Chain | Res | Type | Atom | Shift, ppm | Expected range, ppm | Z-score |
|---------|-------|-----|------|------|------------|---------------------|---------|
| 1       | A     | 55  | GLN  | HB3  | 0.07       | 0.71 – 3.33         | -7.4    |
| 1       | A     | 57  | THR  | HG21 | -0.21      | 0.08 – 2.19         | -6.4    |
| 1       | A     | 57  | THR  | HG22 | -0.21      | 0.08 – 2.19         | -6.4    |
| 1       | A     | 57  | THR  | HG23 | -0.21      | 0.08 – 2.19         | -6.4    |
| 1       | A     | 55  | GLN  | HG3  | 0.61       | 0.91 – 3.68         | -6.1    |
| 1       | A     | 55  | GLN  | HA   | 2.15       | 2.17 – 6.35         | -5.0    |
| 1       | A     | 105 | HIS  | HB3  | 1.17       | 1.18 – 4.91         | -5.0    |

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

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

Random coil index (RCI) for chain A:



## 8 NMR restraints analysis

### 8.1 Conformationally restricting restraints

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

| Description                                              | Value |
|----------------------------------------------------------|-------|
| Total distance restraints                                | 2787  |
| Intra-residue ( $ i-j =0$ )                              | 591   |
| Sequential ( $ i-j =1$ )                                 | 665   |
| Medium range ( $ i-j >1$ and $ i-j <5$ )                 | 508   |
| Long range ( $ i-j \geq 5$ )                             | 961   |
| Inter-chain                                              | 0     |
| Hydrogen bond restraints                                 | 62    |
| Disulfide bond restraints                                | 0     |
| Total dihedral-angle restraints                          | 116   |
| Number of unmapped restraints                            | 0     |
| Number of restraints per residue                         | 26.2  |
| Number of long range restraints per residue <sup>1</sup> | 8.9   |

<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)  | 17.0                                   | 0.2     |
| 0.2-0.5 (Medium) | 13.8                                   | 0.5     |
| >0.5 (Large)     | 0.4                                    | 0.77    |

### 8.2.2 Average number of dihedral-angle violations per model [i](#)

Dihedral-angle violations less than 1° are not included in the calculation.

| Bins (°)           | Average number of violations per model | Max (°) |
|--------------------|----------------------------------------|---------|
| 1.0-10.0 (Small)   | 2.6                                    | 4.74    |
| 10.0-20.0 (Medium) | None                                   | None    |
| >20.0 (Large)      | None                                   | None    |

## 9 Distance violation analysis [i](#)

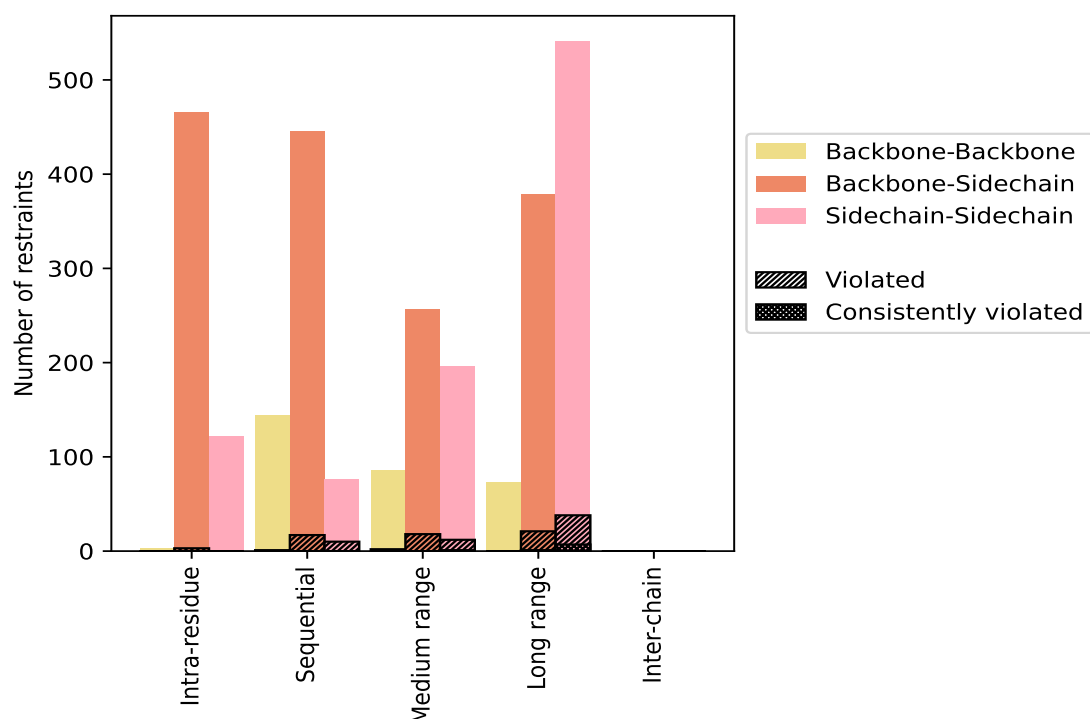
### 9.1 Summary of distance violations [i](#)

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

| Restrains type                                                              | Count       | % <sup>1</sup> | Violated <sup>3</sup> |                |                | Consistently Violated <sup>4</sup> |                |                |
|-----------------------------------------------------------------------------|-------------|----------------|-----------------------|----------------|----------------|------------------------------------|----------------|----------------|
|                                                                             |             |                | Count                 | % <sup>2</sup> | % <sup>1</sup> | Count                              | % <sup>2</sup> | % <sup>1</sup> |
| <b>Intra-residue (<math> i-j =0</math>)</b>                                 | <b>591</b>  | <b>21.2</b>    | <b>3</b>              | <b>0.5</b>     | <b>0.1</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| Backbone-Backbone                                                           | 3           | 0.1            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 466         | 16.7           | 3                     | 0.6            | 0.1            | 0                                  | 0.0            | 0.0            |
| Sidechain-Sidechain                                                         | 122         | 4.4            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| <b>Sequential (<math> i-j =1</math>)</b>                                    | <b>665</b>  | <b>23.9</b>    | <b>28</b>             | <b>4.2</b>     | <b>1.0</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| Backbone-Backbone                                                           | 144         | 5.2            | 1                     | 0.7            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 445         | 16.0           | 17                    | 3.8            | 0.6            | 0                                  | 0.0            | 0.0            |
| Sidechain-Sidechain                                                         | 76          | 2.7            | 10                    | 13.2           | 0.4            | 0                                  | 0.0            | 0.0            |
| <b>Medium range (<math> i-j &gt;1</math> &amp; <math> i-j &lt;5</math>)</b> | <b>508</b>  | <b>18.2</b>    | <b>27</b>             | <b>5.3</b>     | <b>1.0</b>     | <b>1</b>                           | <b>0.2</b>     | <b>0.0</b>     |
| Backbone-Backbone                                                           | 86          | 3.1            | 2                     | 2.3            | 0.1            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 226         | 8.1            | 13                    | 5.8            | 0.5            | 0                                  | 0.0            | 0.0            |
| Sidechain-Sidechain                                                         | 196         | 7.0            | 12                    | 6.1            | 0.4            | 1                                  | 0.5            | 0.0            |
| <b>Long range (<math> i-j \geq 5</math>)</b>                                | <b>961</b>  | <b>34.5</b>    | <b>56</b>             | <b>5.8</b>     | <b>2.0</b>     | <b>8</b>                           | <b>0.8</b>     | <b>0.3</b>     |
| Backbone-Backbone                                                           | 73          | 2.6            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 347         | 12.5           | 18                    | 5.2            | 0.6            | 1                                  | 0.3            | 0.0            |
| Sidechain-Sidechain                                                         | 541         | 19.4           | 38                    | 7.0            | 1.4            | 7                                  | 1.3            | 0.3            |
| <b>Inter-chain</b>                                                          | <b>0</b>    | <b>0.0</b>     | <b>0</b>              | <b>0.0</b>     | <b>0.0</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| Backbone-Backbone                                                           | 0           | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 0           | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Sidechain-Sidechain                                                         | 0           | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| <b>Hydrogen bond</b>                                                        | <b>62</b>   | <b>2.2</b>     | <b>8</b>              | <b>12.9</b>    | <b>0.3</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>2787</b> | <b>100.0</b>   | <b>122</b>            | <b>4.4</b>     | <b>4.4</b>     | <b>9</b>                           | <b>0.3</b>     | <b>0.3</b>     |
| Backbone-Backbone                                                           | 306         | 11.0           | 3                     | 1.0            | 0.1            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 1546        | 55.5           | 59                    | 3.8            | 2.1            | 1                                  | 0.1            | 0.0            |
| Sidechain-Sidechain                                                         | 935         | 33.5           | 60                    | 6.4            | 2.2            | 8                                  | 0.9            | 0.3            |

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

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



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

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

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

| Model ID | Number of violations |                 |                 |                 |                 |       | Mean (Å) | Max (Å) | SD <sup>6</sup> (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
|          | IR <sup>1</sup>      | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total |          |         |                     |            |
| 1        | 0                    | 7               | 8               | 15              | 0               | 30    | 0.23     | 0.45    | 0.1                 | 0.22       |
| 2        | 0                    | 9               | 6               | 14              | 0               | 29    | 0.22     | 0.47    | 0.09                | 0.2        |
| 3        | 0                    | 8               | 7               | 19              | 0               | 34    | 0.21     | 0.49    | 0.11                | 0.16       |
| 4        | 0                    | 9               | 6               | 14              | 0               | 29    | 0.21     | 0.44    | 0.1                 | 0.19       |
| 5        | 0                    | 7               | 9               | 18              | 0               | 34    | 0.21     | 0.48    | 0.1                 | 0.18       |
| 6        | 0                    | 8               | 9               | 18              | 0               | 35    | 0.21     | 0.46    | 0.1                 | 0.16       |
| 7        | 1                    | 5               | 6               | 18              | 0               | 30    | 0.21     | 0.5     | 0.1                 | 0.16       |
| 8        | 0                    | 7               | 8               | 16              | 0               | 31    | 0.22     | 0.44    | 0.1                 | 0.21       |
| 9        | 0                    | 7               | 7               | 14              | 0               | 28    | 0.23     | 0.58    | 0.12                | 0.23       |
| 10       | 0                    | 7               | 6               | 15              | 0               | 28    | 0.22     | 0.55    | 0.11                | 0.2        |

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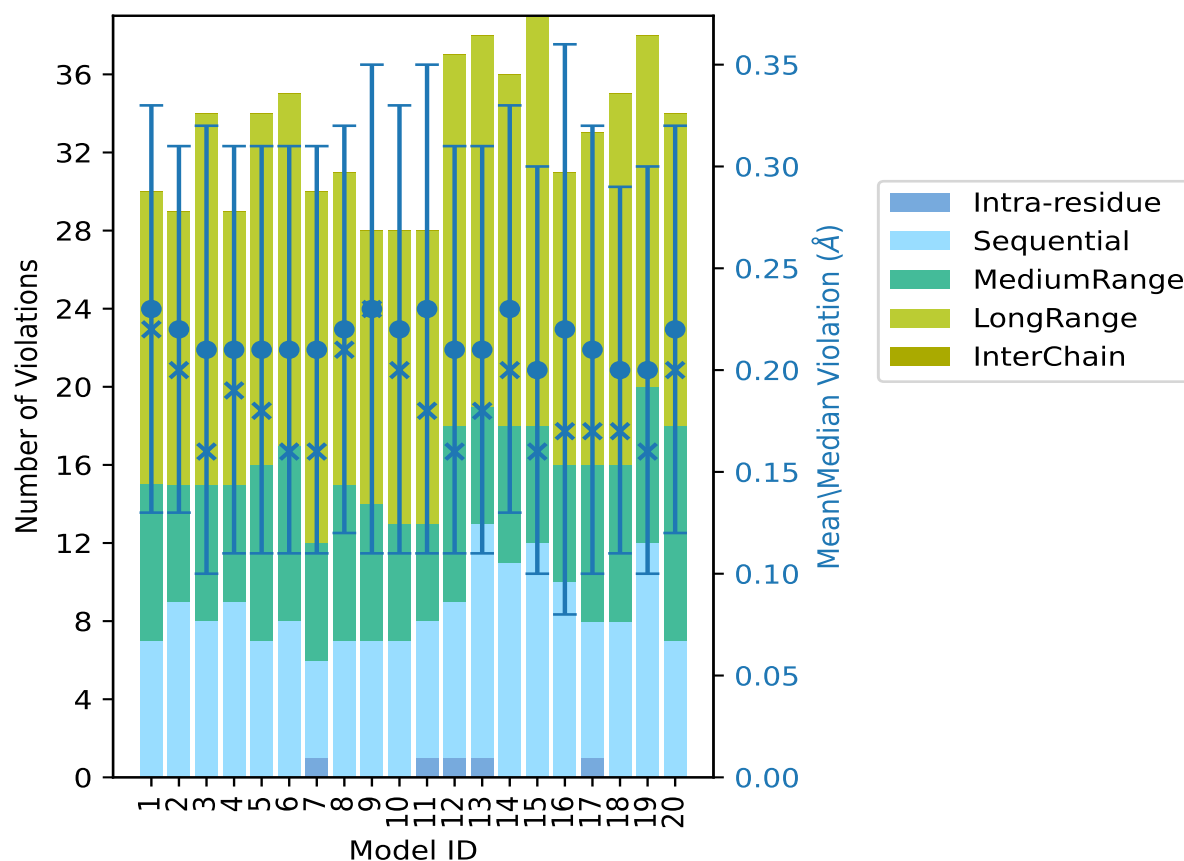
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| Model ID | Number of violations |                 |                 |                 |                 |       | Mean (Å) | Max (Å) | SD <sup>6</sup> (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
|          | IR <sup>1</sup>      | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total |          |         |                     |            |
| 11       | 1                    | 7               | 5               | 15              | 0               | 28    | 0.23     | 0.58    | 0.12                | 0.18       |
| 12       | 1                    | 8               | 9               | 19              | 0               | 37    | 0.21     | 0.48    | 0.1                 | 0.16       |
| 13       | 1                    | 12              | 6               | 19              | 0               | 38    | 0.21     | 0.54    | 0.1                 | 0.18       |
| 14       | 0                    | 11              | 7               | 18              | 0               | 36    | 0.23     | 0.58    | 0.1                 | 0.2        |
| 15       | 0                    | 12              | 6               | 21              | 0               | 39    | 0.2      | 0.46    | 0.1                 | 0.16       |
| 16       | 0                    | 10              | 6               | 15              | 0               | 31    | 0.22     | 0.77    | 0.14                | 0.17       |
| 17       | 1                    | 7               | 8               | 17              | 0               | 33    | 0.21     | 0.52    | 0.11                | 0.17       |
| 18       | 0                    | 8               | 8               | 19              | 0               | 35    | 0.2      | 0.46    | 0.09                | 0.17       |
| 19       | 0                    | 12              | 8               | 18              | 0               | 38    | 0.2      | 0.47    | 0.1                 | 0.16       |
| 20       | 0                    | 7               | 11              | 16              | 0               | 34    | 0.22     | 0.55    | 0.1                 | 0.2        |

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

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

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



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

### 9.3 Distance violation statistics for the ensemble

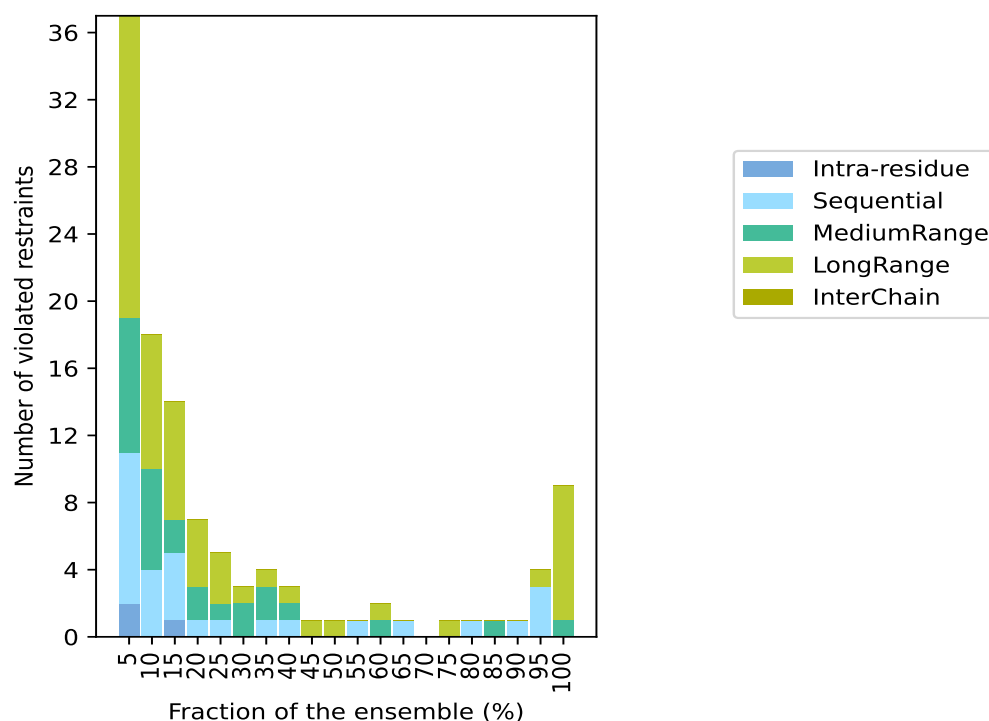
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 2611(IR:588, SQ:637, MR:481, LR:905, IC:0) restraints are not violated in the ensemble.

| Number of violated restraints |                 |                 |                 |                 |       | Fraction of the ensemble |       |
|-------------------------------|-----------------|-----------------|-----------------|-----------------|-------|--------------------------|-------|
| IR <sup>1</sup>               | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total | Count <sup>6</sup>       | %     |
| 2                             | 9               | 8               | 18              | 0               | 37    | 1                        | 5.0   |
| 0                             | 4               | 6               | 8               | 0               | 18    | 2                        | 10.0  |
| 1                             | 4               | 2               | 7               | 0               | 14    | 3                        | 15.0  |
| 0                             | 1               | 2               | 4               | 0               | 7     | 4                        | 20.0  |
| 0                             | 1               | 1               | 3               | 0               | 5     | 5                        | 25.0  |
| 0                             | 0               | 2               | 1               | 0               | 3     | 6                        | 30.0  |
| 0                             | 1               | 2               | 1               | 0               | 4     | 7                        | 35.0  |
| 0                             | 1               | 1               | 1               | 0               | 3     | 8                        | 40.0  |
| 0                             | 0               | 0               | 1               | 0               | 1     | 9                        | 45.0  |
| 0                             | 0               | 0               | 1               | 0               | 1     | 10                       | 50.0  |
| 0                             | 1               | 0               | 0               | 0               | 1     | 11                       | 55.0  |
| 0                             | 0               | 1               | 1               | 0               | 2     | 12                       | 60.0  |
| 0                             | 1               | 0               | 0               | 0               | 1     | 13                       | 65.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 14                       | 70.0  |
| 0                             | 0               | 0               | 1               | 0               | 1     | 15                       | 75.0  |
| 0                             | 1               | 0               | 0               | 0               | 1     | 16                       | 80.0  |
| 0                             | 0               | 1               | 0               | 0               | 1     | 17                       | 85.0  |
| 0                             | 1               | 0               | 0               | 0               | 1     | 18                       | 90.0  |
| 0                             | 3               | 0               | 1               | 0               | 4     | 19                       | 95.0  |
| 0                             | 0               | 1               | 8               | 0               | 9     | 20                       | 100.0 |

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

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

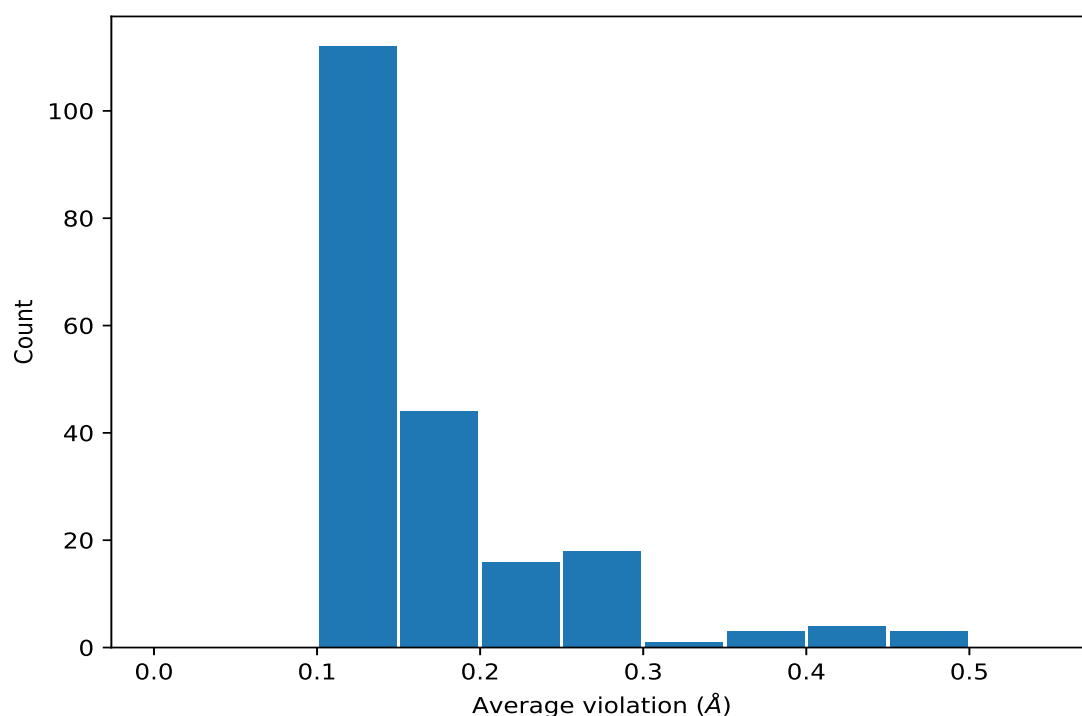
### 9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

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

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



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

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

| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,2011) | 1:56:A:ALA:HB1  | 1:79:A:PHE:HE1  | 20                  | 0.48     | 0.1                 | 0.48       |
| (1,2011) | 1:56:A:ALA:HB2  | 1:79:A:PHE:HE1  | 20                  | 0.48     | 0.1                 | 0.48       |
| (1,2011) | 1:56:A:ALA:HB3  | 1:79:A:PHE:HE1  | 20                  | 0.48     | 0.1                 | 0.48       |
| (1,1300) | 1:68:A:ILE:HG13 | 1:79:A:PHE:HE2  | 20                  | 0.42     | 0.06                | 0.42       |
| (1,1281) | 1:68:A:ILE:HG21 | 1:79:A:PHE:HD2  | 20                  | 0.36     | 0.03                | 0.36       |
| (1,1281) | 1:68:A:ILE:HG22 | 1:79:A:PHE:HD2  | 20                  | 0.36     | 0.03                | 0.36       |
| (1,1281) | 1:68:A:ILE:HG23 | 1:79:A:PHE:HD2  | 20                  | 0.36     | 0.03                | 0.36       |
| (1,1641) | 1:77:A:VAL:HB   | 1:79:A:PHE:HE2  | 20                  | 0.32     | 0.03                | 0.32       |
| (1,1530) | 1:65:A:LEU:HA   | 1:79:A:PHE:HE1  | 20                  | 0.3      | 0.07                | 0.29       |
| (1,1871) | 1:79:A:PHE:HE1  | 1:86:A:VAL:HB   | 20                  | 0.28     | 0.03                | 0.28       |
| (1,1876) | 1:56:A:ALA:HB1  | 1:86:A:VAL:HG11 | 20                  | 0.28     | 0.05                | 0.26       |
| (1,1876) | 1:56:A:ALA:HB1  | 1:86:A:VAL:HG12 | 20                  | 0.28     | 0.05                | 0.26       |
| (1,1876) | 1:56:A:ALA:HB1  | 1:86:A:VAL:HG13 | 20                  | 0.28     | 0.05                | 0.26       |
| (1,1876) | 1:56:A:ALA:HB2  | 1:86:A:VAL:HG11 | 20                  | 0.28     | 0.05                | 0.26       |
| (1,1876) | 1:56:A:ALA:HB2  | 1:86:A:VAL:HG12 | 20                  | 0.28     | 0.05                | 0.26       |
| (1,1876) | 1:56:A:ALA:HB2  | 1:86:A:VAL:HG13 | 20                  | 0.28     | 0.05                | 0.26       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1876) | 1:56:A:ALA:HB3  | 1:86:A:VAL:HG11 | 20                  | 0.28     | 0.05                | 0.26       |
| (1,1876) | 1:56:A:ALA:HB3  | 1:86:A:VAL:HG12 | 20                  | 0.28     | 0.05                | 0.26       |
| (1,1876) | 1:56:A:ALA:HB3  | 1:86:A:VAL:HG13 | 20                  | 0.28     | 0.05                | 0.26       |
| (1,1283) | 1:68:A:ILE:HG21 | 1:79:A:PHE:HE2  | 20                  | 0.26     | 0.02                | 0.26       |
| (1,1283) | 1:68:A:ILE:HG22 | 1:79:A:PHE:HE2  | 20                  | 0.26     | 0.02                | 0.26       |
| (1,1283) | 1:68:A:ILE:HG23 | 1:79:A:PHE:HE2  | 20                  | 0.26     | 0.02                | 0.26       |
| (1,2118) | 1:57:A:THR:HG21 | 1:79:A:PHE:HD1  | 20                  | 0.26     | 0.07                | 0.24       |
| (1,2118) | 1:57:A:THR:HG22 | 1:79:A:PHE:HD1  | 20                  | 0.26     | 0.07                | 0.24       |
| (1,2118) | 1:57:A:THR:HG23 | 1:79:A:PHE:HD1  | 20                  | 0.26     | 0.07                | 0.24       |
| (1,911)  | 1:79:A:PHE:HD2  | 1:80:A:GLU:H    | 19                  | 0.3      | 0.1                 | 0.33       |
| (1,2270) | 1:103:A:ALA:H   | 1:104:A:GLU:HG2 | 19                  | 0.23     | 0.03                | 0.23       |
| (1,2009) | 1:56:A:ALA:HB1  | 1:79:A:PHE:HD1  | 19                  | 0.22     | 0.07                | 0.22       |
| (1,2009) | 1:56:A:ALA:HB2  | 1:79:A:PHE:HD1  | 19                  | 0.22     | 0.07                | 0.22       |
| (1,2009) | 1:56:A:ALA:HB3  | 1:79:A:PHE:HD1  | 19                  | 0.22     | 0.07                | 0.22       |
| (1,1575) | 1:67:A:GLU:HA   | 1:68:A:ILE:HD11 | 19                  | 0.21     | 0.05                | 0.21       |
| (1,1575) | 1:67:A:GLU:HA   | 1:68:A:ILE:HD12 | 19                  | 0.21     | 0.05                | 0.21       |
| (1,1575) | 1:67:A:GLU:HA   | 1:68:A:ILE:HD13 | 19                  | 0.21     | 0.05                | 0.21       |
| (1,2225) | 1:47:A:LEU:HD21 | 1:48:A:LYS:HB3  | 18                  | 0.17     | 0.04                | 0.16       |
| (1,2225) | 1:47:A:LEU:HD22 | 1:48:A:LYS:HB3  | 18                  | 0.17     | 0.04                | 0.16       |
| (1,2225) | 1:47:A:LEU:HD23 | 1:48:A:LYS:HB3  | 18                  | 0.17     | 0.04                | 0.16       |
| (1,1713) | 1:70:A:ILE:HG21 | 1:74:A:GLY:HA3  | 17                  | 0.16     | 0.04                | 0.16       |
| (1,1713) | 1:70:A:ILE:HG22 | 1:74:A:GLY:HA3  | 17                  | 0.16     | 0.04                | 0.16       |
| (1,1713) | 1:70:A:ILE:HG23 | 1:74:A:GLY:HA3  | 17                  | 0.16     | 0.04                | 0.16       |
| (1,179)  | 1:29:A:GLN:HG2  | 1:30:A:TYR:H    | 16                  | 0.18     | 0.04                | 0.18       |
| (1,1528) | 1:65:A:LEU:HA   | 1:79:A:PHE:HD1  | 15                  | 0.13     | 0.02                | 0.13       |
| (1,288)  | 1:47:A:LEU:HD11 | 1:48:A:LYS:H    | 13                  | 0.15     | 0.03                | 0.15       |
| (1,288)  | 1:47:A:LEU:HD12 | 1:48:A:LYS:H    | 13                  | 0.15     | 0.03                | 0.15       |
| (1,288)  | 1:47:A:LEU:HD13 | 1:48:A:LYS:H    | 13                  | 0.15     | 0.03                | 0.15       |
| (1,1424) | 1:79:A:PHE:HD1  | 1:82:A:LEU:HD21 | 12                  | 0.4      | 0.08                | 0.38       |
| (1,1424) | 1:79:A:PHE:HD1  | 1:82:A:LEU:HD22 | 12                  | 0.4      | 0.08                | 0.38       |
| (1,1424) | 1:79:A:PHE:HD1  | 1:82:A:LEU:HD23 | 12                  | 0.4      | 0.08                | 0.38       |
| (1,1993) | 1:72:A:PRO:HB3  | 1:78:A:TYR:HB2  | 12                  | 0.14     | 0.02                | 0.14       |
| (2,13)   | 1:16:A:GLU:O    | 1:20:A:ARG:H    | 12                  | 0.14     | 0.03                | 0.12       |
| (1,2271) | 1:9:A:GLU:HG3   | 1:10:A:ALA:HB1  | 11                  | 0.19     | 0.05                | 0.17       |
| (1,2271) | 1:9:A:GLU:HG3   | 1:10:A:ALA:HB2  | 11                  | 0.19     | 0.05                | 0.17       |
| (1,2271) | 1:9:A:GLU:HG3   | 1:10:A:ALA:HB3  | 11                  | 0.19     | 0.05                | 0.17       |
| (1,1298) | 1:68:A:ILE:HG13 | 1:79:A:PHE:HD2  | 10                  | 0.13     | 0.02                | 0.12       |
| (1,1529) | 1:65:A:LEU:HA   | 1:79:A:PHE:HD2  | 9                   | 0.21     | 0.07                | 0.21       |
| (1,2196) | 1:61:A:THR:HG21 | 1:63:A:GLU:HB2  | 8                   | 0.23     | 0.07                | 0.24       |
| (1,2196) | 1:61:A:THR:HG21 | 1:63:A:GLU:HB3  | 8                   | 0.23     | 0.07                | 0.24       |
| (1,2196) | 1:61:A:THR:HG22 | 1:63:A:GLU:HB2  | 8                   | 0.23     | 0.07                | 0.24       |
| (1,2196) | 1:61:A:THR:HG22 | 1:63:A:GLU:HB3  | 8                   | 0.23     | 0.07                | 0.24       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,2196) | 1:61:A:THR:HG23 | 1:63:A:GLU:HB2  | 8                   | 0.23     | 0.07                | 0.24       |
| (1,2196) | 1:61:A:THR:HG23 | 1:63:A:GLU:HB3  | 8                   | 0.23     | 0.07                | 0.24       |
| (1,231)  | 1:106:A:PRO:HB3 | 1:107:A:LEU:H   | 8                   | 0.15     | 0.04                | 0.15       |
| (1,1950) | 1:15:A:MET:HE1  | 1:89:A:ILE:HD11 | 8                   | 0.15     | 0.04                | 0.13       |
| (1,1950) | 1:15:A:MET:HE1  | 1:89:A:ILE:HD12 | 8                   | 0.15     | 0.04                | 0.13       |
| (1,1950) | 1:15:A:MET:HE1  | 1:89:A:ILE:HD13 | 8                   | 0.15     | 0.04                | 0.13       |
| (1,1950) | 1:15:A:MET:HE2  | 1:89:A:ILE:HD11 | 8                   | 0.15     | 0.04                | 0.13       |
| (1,1950) | 1:15:A:MET:HE2  | 1:89:A:ILE:HD12 | 8                   | 0.15     | 0.04                | 0.13       |
| (1,1950) | 1:15:A:MET:HE2  | 1:89:A:ILE:HD13 | 8                   | 0.15     | 0.04                | 0.13       |
| (1,1950) | 1:15:A:MET:HE3  | 1:89:A:ILE:HD11 | 8                   | 0.15     | 0.04                | 0.13       |
| (1,1950) | 1:15:A:MET:HE3  | 1:89:A:ILE:HD12 | 8                   | 0.15     | 0.04                | 0.13       |
| (1,1950) | 1:15:A:MET:HE3  | 1:89:A:ILE:HD13 | 8                   | 0.15     | 0.04                | 0.13       |
| (1,1960) | 1:33:A:GLU:HA   | 1:34:A:GLU:HG2  | 7                   | 0.17     | 0.03                | 0.16       |
| (1,2133) | 1:57:A:THR:HG21 | 1:84:A:GLU:HB2  | 7                   | 0.16     | 0.03                | 0.16       |
| (1,2133) | 1:57:A:THR:HG22 | 1:84:A:GLU:HB2  | 7                   | 0.16     | 0.03                | 0.16       |
| (1,2133) | 1:57:A:THR:HG23 | 1:84:A:GLU:HB2  | 7                   | 0.16     | 0.03                | 0.16       |
| (2,23)   | 1:99:A:ALA:O    | 1:103:A:ALA:H   | 7                   | 0.15     | 0.04                | 0.14       |
| (1,528)  | 1:61:A:THR:H    | 1:64:A:GLN:HA   | 7                   | 0.13     | 0.03                | 0.12       |
| (1,2034) | 1:104:A:GLU:HA  | 1:106:A:PRO:HD2 | 7                   | 0.12     | 0.01                | 0.12       |
| (1,2040) | 1:43:A:ASN:HA   | 1:45:A:ARG:H    | 6                   | 0.16     | 0.03                | 0.16       |
| (1,2120) | 1:57:A:THR:HG21 | 1:79:A:PHE:HE1  | 6                   | 0.13     | 0.01                | 0.14       |
| (1,2120) | 1:57:A:THR:HG22 | 1:79:A:PHE:HE1  | 6                   | 0.13     | 0.01                | 0.14       |
| (1,2120) | 1:57:A:THR:HG23 | 1:79:A:PHE:HE1  | 6                   | 0.13     | 0.01                | 0.14       |
| (1,864)  | 1:25:A:LEU:HD21 | 1:28:A:VAL:H    | 6                   | 0.11     | 0.01                | 0.11       |
| (1,864)  | 1:25:A:LEU:HD22 | 1:28:A:VAL:H    | 6                   | 0.11     | 0.01                | 0.11       |
| (1,864)  | 1:25:A:LEU:HD23 | 1:28:A:VAL:H    | 6                   | 0.11     | 0.01                | 0.11       |
| (1,2615) | 1:54:A:LEU:HD21 | 1:96:A:ARG:HG2  | 5                   | 0.18     | 0.05                | 0.16       |
| (1,2615) | 1:54:A:LEU:HD21 | 1:96:A:ARG:HG3  | 5                   | 0.18     | 0.05                | 0.16       |
| (1,2615) | 1:54:A:LEU:HD22 | 1:96:A:ARG:HG2  | 5                   | 0.18     | 0.05                | 0.16       |
| (1,2615) | 1:54:A:LEU:HD22 | 1:96:A:ARG:HG3  | 5                   | 0.18     | 0.05                | 0.16       |
| (1,2615) | 1:54:A:LEU:HD23 | 1:96:A:ARG:HG2  | 5                   | 0.18     | 0.05                | 0.16       |
| (1,2615) | 1:54:A:LEU:HD23 | 1:96:A:ARG:HG3  | 5                   | 0.18     | 0.05                | 0.16       |
| (1,932)  | 1:79:A:PHE:H    | 1:82:A:LEU:HB2  | 5                   | 0.16     | 0.06                | 0.15       |
| (1,932)  | 1:79:A:PHE:H    | 1:82:A:LEU:HB3  | 5                   | 0.16     | 0.06                | 0.15       |
| (1,793)  | 1:67:A:GLU:H    | 1:81:A:THR:HG21 | 5                   | 0.15     | 0.04                | 0.15       |
| (1,793)  | 1:67:A:GLU:H    | 1:81:A:THR:HG22 | 5                   | 0.15     | 0.04                | 0.15       |
| (1,793)  | 1:67:A:GLU:H    | 1:81:A:THR:HG23 | 5                   | 0.15     | 0.04                | 0.15       |
| (1,376)  | 1:65:A:LEU:H    | 1:66:A:ARG:HG2  | 5                   | 0.14     | 0.04                | 0.11       |
| (1,1293) | 1:68:A:ILE:HD11 | 1:79:A:PHE:HD2  | 5                   | 0.12     | 0.02                | 0.11       |
| (1,1293) | 1:68:A:ILE:HD12 | 1:79:A:PHE:HD2  | 5                   | 0.12     | 0.02                | 0.11       |
| (1,1293) | 1:68:A:ILE:HD13 | 1:79:A:PHE:HD2  | 5                   | 0.12     | 0.02                | 0.11       |
| (1,2335) | 1:41:A:LEU:HB3  | 1:45:A:ARG:HB2  | 4                   | 0.14     | 0.02                | 0.14       |

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| Key      | Atom-1          | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,2335) | 1:41:A:LEU:HB3  | 1:45:A:ARG:HB3   | 4                   | 0.14     | 0.02                | 0.14       |
| (1,1420) | 1:82:A:LEU:HB2  | 1:84:A:GLU:HG3   | 4                   | 0.14     | 0.04                | 0.12       |
| (1,1420) | 1:82:A:LEU:HB3  | 1:84:A:GLU:HG3   | 4                   | 0.14     | 0.04                | 0.12       |
| (1,928)  | 1:52:A:ASP:H    | 1:58:A:TYR:HE1   | 4                   | 0.13     | 0.02                | 0.13       |
| (1,1671) | 1:71:A:SER:HA   | 1:77:A:VAL:HG11  | 4                   | 0.12     | 0.01                | 0.12       |
| (1,1671) | 1:71:A:SER:HA   | 1:77:A:VAL:HG12  | 4                   | 0.12     | 0.01                | 0.12       |
| (1,1671) | 1:71:A:SER:HA   | 1:77:A:VAL:HG13  | 4                   | 0.12     | 0.01                | 0.12       |
| (1,456)  | 1:25:A:LEU:H    | 1:88:A:LEU:HG    | 4                   | 0.12     | 0.02                | 0.12       |
| (1,1996) | 1:78:A:TYR:HA   | 1:79:A:PHE:HD2   | 4                   | 0.12     | 0.01                | 0.11       |
| (1,2057) | 1:25:A:LEU:HD11 | 1:88:A:LEU:H     | 4                   | 0.12     | 0.01                | 0.12       |
| (1,2057) | 1:25:A:LEU:HD12 | 1:88:A:LEU:H     | 4                   | 0.12     | 0.01                | 0.12       |
| (1,2057) | 1:25:A:LEU:HD13 | 1:88:A:LEU:H     | 4                   | 0.12     | 0.01                | 0.12       |
| (1,2619) | 1:55:A:GLN:HG2  | 1:101:A:TRP:HE1  | 3                   | 0.2      | 0.06                | 0.24       |
| (1,2619) | 1:55:A:GLN:HG3  | 1:101:A:TRP:HE1  | 3                   | 0.2      | 0.06                | 0.24       |
| (1,2456) | 1:8:A:LEU:HB2   | 1:9:A:GLU:H      | 3                   | 0.17     | 0.04                | 0.17       |
| (1,2456) | 1:8:A:LEU:HB3   | 1:9:A:GLU:H      | 3                   | 0.17     | 0.04                | 0.17       |
| (1,930)  | 1:105:A:HIS:H   | 1:106:A:PRO:HB3  | 3                   | 0.16     | 0.03                | 0.17       |
| (1,1236) | 1:100:A:LYS:HA  | 1:100:A:LYS:HE2  | 3                   | 0.16     | 0.01                | 0.15       |
| (1,1236) | 1:100:A:LYS:HA  | 1:100:A:LYS:HE3  | 3                   | 0.16     | 0.01                | 0.15       |
| (2,51)   | 1:78:A:TYR:O    | 1:69:A:GLU:H     | 3                   | 0.15     | 0.03                | 0.15       |
| (1,1553) | 1:65:A:LEU:HD21 | 1:79:A:PHE:HE1   | 3                   | 0.14     | 0.0                 | 0.14       |
| (1,1553) | 1:65:A:LEU:HD22 | 1:79:A:PHE:HE1   | 3                   | 0.14     | 0.0                 | 0.14       |
| (1,1553) | 1:65:A:LEU:HD23 | 1:79:A:PHE:HE1   | 3                   | 0.14     | 0.0                 | 0.14       |
| (1,2079) | 1:53:A:ASP:HB3  | 1:107:A:LEU:HD21 | 3                   | 0.14     | 0.01                | 0.15       |
| (1,2079) | 1:53:A:ASP:HB3  | 1:107:A:LEU:HD22 | 3                   | 0.14     | 0.01                | 0.15       |
| (1,2079) | 1:53:A:ASP:HB3  | 1:107:A:LEU:HD23 | 3                   | 0.14     | 0.01                | 0.15       |
| (1,1277) | 1:67:A:GLU:HG2  | 1:68:A:ILE:HA    | 3                   | 0.14     | 0.01                | 0.13       |
| (1,1277) | 1:67:A:GLU:HG3  | 1:68:A:ILE:HA    | 3                   | 0.14     | 0.01                | 0.13       |
| (1,868)  | 1:55:A:GLN:H    | 1:58:A:TYR:HB2   | 3                   | 0.13     | 0.04                | 0.11       |
| (1,1434) | 1:65:A:LEU:HG   | 1:82:A:LEU:HD11  | 3                   | 0.13     | 0.02                | 0.12       |
| (1,1434) | 1:65:A:LEU:HG   | 1:82:A:LEU:HD12  | 3                   | 0.13     | 0.02                | 0.12       |
| (1,1434) | 1:65:A:LEU:HG   | 1:82:A:LEU:HD13  | 3                   | 0.13     | 0.02                | 0.12       |
| (1,2267) | 1:43:A:ASN:HD21 | 1:45:A:ARG:HD3   | 3                   | 0.13     | 0.01                | 0.14       |
| (1,2606) | 1:52:A:ASP:HB2  | 1:59:A:GLY:H     | 3                   | 0.13     | 0.01                | 0.13       |
| (1,2606) | 1:52:A:ASP:HB3  | 1:59:A:GLY:H     | 3                   | 0.13     | 0.01                | 0.13       |
| (1,2320) | 1:25:A:LEU:HB3  | 1:70:A:ILE:HG12  | 3                   | 0.13     | 0.01                | 0.13       |
| (1,1903) | 1:15:A:MET:HE1  | 1:75:A:LEU:HD21  | 3                   | 0.12     | 0.0                 | 0.12       |
| (1,1903) | 1:15:A:MET:HE1  | 1:75:A:LEU:HD22  | 3                   | 0.12     | 0.0                 | 0.12       |
| (1,1903) | 1:15:A:MET:HE1  | 1:75:A:LEU:HD23  | 3                   | 0.12     | 0.0                 | 0.12       |
| (1,1903) | 1:15:A:MET:HE2  | 1:75:A:LEU:HD21  | 3                   | 0.12     | 0.0                 | 0.12       |
| (1,1903) | 1:15:A:MET:HE2  | 1:75:A:LEU:HD22  | 3                   | 0.12     | 0.0                 | 0.12       |
| (1,1903) | 1:15:A:MET:HE2  | 1:75:A:LEU:HD23  | 3                   | 0.12     | 0.0                 | 0.12       |

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| Key      | Atom-1          | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,1903) | 1:15:A:MET:HE3  | 1:75:A:LEU:HD21  | 3                   | 0.12     | 0.0                 | 0.12       |
| (1,1903) | 1:15:A:MET:HE3  | 1:75:A:LEU:HD22  | 3                   | 0.12     | 0.0                 | 0.12       |
| (1,1903) | 1:15:A:MET:HE3  | 1:75:A:LEU:HD23  | 3                   | 0.12     | 0.0                 | 0.12       |
| (1,2194) | 1:61:A:THR:HG21 | 1:62:A:PRO:HG2   | 3                   | 0.11     | 0.01                | 0.11       |
| (1,2194) | 1:61:A:THR:HG22 | 1:62:A:PRO:HG2   | 3                   | 0.11     | 0.01                | 0.11       |
| (1,2194) | 1:61:A:THR:HG23 | 1:62:A:PRO:HG2   | 3                   | 0.11     | 0.01                | 0.11       |
| (1,943)  | 1:23:A:SER:HB2  | 1:43:A:ASN:HD21  | 2                   | 0.18     | 0.01                | 0.18       |
| (1,1572) | 1:8:A:LEU:HD11  | 1:10:A:ALA:HA    | 2                   | 0.18     | 0.01                | 0.18       |
| (1,1572) | 1:8:A:LEU:HD12  | 1:10:A:ALA:HA    | 2                   | 0.18     | 0.01                | 0.18       |
| (1,1572) | 1:8:A:LEU:HD13  | 1:10:A:ALA:HA    | 2                   | 0.18     | 0.01                | 0.18       |
| (1,1312) | 1:7:A:GLU:HG2   | 1:8:A:LEU:HG     | 2                   | 0.17     | 0.01                | 0.17       |
| (1,1312) | 1:7:A:GLU:HG3   | 1:8:A:LEU:HG     | 2                   | 0.17     | 0.01                | 0.17       |
| (1,2078) | 1:53:A:ASP:HB2  | 1:107:A:LEU:HD21 | 2                   | 0.17     | 0.02                | 0.17       |
| (1,2078) | 1:53:A:ASP:HB2  | 1:107:A:LEU:HD22 | 2                   | 0.17     | 0.02                | 0.17       |
| (1,2078) | 1:53:A:ASP:HB2  | 1:107:A:LEU:HD23 | 2                   | 0.17     | 0.02                | 0.17       |
| (1,1500) | 1:36:A:VAL:HG21 | 1:48:A:LYS:HD2   | 2                   | 0.16     | 0.02                | 0.16       |
| (1,1500) | 1:36:A:VAL:HG21 | 1:48:A:LYS:HD3   | 2                   | 0.16     | 0.02                | 0.16       |
| (1,1500) | 1:36:A:VAL:HG22 | 1:48:A:LYS:HD2   | 2                   | 0.16     | 0.02                | 0.16       |
| (1,1500) | 1:36:A:VAL:HG22 | 1:48:A:LYS:HD3   | 2                   | 0.16     | 0.02                | 0.16       |
| (1,1500) | 1:36:A:VAL:HG23 | 1:48:A:LYS:HD2   | 2                   | 0.16     | 0.02                | 0.16       |
| (1,1500) | 1:36:A:VAL:HG23 | 1:48:A:LYS:HD3   | 2                   | 0.16     | 0.02                | 0.16       |
| (1,1489) | 1:39:A:PHE:HE2  | 1:48:A:LYS:HA    | 2                   | 0.16     | 0.0                 | 0.16       |
| (1,2576) | 1:45:A:ARG:HD2  | 1:47:A:LEU:HG    | 2                   | 0.15     | 0.01                | 0.15       |
| (1,2576) | 1:45:A:ARG:HD3  | 1:47:A:LEU:HG    | 2                   | 0.15     | 0.01                | 0.15       |
| (1,918)  | 1:65:A:LEU:H    | 1:66:A:ARG:HG3   | 2                   | 0.15     | 0.0                 | 0.15       |
| (1,1599) | 1:54:A:LEU:HD21 | 1:96:A:ARG:HD2   | 2                   | 0.15     | 0.0                 | 0.15       |
| (1,1599) | 1:54:A:LEU:HD22 | 1:96:A:ARG:HD2   | 2                   | 0.15     | 0.0                 | 0.15       |
| (1,1599) | 1:54:A:LEU:HD23 | 1:96:A:ARG:HD2   | 2                   | 0.15     | 0.0                 | 0.15       |
| (2,14)   | 1:16:A:GLU:O    | 1:20:A:ARG:N     | 2                   | 0.14     | 0.0                 | 0.14       |
| (1,1416) | 1:7:A:GLU:HG2   | 1:8:A:LEU:HD21   | 2                   | 0.14     | 0.02                | 0.14       |
| (1,1416) | 1:7:A:GLU:HG2   | 1:8:A:LEU:HD22   | 2                   | 0.14     | 0.02                | 0.14       |
| (1,1416) | 1:7:A:GLU:HG2   | 1:8:A:LEU:HD23   | 2                   | 0.14     | 0.02                | 0.14       |
| (1,1416) | 1:7:A:GLU:HG3   | 1:8:A:LEU:HD21   | 2                   | 0.14     | 0.02                | 0.14       |
| (1,1416) | 1:7:A:GLU:HG3   | 1:8:A:LEU:HD22   | 2                   | 0.14     | 0.02                | 0.14       |
| (1,1416) | 1:7:A:GLU:HG3   | 1:8:A:LEU:HD23   | 2                   | 0.14     | 0.02                | 0.14       |
| (1,1726) | 1:11:A:ALA:HA   | 1:15:A:MET:HE1   | 2                   | 0.13     | 0.02                | 0.13       |
| (1,1726) | 1:11:A:ALA:HA   | 1:15:A:MET:HE2   | 2                   | 0.13     | 0.02                | 0.13       |
| (1,1726) | 1:11:A:ALA:HA   | 1:15:A:MET:HE3   | 2                   | 0.13     | 0.02                | 0.13       |
| (1,2229) | 1:39:A:PHE:HD2  | 1:47:A:LEU:HD21  | 2                   | 0.13     | 0.01                | 0.13       |
| (1,2229) | 1:39:A:PHE:HD2  | 1:47:A:LEU:HD22  | 2                   | 0.13     | 0.01                | 0.13       |
| (1,2229) | 1:39:A:PHE:HD2  | 1:47:A:LEU:HD23  | 2                   | 0.13     | 0.01                | 0.13       |
| (1,1894) | 1:84:A:GLU:HB3  | 1:86:A:VAL:HG21  | 2                   | 0.12     | 0.01                | 0.12       |

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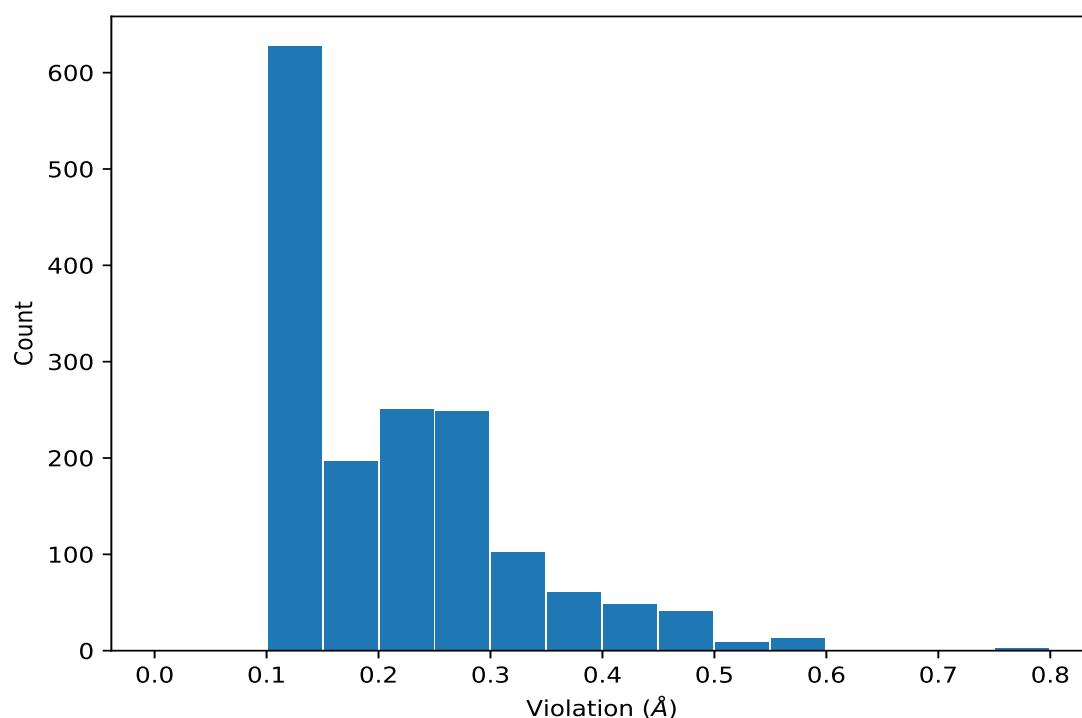
| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1894) | 1:84:A:GLU:HB3  | 1:86:A:VAL:HG22 | 2                   | 0.12     | 0.01                | 0.12       |
| (1,1894) | 1:84:A:GLU:HB3  | 1:86:A:VAL:HG23 | 2                   | 0.12     | 0.01                | 0.12       |
| (1,443)  | 1:24:A:THR:H    | 1:41:A:LEU:HB3  | 2                   | 0.12     | 0.01                | 0.12       |
| (1,1444) | 1:79:A:PHE:HD1  | 1:82:A:LEU:HD11 | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,1444) | 1:79:A:PHE:HD1  | 1:82:A:LEU:HD12 | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,1444) | 1:79:A:PHE:HD1  | 1:82:A:LEU:HD13 | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,1756) | 1:38:A:VAL:HG11 | 1:39:A:PHE:HD2  | 2                   | 0.12     | 0.01                | 0.12       |
| (1,1756) | 1:38:A:VAL:HG12 | 1:39:A:PHE:HD2  | 2                   | 0.12     | 0.01                | 0.12       |
| (1,1756) | 1:38:A:VAL:HG13 | 1:39:A:PHE:HD2  | 2                   | 0.12     | 0.01                | 0.12       |
| (1,2216) | 1:47:A:LEU:HD11 | 1:92:A:LEU:HB2  | 2                   | 0.12     | 0.01                | 0.12       |
| (1,2216) | 1:47:A:LEU:HD12 | 1:92:A:LEU:HB2  | 2                   | 0.12     | 0.01                | 0.12       |
| (1,2216) | 1:47:A:LEU:HD13 | 1:92:A:LEU:HB2  | 2                   | 0.12     | 0.01                | 0.12       |
| (2,5)    | 1:12:A:SER:O    | 1:16:A:GLU:H    | 2                   | 0.12     | 0.02                | 0.12       |
| (1,521)  | 1:18:A:LEU:HD21 | 1:21:A:GLU:H    | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,521)  | 1:18:A:LEU:HD22 | 1:21:A:GLU:H    | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,521)  | 1:18:A:LEU:HD23 | 1:21:A:GLU:H    | 2                   | 0.12     | 0.0                 | 0.12       |
| (2,55)   | 1:79:A:PHE:O    | 1:84:A:GLU:H    | 2                   | 0.11     | 0.0                 | 0.11       |

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

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

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

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



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

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

| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2011) | 1:56:A:ALA:HB1  | 1:79:A:PHE:HE1  | 16       | 0.77          |
| (1,2011) | 1:56:A:ALA:HB2  | 1:79:A:PHE:HE1  | 16       | 0.77          |
| (1,2011) | 1:56:A:ALA:HB3  | 1:79:A:PHE:HE1  | 16       | 0.77          |
| (1,2011) | 1:56:A:ALA:HB1  | 1:79:A:PHE:HE1  | 9        | 0.58          |
| (1,2011) | 1:56:A:ALA:HB2  | 1:79:A:PHE:HE1  | 9        | 0.58          |
| (1,2011) | 1:56:A:ALA:HB3  | 1:79:A:PHE:HE1  | 9        | 0.58          |
| (1,1424) | 1:79:A:PHE:HD1  | 1:82:A:LEU:HD21 | 14       | 0.58          |
| (1,1424) | 1:79:A:PHE:HD1  | 1:82:A:LEU:HD22 | 14       | 0.58          |
| (1,1424) | 1:79:A:PHE:HD1  | 1:82:A:LEU:HD23 | 14       | 0.58          |
| (1,1300) | 1:68:A:ILE:HG13 | 1:79:A:PHE:HE2  | 11       | 0.58          |
| (1,2011) | 1:56:A:ALA:HB1  | 1:79:A:PHE:HE1  | 10       | 0.55          |
| (1,2011) | 1:56:A:ALA:HB2  | 1:79:A:PHE:HE1  | 10       | 0.55          |
| (1,2011) | 1:56:A:ALA:HB3  | 1:79:A:PHE:HE1  | 10       | 0.55          |
| (1,2011) | 1:56:A:ALA:HB1  | 1:79:A:PHE:HE1  | 20       | 0.55          |
| (1,2011) | 1:56:A:ALA:HB2  | 1:79:A:PHE:HE1  | 20       | 0.55          |
| (1,2011) | 1:56:A:ALA:HB3  | 1:79:A:PHE:HE1  | 20       | 0.55          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2011) | 1:56:A:ALA:HB1  | 1:79:A:PHE:HE1  | 13       | 0.54          |
| (1,2011) | 1:56:A:ALA:HB2  | 1:79:A:PHE:HE1  | 13       | 0.54          |
| (1,2011) | 1:56:A:ALA:HB3  | 1:79:A:PHE:HE1  | 13       | 0.54          |
| (1,2011) | 1:56:A:ALA:HB1  | 1:79:A:PHE:HE1  | 17       | 0.52          |
| (1,2011) | 1:56:A:ALA:HB2  | 1:79:A:PHE:HE1  | 17       | 0.52          |
| (1,2011) | 1:56:A:ALA:HB3  | 1:79:A:PHE:HE1  | 17       | 0.52          |
| (1,2011) | 1:56:A:ALA:HB1  | 1:79:A:PHE:HE1  | 7        | 0.5           |
| (1,2011) | 1:56:A:ALA:HB2  | 1:79:A:PHE:HE1  | 7        | 0.5           |
| (1,2011) | 1:56:A:ALA:HB3  | 1:79:A:PHE:HE1  | 7        | 0.5           |
| (1,2011) | 1:56:A:ALA:HB1  | 1:79:A:PHE:HE1  | 3        | 0.49          |
| (1,2011) | 1:56:A:ALA:HB2  | 1:79:A:PHE:HE1  | 3        | 0.49          |
| (1,2011) | 1:56:A:ALA:HB3  | 1:79:A:PHE:HE1  | 3        | 0.49          |
| (1,2011) | 1:56:A:ALA:HB1  | 1:79:A:PHE:HE1  | 11       | 0.48          |
| (1,2011) | 1:56:A:ALA:HB2  | 1:79:A:PHE:HE1  | 11       | 0.48          |
| (1,2011) | 1:56:A:ALA:HB3  | 1:79:A:PHE:HE1  | 11       | 0.48          |
| (1,2011) | 1:56:A:ALA:HB1  | 1:79:A:PHE:HE1  | 12       | 0.48          |
| (1,2011) | 1:56:A:ALA:HB2  | 1:79:A:PHE:HE1  | 12       | 0.48          |
| (1,2011) | 1:56:A:ALA:HB3  | 1:79:A:PHE:HE1  | 12       | 0.48          |
| (1,1300) | 1:68:A:ILE:HG13 | 1:79:A:PHE:HE2  | 5        | 0.48          |
| (1,2011) | 1:56:A:ALA:HB1  | 1:79:A:PHE:HE1  | 2        | 0.47          |
| (1,2011) | 1:56:A:ALA:HB2  | 1:79:A:PHE:HE1  | 2        | 0.47          |
| (1,2011) | 1:56:A:ALA:HB3  | 1:79:A:PHE:HE1  | 2        | 0.47          |
| (1,1424) | 1:79:A:PHE:HD1  | 1:82:A:LEU:HD21 | 3        | 0.47          |
| (1,1424) | 1:79:A:PHE:HD1  | 1:82:A:LEU:HD22 | 3        | 0.47          |
| (1,1424) | 1:79:A:PHE:HD1  | 1:82:A:LEU:HD23 | 3        | 0.47          |
| (1,1300) | 1:68:A:ILE:HG13 | 1:79:A:PHE:HE2  | 19       | 0.47          |
| (1,2118) | 1:57:A:THR:HG21 | 1:79:A:PHE:HD1  | 5        | 0.46          |
| (1,2118) | 1:57:A:THR:HG22 | 1:79:A:PHE:HD1  | 5        | 0.46          |
| (1,2118) | 1:57:A:THR:HG23 | 1:79:A:PHE:HD1  | 5        | 0.46          |
| (1,2118) | 1:57:A:THR:HG21 | 1:79:A:PHE:HD1  | 6        | 0.46          |
| (1,2118) | 1:57:A:THR:HG22 | 1:79:A:PHE:HD1  | 6        | 0.46          |
| (1,2118) | 1:57:A:THR:HG23 | 1:79:A:PHE:HD1  | 6        | 0.46          |
| (1,2011) | 1:56:A:ALA:HB1  | 1:79:A:PHE:HE1  | 15       | 0.46          |
| (1,2011) | 1:56:A:ALA:HB2  | 1:79:A:PHE:HE1  | 15       | 0.46          |
| (1,2011) | 1:56:A:ALA:HB3  | 1:79:A:PHE:HE1  | 15       | 0.46          |
| (1,2011) | 1:56:A:ALA:HB1  | 1:79:A:PHE:HE1  | 18       | 0.46          |
| (1,2011) | 1:56:A:ALA:HB2  | 1:79:A:PHE:HE1  | 18       | 0.46          |
| (1,2011) | 1:56:A:ALA:HB3  | 1:79:A:PHE:HE1  | 18       | 0.46          |
| (1,2011) | 1:56:A:ALA:HB1  | 1:79:A:PHE:HE1  | 19       | 0.46          |
| (1,2011) | 1:56:A:ALA:HB2  | 1:79:A:PHE:HE1  | 19       | 0.46          |
| (1,2011) | 1:56:A:ALA:HB3  | 1:79:A:PHE:HE1  | 19       | 0.46          |
| (1,1424) | 1:79:A:PHE:HD1  | 1:82:A:LEU:HD21 | 15       | 0.46          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1424) | 1:79:A:PHE:HD1  | 1:82:A:LEU:HD22 | 15       | 0.46          |
| (1,1424) | 1:79:A:PHE:HD1  | 1:82:A:LEU:HD23 | 15       | 0.46          |
| (1,1300) | 1:68:A:ILE:HG13 | 1:79:A:PHE:HE2  | 14       | 0.46          |
| (1,2011) | 1:56:A:ALA:HB1  | 1:79:A:PHE:HE1  | 1        | 0.45          |
| (1,2011) | 1:56:A:ALA:HB2  | 1:79:A:PHE:HE1  | 1        | 0.45          |
| (1,2011) | 1:56:A:ALA:HB3  | 1:79:A:PHE:HE1  | 1        | 0.45          |
| (1,1300) | 1:68:A:ILE:HG13 | 1:79:A:PHE:HE2  | 9        | 0.45          |
| (1,1300) | 1:68:A:ILE:HG13 | 1:79:A:PHE:HE2  | 16       | 0.45          |
| (1,2011) | 1:56:A:ALA:HB1  | 1:79:A:PHE:HE1  | 4        | 0.44          |
| (1,2011) | 1:56:A:ALA:HB2  | 1:79:A:PHE:HE1  | 4        | 0.44          |
| (1,2011) | 1:56:A:ALA:HB3  | 1:79:A:PHE:HE1  | 4        | 0.44          |
| (1,2011) | 1:56:A:ALA:HB1  | 1:79:A:PHE:HE1  | 8        | 0.44          |
| (1,2011) | 1:56:A:ALA:HB2  | 1:79:A:PHE:HE1  | 8        | 0.44          |
| (1,2011) | 1:56:A:ALA:HB3  | 1:79:A:PHE:HE1  | 8        | 0.44          |
| (1,1530) | 1:65:A:LEU:HA   | 1:79:A:PHE:HE1  | 16       | 0.44          |
| (1,1424) | 1:79:A:PHE:HD1  | 1:82:A:LEU:HD21 | 9        | 0.44          |
| (1,1424) | 1:79:A:PHE:HD1  | 1:82:A:LEU:HD22 | 9        | 0.44          |
| (1,1424) | 1:79:A:PHE:HD1  | 1:82:A:LEU:HD23 | 9        | 0.44          |
| (1,1281) | 1:68:A:ILE:HG21 | 1:79:A:PHE:HD2  | 3        | 0.44          |
| (1,1281) | 1:68:A:ILE:HG22 | 1:79:A:PHE:HD2  | 3        | 0.44          |
| (1,1281) | 1:68:A:ILE:HG23 | 1:79:A:PHE:HD2  | 3        | 0.44          |
| (1,2011) | 1:56:A:ALA:HB1  | 1:79:A:PHE:HE1  | 14       | 0.43          |
| (1,2011) | 1:56:A:ALA:HB2  | 1:79:A:PHE:HE1  | 14       | 0.43          |
| (1,2011) | 1:56:A:ALA:HB3  | 1:79:A:PHE:HE1  | 14       | 0.43          |
| (1,1300) | 1:68:A:ILE:HG13 | 1:79:A:PHE:HE2  | 4        | 0.43          |
| (1,1300) | 1:68:A:ILE:HG13 | 1:79:A:PHE:HE2  | 15       | 0.43          |
| (1,911)  | 1:79:A:PHE:HD2  | 1:80:A:GLU:H    | 1        | 0.43          |
| (1,2009) | 1:56:A:ALA:HB1  | 1:79:A:PHE:HD1  | 16       | 0.42          |
| (1,2009) | 1:56:A:ALA:HB2  | 1:79:A:PHE:HD1  | 16       | 0.42          |
| (1,2009) | 1:56:A:ALA:HB3  | 1:79:A:PHE:HD1  | 16       | 0.42          |
| (1,1876) | 1:56:A:ALA:HB1  | 1:86:A:VAL:HG11 | 6        | 0.42          |
| (1,1876) | 1:56:A:ALA:HB1  | 1:86:A:VAL:HG12 | 6        | 0.42          |
| (1,1876) | 1:56:A:ALA:HB1  | 1:86:A:VAL:HG13 | 6        | 0.42          |
| (1,1876) | 1:56:A:ALA:HB2  | 1:86:A:VAL:HG11 | 6        | 0.42          |
| (1,1876) | 1:56:A:ALA:HB2  | 1:86:A:VAL:HG12 | 6        | 0.42          |
| (1,1876) | 1:56:A:ALA:HB2  | 1:86:A:VAL:HG13 | 6        | 0.42          |
| (1,1876) | 1:56:A:ALA:HB3  | 1:86:A:VAL:HG11 | 6        | 0.42          |
| (1,1876) | 1:56:A:ALA:HB3  | 1:86:A:VAL:HG12 | 6        | 0.42          |
| (1,1876) | 1:56:A:ALA:HB3  | 1:86:A:VAL:HG13 | 6        | 0.42          |
| (1,1530) | 1:65:A:LEU:HA   | 1:79:A:PHE:HE1  | 11       | 0.42          |
| (1,1300) | 1:68:A:ILE:HG13 | 1:79:A:PHE:HE2  | 10       | 0.42          |
| (1,1300) | 1:68:A:ILE:HG13 | 1:79:A:PHE:HE2  | 13       | 0.42          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1300) | 1:68:A:ILE:HG13 | 1:79:A:PHE:HE2  | 20       | 0.42          |
| (1,911)  | 1:79:A:PHE:HD2  | 1:80:A:GLU:H    | 13       | 0.42          |
| (1,1300) | 1:68:A:ILE:HG13 | 1:79:A:PHE:HE2  | 7        | 0.41          |
| (1,1281) | 1:68:A:ILE:HG21 | 1:79:A:PHE:HD2  | 2        | 0.41          |
| (1,1281) | 1:68:A:ILE:HG22 | 1:79:A:PHE:HD2  | 2        | 0.41          |
| (1,1281) | 1:68:A:ILE:HG23 | 1:79:A:PHE:HD2  | 2        | 0.41          |
| (1,911)  | 1:79:A:PHE:HD2  | 1:80:A:GLU:H    | 8        | 0.41          |
| (1,911)  | 1:79:A:PHE:HD2  | 1:80:A:GLU:H    | 12       | 0.41          |
| (1,911)  | 1:79:A:PHE:HD2  | 1:80:A:GLU:H    | 17       | 0.41          |
| (1,911)  | 1:79:A:PHE:HD2  | 1:80:A:GLU:H    | 20       | 0.41          |
| (1,1300) | 1:68:A:ILE:HG13 | 1:79:A:PHE:HE2  | 8        | 0.4           |
| (1,1281) | 1:68:A:ILE:HG21 | 1:79:A:PHE:HD2  | 10       | 0.4           |
| (1,1281) | 1:68:A:ILE:HG22 | 1:79:A:PHE:HD2  | 10       | 0.4           |
| (1,1281) | 1:68:A:ILE:HG23 | 1:79:A:PHE:HD2  | 10       | 0.4           |
| (1,1530) | 1:65:A:LEU:HA   | 1:79:A:PHE:HE1  | 4        | 0.39          |
| (1,1300) | 1:68:A:ILE:HG13 | 1:79:A:PHE:HE2  | 1        | 0.39          |
| (1,1300) | 1:68:A:ILE:HG13 | 1:79:A:PHE:HE2  | 17       | 0.39          |
| (1,1281) | 1:68:A:ILE:HG21 | 1:79:A:PHE:HD2  | 18       | 0.39          |
| (1,1281) | 1:68:A:ILE:HG22 | 1:79:A:PHE:HD2  | 18       | 0.39          |
| (1,1281) | 1:68:A:ILE:HG23 | 1:79:A:PHE:HD2  | 18       | 0.39          |
| (1,1641) | 1:77:A:VAL:HB   | 1:79:A:PHE:HE2  | 5        | 0.38          |
| (1,1641) | 1:77:A:VAL:HB   | 1:79:A:PHE:HE2  | 10       | 0.38          |
| (1,1424) | 1:79:A:PHE:HD1  | 1:82:A:LEU:HD21 | 1        | 0.38          |
| (1,1424) | 1:79:A:PHE:HD1  | 1:82:A:LEU:HD22 | 1        | 0.38          |
| (1,1424) | 1:79:A:PHE:HD1  | 1:82:A:LEU:HD23 | 1        | 0.38          |
| (1,1424) | 1:79:A:PHE:HD1  | 1:82:A:LEU:HD21 | 12       | 0.38          |
| (1,1424) | 1:79:A:PHE:HD1  | 1:82:A:LEU:HD22 | 12       | 0.38          |
| (1,1424) | 1:79:A:PHE:HD1  | 1:82:A:LEU:HD23 | 12       | 0.38          |
| (1,1300) | 1:68:A:ILE:HG13 | 1:79:A:PHE:HE2  | 3        | 0.38          |
| (1,1876) | 1:56:A:ALA:HB1  | 1:86:A:VAL:HG11 | 17       | 0.37          |
| (1,1876) | 1:56:A:ALA:HB1  | 1:86:A:VAL:HG12 | 17       | 0.37          |
| (1,1876) | 1:56:A:ALA:HB1  | 1:86:A:VAL:HG13 | 17       | 0.37          |
| (1,1876) | 1:56:A:ALA:HB2  | 1:86:A:VAL:HG11 | 17       | 0.37          |
| (1,1876) | 1:56:A:ALA:HB2  | 1:86:A:VAL:HG12 | 17       | 0.37          |
| (1,1876) | 1:56:A:ALA:HB2  | 1:86:A:VAL:HG13 | 17       | 0.37          |
| (1,1876) | 1:56:A:ALA:HB3  | 1:86:A:VAL:HG11 | 17       | 0.37          |
| (1,1876) | 1:56:A:ALA:HB3  | 1:86:A:VAL:HG12 | 17       | 0.37          |
| (1,1876) | 1:56:A:ALA:HB3  | 1:86:A:VAL:HG13 | 17       | 0.37          |
| (1,1641) | 1:77:A:VAL:HB   | 1:79:A:PHE:HE2  | 7        | 0.37          |
| (1,1424) | 1:79:A:PHE:HD1  | 1:82:A:LEU:HD21 | 17       | 0.37          |
| (1,1424) | 1:79:A:PHE:HD1  | 1:82:A:LEU:HD22 | 17       | 0.37          |
| (1,1424) | 1:79:A:PHE:HD1  | 1:82:A:LEU:HD23 | 17       | 0.37          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1281) | 1:68:A:ILE:HG21 | 1:79:A:PHE:HD2  | 12       | 0.37          |
| (1,1281) | 1:68:A:ILE:HG22 | 1:79:A:PHE:HD2  | 12       | 0.37          |
| (1,1281) | 1:68:A:ILE:HG23 | 1:79:A:PHE:HD2  | 12       | 0.37          |
| (1,1281) | 1:68:A:ILE:HG21 | 1:79:A:PHE:HD2  | 13       | 0.37          |
| (1,1281) | 1:68:A:ILE:HG22 | 1:79:A:PHE:HD2  | 13       | 0.37          |
| (1,1281) | 1:68:A:ILE:HG23 | 1:79:A:PHE:HD2  | 13       | 0.37          |
| (1,1281) | 1:68:A:ILE:HG21 | 1:79:A:PHE:HD2  | 19       | 0.37          |
| (1,1281) | 1:68:A:ILE:HG22 | 1:79:A:PHE:HD2  | 19       | 0.37          |
| (1,1281) | 1:68:A:ILE:HG23 | 1:79:A:PHE:HD2  | 19       | 0.37          |
| (1,1424) | 1:79:A:PHE:HD1  | 1:82:A:LEU:HD21 | 8        | 0.36          |
| (1,1424) | 1:79:A:PHE:HD1  | 1:82:A:LEU:HD22 | 8        | 0.36          |
| (1,1424) | 1:79:A:PHE:HD1  | 1:82:A:LEU:HD23 | 8        | 0.36          |
| (1,1424) | 1:79:A:PHE:HD1  | 1:82:A:LEU:HD21 | 20       | 0.36          |
| (1,1424) | 1:79:A:PHE:HD1  | 1:82:A:LEU:HD22 | 20       | 0.36          |
| (1,1424) | 1:79:A:PHE:HD1  | 1:82:A:LEU:HD23 | 20       | 0.36          |
| (1,1300) | 1:68:A:ILE:HG13 | 1:79:A:PHE:HE2  | 6        | 0.36          |
| (1,1281) | 1:68:A:ILE:HG21 | 1:79:A:PHE:HD2  | 6        | 0.36          |
| (1,1281) | 1:68:A:ILE:HG22 | 1:79:A:PHE:HD2  | 6        | 0.36          |
| (1,1281) | 1:68:A:ILE:HG23 | 1:79:A:PHE:HD2  | 6        | 0.36          |
| (1,1281) | 1:68:A:ILE:HG21 | 1:79:A:PHE:HD2  | 8        | 0.36          |
| (1,1281) | 1:68:A:ILE:HG22 | 1:79:A:PHE:HD2  | 8        | 0.36          |
| (1,1281) | 1:68:A:ILE:HG23 | 1:79:A:PHE:HD2  | 8        | 0.36          |
| (1,1281) | 1:68:A:ILE:HG21 | 1:79:A:PHE:HD2  | 15       | 0.36          |
| (1,1281) | 1:68:A:ILE:HG22 | 1:79:A:PHE:HD2  | 15       | 0.36          |
| (1,1281) | 1:68:A:ILE:HG23 | 1:79:A:PHE:HD2  | 15       | 0.36          |
| (1,1281) | 1:68:A:ILE:HG21 | 1:79:A:PHE:HD2  | 17       | 0.36          |
| (1,1281) | 1:68:A:ILE:HG22 | 1:79:A:PHE:HD2  | 17       | 0.36          |
| (1,1281) | 1:68:A:ILE:HG23 | 1:79:A:PHE:HD2  | 17       | 0.36          |
| (1,1281) | 1:68:A:ILE:HG21 | 1:79:A:PHE:HD2  | 20       | 0.36          |
| (1,1281) | 1:68:A:ILE:HG22 | 1:79:A:PHE:HD2  | 20       | 0.36          |
| (1,1281) | 1:68:A:ILE:HG23 | 1:79:A:PHE:HD2  | 20       | 0.36          |
| (1,911)  | 1:79:A:PHE:HD2  | 1:80:A:GLU:H    | 6        | 0.36          |
| (1,911)  | 1:79:A:PHE:HD2  | 1:80:A:GLU:H    | 7        | 0.36          |
| (1,1641) | 1:77:A:VAL:HB   | 1:79:A:PHE:HE2  | 8        | 0.35          |
| (1,1530) | 1:65:A:LEU:HA   | 1:79:A:PHE:HE1  | 3        | 0.35          |
| (1,1530) | 1:65:A:LEU:HA   | 1:79:A:PHE:HE1  | 10       | 0.35          |
| (1,1424) | 1:79:A:PHE:HD1  | 1:82:A:LEU:HD21 | 13       | 0.35          |
| (1,1424) | 1:79:A:PHE:HD1  | 1:82:A:LEU:HD22 | 13       | 0.35          |
| (1,1424) | 1:79:A:PHE:HD1  | 1:82:A:LEU:HD23 | 13       | 0.35          |
| (1,1300) | 1:68:A:ILE:HG13 | 1:79:A:PHE:HE2  | 12       | 0.35          |
| (1,1281) | 1:68:A:ILE:HG21 | 1:79:A:PHE:HD2  | 1        | 0.35          |
| (1,1281) | 1:68:A:ILE:HG22 | 1:79:A:PHE:HD2  | 1        | 0.35          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1281) | 1:68:A:ILE:HG23 | 1:79:A:PHE:HD2  | 1        | 0.35          |
| (1,1281) | 1:68:A:ILE:HG21 | 1:79:A:PHE:HD2  | 7        | 0.35          |
| (1,1281) | 1:68:A:ILE:HG22 | 1:79:A:PHE:HD2  | 7        | 0.35          |
| (1,1281) | 1:68:A:ILE:HG23 | 1:79:A:PHE:HD2  | 7        | 0.35          |
| (1,1281) | 1:68:A:ILE:HG21 | 1:79:A:PHE:HD2  | 9        | 0.35          |
| (1,1281) | 1:68:A:ILE:HG22 | 1:79:A:PHE:HD2  | 9        | 0.35          |
| (1,1281) | 1:68:A:ILE:HG23 | 1:79:A:PHE:HD2  | 9        | 0.35          |
| (1,911)  | 1:79:A:PHE:HD2  | 1:80:A:GLU:H    | 2        | 0.35          |
| (1,1876) | 1:56:A:ALA:HB1  | 1:86:A:VAL:HG11 | 18       | 0.34          |
| (1,1876) | 1:56:A:ALA:HB1  | 1:86:A:VAL:HG12 | 18       | 0.34          |
| (1,1876) | 1:56:A:ALA:HB1  | 1:86:A:VAL:HG13 | 18       | 0.34          |
| (1,1876) | 1:56:A:ALA:HB2  | 1:86:A:VAL:HG11 | 18       | 0.34          |
| (1,1876) | 1:56:A:ALA:HB2  | 1:86:A:VAL:HG12 | 18       | 0.34          |
| (1,1876) | 1:56:A:ALA:HB2  | 1:86:A:VAL:HG13 | 18       | 0.34          |
| (1,1876) | 1:56:A:ALA:HB3  | 1:86:A:VAL:HG11 | 18       | 0.34          |
| (1,1876) | 1:56:A:ALA:HB3  | 1:86:A:VAL:HG12 | 18       | 0.34          |
| (1,1876) | 1:56:A:ALA:HB3  | 1:86:A:VAL:HG13 | 18       | 0.34          |
| (1,1871) | 1:79:A:PHE:HE1  | 1:86:A:VAL:HB   | 2        | 0.34          |
| (1,1871) | 1:79:A:PHE:HE1  | 1:86:A:VAL:HB   | 12       | 0.34          |
| (1,1641) | 1:77:A:VAL:HB   | 1:79:A:PHE:HE2  | 3        | 0.34          |
| (1,1300) | 1:68:A:ILE:HG13 | 1:79:A:PHE:HE2  | 2        | 0.34          |
| (1,1281) | 1:68:A:ILE:HG21 | 1:79:A:PHE:HD2  | 5        | 0.34          |
| (1,1281) | 1:68:A:ILE:HG22 | 1:79:A:PHE:HD2  | 5        | 0.34          |
| (1,1281) | 1:68:A:ILE:HG23 | 1:79:A:PHE:HD2  | 5        | 0.34          |
| (1,1281) | 1:68:A:ILE:HG21 | 1:79:A:PHE:HD2  | 11       | 0.34          |
| (1,1281) | 1:68:A:ILE:HG22 | 1:79:A:PHE:HD2  | 11       | 0.34          |
| (1,1281) | 1:68:A:ILE:HG23 | 1:79:A:PHE:HD2  | 11       | 0.34          |
| (1,1281) | 1:68:A:ILE:HG21 | 1:79:A:PHE:HD2  | 14       | 0.34          |
| (1,1281) | 1:68:A:ILE:HG22 | 1:79:A:PHE:HD2  | 14       | 0.34          |
| (1,1281) | 1:68:A:ILE:HG23 | 1:79:A:PHE:HD2  | 14       | 0.34          |
| (1,1281) | 1:68:A:ILE:HG21 | 1:79:A:PHE:HD2  | 16       | 0.34          |
| (1,1281) | 1:68:A:ILE:HG22 | 1:79:A:PHE:HD2  | 16       | 0.34          |
| (1,1281) | 1:68:A:ILE:HG23 | 1:79:A:PHE:HD2  | 16       | 0.34          |
| (1,1871) | 1:79:A:PHE:HE1  | 1:86:A:VAL:HB   | 8        | 0.33          |
| (1,1641) | 1:77:A:VAL:HB   | 1:79:A:PHE:HE2  | 11       | 0.33          |
| (1,1641) | 1:77:A:VAL:HB   | 1:79:A:PHE:HE2  | 19       | 0.33          |
| (1,1424) | 1:79:A:PHE:HD1  | 1:82:A:LEU:HD21 | 6        | 0.33          |
| (1,1424) | 1:79:A:PHE:HD1  | 1:82:A:LEU:HD22 | 6        | 0.33          |
| (1,1424) | 1:79:A:PHE:HD1  | 1:82:A:LEU:HD23 | 6        | 0.33          |
| (1,911)  | 1:79:A:PHE:HD2  | 1:80:A:GLU:H    | 18       | 0.33          |
| (1,1871) | 1:79:A:PHE:HE1  | 1:86:A:VAL:HB   | 6        | 0.32          |
| (1,1641) | 1:77:A:VAL:HB   | 1:79:A:PHE:HE2  | 2        | 0.32          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1641) | 1:77:A:VAL:HB   | 1:79:A:PHE:HE2  | 12       | 0.32          |
| (1,1641) | 1:77:A:VAL:HB   | 1:79:A:PHE:HE2  | 16       | 0.32          |
| (1,1641) | 1:77:A:VAL:HB   | 1:79:A:PHE:HE2  | 20       | 0.32          |
| (1,1575) | 1:67:A:GLU:HA   | 1:68:A:ILE:HD11 | 5        | 0.32          |
| (1,1575) | 1:67:A:GLU:HA   | 1:68:A:ILE:HD12 | 5        | 0.32          |
| (1,1575) | 1:67:A:GLU:HA   | 1:68:A:ILE:HD13 | 5        | 0.32          |
| (1,1530) | 1:65:A:LEU:HA   | 1:79:A:PHE:HE1  | 19       | 0.32          |
| (1,1300) | 1:68:A:ILE:HG13 | 1:79:A:PHE:HE2  | 18       | 0.32          |
| (1,1281) | 1:68:A:ILE:HG21 | 1:79:A:PHE:HD2  | 4        | 0.32          |
| (1,1281) | 1:68:A:ILE:HG22 | 1:79:A:PHE:HD2  | 4        | 0.32          |
| (1,1281) | 1:68:A:ILE:HG23 | 1:79:A:PHE:HD2  | 4        | 0.32          |
| (1,911)  | 1:79:A:PHE:HD2  | 1:80:A:GLU:H    | 3        | 0.32          |
| (1,2621) | 1:55:A:GLN:HE21 | 1:101:A:TRP:HE1 | 14       | 0.31          |
| (1,2621) | 1:55:A:GLN:HE22 | 1:101:A:TRP:HE1 | 14       | 0.31          |
| (1,2196) | 1:61:A:THR:HG21 | 1:63:A:GLU:HB2  | 10       | 0.31          |
| (1,2196) | 1:61:A:THR:HG21 | 1:63:A:GLU:HB3  | 10       | 0.31          |
| (1,2196) | 1:61:A:THR:HG22 | 1:63:A:GLU:HB2  | 10       | 0.31          |
| (1,2196) | 1:61:A:THR:HG22 | 1:63:A:GLU:HB3  | 10       | 0.31          |
| (1,2196) | 1:61:A:THR:HG23 | 1:63:A:GLU:HB2  | 10       | 0.31          |
| (1,2196) | 1:61:A:THR:HG23 | 1:63:A:GLU:HB3  | 10       | 0.31          |
| (1,2009) | 1:56:A:ALA:HB1  | 1:79:A:PHE:HD1  | 19       | 0.31          |
| (1,2009) | 1:56:A:ALA:HB2  | 1:79:A:PHE:HD1  | 19       | 0.31          |
| (1,2009) | 1:56:A:ALA:HB3  | 1:79:A:PHE:HD1  | 19       | 0.31          |
| (1,1876) | 1:56:A:ALA:HB1  | 1:86:A:VAL:HG11 | 12       | 0.31          |
| (1,1876) | 1:56:A:ALA:HB1  | 1:86:A:VAL:HG12 | 12       | 0.31          |
| (1,1876) | 1:56:A:ALA:HB1  | 1:86:A:VAL:HG13 | 12       | 0.31          |
| (1,1876) | 1:56:A:ALA:HB2  | 1:86:A:VAL:HG11 | 12       | 0.31          |
| (1,1876) | 1:56:A:ALA:HB2  | 1:86:A:VAL:HG12 | 12       | 0.31          |
| (1,1876) | 1:56:A:ALA:HB2  | 1:86:A:VAL:HG13 | 12       | 0.31          |
| (1,1876) | 1:56:A:ALA:HB3  | 1:86:A:VAL:HG11 | 12       | 0.31          |
| (1,1876) | 1:56:A:ALA:HB3  | 1:86:A:VAL:HG12 | 12       | 0.31          |
| (1,1876) | 1:56:A:ALA:HB3  | 1:86:A:VAL:HG13 | 12       | 0.31          |
| (1,1876) | 1:56:A:ALA:HB1  | 1:86:A:VAL:HG11 | 15       | 0.31          |
| (1,1876) | 1:56:A:ALA:HB1  | 1:86:A:VAL:HG12 | 15       | 0.31          |
| (1,1876) | 1:56:A:ALA:HB1  | 1:86:A:VAL:HG13 | 15       | 0.31          |
| (1,1876) | 1:56:A:ALA:HB2  | 1:86:A:VAL:HG11 | 15       | 0.31          |
| (1,1876) | 1:56:A:ALA:HB2  | 1:86:A:VAL:HG12 | 15       | 0.31          |
| (1,1876) | 1:56:A:ALA:HB2  | 1:86:A:VAL:HG13 | 15       | 0.31          |
| (1,1876) | 1:56:A:ALA:HB3  | 1:86:A:VAL:HG11 | 15       | 0.31          |
| (1,1876) | 1:56:A:ALA:HB3  | 1:86:A:VAL:HG12 | 15       | 0.31          |
| (1,1876) | 1:56:A:ALA:HB3  | 1:86:A:VAL:HG13 | 15       | 0.31          |
| (1,1871) | 1:79:A:PHE:HE1  | 1:86:A:VAL:HB   | 3        | 0.31          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1641) | 1:77:A:VAL:HB   | 1:79:A:PHE:HE2  | 18       | 0.31          |
| (1,1530) | 1:65:A:LEU:HA   | 1:79:A:PHE:HE1  | 14       | 0.31          |
| (1,1529) | 1:65:A:LEU:HA   | 1:79:A:PHE:HD2  | 13       | 0.31          |
| (1,1283) | 1:68:A:ILE:HG21 | 1:79:A:PHE:HE2  | 11       | 0.31          |
| (1,1283) | 1:68:A:ILE:HG22 | 1:79:A:PHE:HE2  | 11       | 0.31          |
| (1,1283) | 1:68:A:ILE:HG23 | 1:79:A:PHE:HE2  | 11       | 0.31          |
| (1,1283) | 1:68:A:ILE:HG21 | 1:79:A:PHE:HE2  | 15       | 0.31          |
| (1,1283) | 1:68:A:ILE:HG22 | 1:79:A:PHE:HE2  | 15       | 0.31          |
| (1,1283) | 1:68:A:ILE:HG23 | 1:79:A:PHE:HE2  | 15       | 0.31          |
| (1,2270) | 1:103:A:ALA:H   | 1:104:A:GLU:HG2 | 6        | 0.3           |
| (1,2196) | 1:61:A:THR:HG21 | 1:63:A:GLU:HB2  | 15       | 0.3           |
| (1,2196) | 1:61:A:THR:HG21 | 1:63:A:GLU:HB3  | 15       | 0.3           |
| (1,2196) | 1:61:A:THR:HG22 | 1:63:A:GLU:HB2  | 15       | 0.3           |
| (1,2196) | 1:61:A:THR:HG22 | 1:63:A:GLU:HB3  | 15       | 0.3           |
| (1,2196) | 1:61:A:THR:HG23 | 1:63:A:GLU:HB2  | 15       | 0.3           |
| (1,2196) | 1:61:A:THR:HG23 | 1:63:A:GLU:HB3  | 15       | 0.3           |
| (1,1876) | 1:56:A:ALA:HB1  | 1:86:A:VAL:HG11 | 2        | 0.3           |
| (1,1876) | 1:56:A:ALA:HB1  | 1:86:A:VAL:HG12 | 2        | 0.3           |
| (1,1876) | 1:56:A:ALA:HB1  | 1:86:A:VAL:HG13 | 2        | 0.3           |
| (1,1876) | 1:56:A:ALA:HB2  | 1:86:A:VAL:HG11 | 2        | 0.3           |
| (1,1876) | 1:56:A:ALA:HB2  | 1:86:A:VAL:HG12 | 2        | 0.3           |
| (1,1876) | 1:56:A:ALA:HB2  | 1:86:A:VAL:HG13 | 2        | 0.3           |
| (1,1876) | 1:56:A:ALA:HB3  | 1:86:A:VAL:HG11 | 2        | 0.3           |
| (1,1876) | 1:56:A:ALA:HB3  | 1:86:A:VAL:HG12 | 2        | 0.3           |
| (1,1876) | 1:56:A:ALA:HB3  | 1:86:A:VAL:HG13 | 2        | 0.3           |
| (1,1871) | 1:79:A:PHE:HE1  | 1:86:A:VAL:HB   | 14       | 0.3           |
| (1,1871) | 1:79:A:PHE:HE1  | 1:86:A:VAL:HB   | 15       | 0.3           |
| (1,1641) | 1:77:A:VAL:HB   | 1:79:A:PHE:HE2  | 1        | 0.3           |
| (1,1641) | 1:77:A:VAL:HB   | 1:79:A:PHE:HE2  | 4        | 0.3           |
| (1,1641) | 1:77:A:VAL:HB   | 1:79:A:PHE:HE2  | 9        | 0.3           |
| (1,1641) | 1:77:A:VAL:HB   | 1:79:A:PHE:HE2  | 13       | 0.3           |
| (1,1530) | 1:65:A:LEU:HA   | 1:79:A:PHE:HE1  | 1        | 0.3           |
| (1,1530) | 1:65:A:LEU:HA   | 1:79:A:PHE:HE1  | 7        | 0.3           |
| (1,2011) | 1:56:A:ALA:HB1  | 1:79:A:PHE:HE1  | 6        | 0.29          |
| (1,2011) | 1:56:A:ALA:HB2  | 1:79:A:PHE:HE1  | 6        | 0.29          |
| (1,2011) | 1:56:A:ALA:HB3  | 1:79:A:PHE:HE1  | 6        | 0.29          |
| (1,2009) | 1:56:A:ALA:HB1  | 1:79:A:PHE:HD1  | 9        | 0.29          |
| (1,2009) | 1:56:A:ALA:HB2  | 1:79:A:PHE:HD1  | 9        | 0.29          |
| (1,2009) | 1:56:A:ALA:HB3  | 1:79:A:PHE:HD1  | 9        | 0.29          |
| (1,2009) | 1:56:A:ALA:HB1  | 1:79:A:PHE:HD1  | 11       | 0.29          |
| (1,2009) | 1:56:A:ALA:HB2  | 1:79:A:PHE:HD1  | 11       | 0.29          |
| (1,2009) | 1:56:A:ALA:HB3  | 1:79:A:PHE:HD1  | 11       | 0.29          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1876) | 1:56:A:ALA:HB1  | 1:86:A:VAL:HG11 | 5        | 0.29          |
| (1,1876) | 1:56:A:ALA:HB1  | 1:86:A:VAL:HG12 | 5        | 0.29          |
| (1,1876) | 1:56:A:ALA:HB1  | 1:86:A:VAL:HG13 | 5        | 0.29          |
| (1,1876) | 1:56:A:ALA:HB2  | 1:86:A:VAL:HG11 | 5        | 0.29          |
| (1,1876) | 1:56:A:ALA:HB2  | 1:86:A:VAL:HG12 | 5        | 0.29          |
| (1,1876) | 1:56:A:ALA:HB2  | 1:86:A:VAL:HG13 | 5        | 0.29          |
| (1,1876) | 1:56:A:ALA:HB3  | 1:86:A:VAL:HG11 | 5        | 0.29          |
| (1,1876) | 1:56:A:ALA:HB3  | 1:86:A:VAL:HG12 | 5        | 0.29          |
| (1,1876) | 1:56:A:ALA:HB3  | 1:86:A:VAL:HG13 | 5        | 0.29          |
| (1,1871) | 1:79:A:PHE:HE1  | 1:86:A:VAL:HB   | 1        | 0.29          |
| (1,1871) | 1:79:A:PHE:HE1  | 1:86:A:VAL:HB   | 20       | 0.29          |
| (1,1641) | 1:77:A:VAL:HB   | 1:79:A:PHE:HE2  | 14       | 0.29          |
| (1,1641) | 1:77:A:VAL:HB   | 1:79:A:PHE:HE2  | 17       | 0.29          |
| (1,1530) | 1:65:A:LEU:HA   | 1:79:A:PHE:HE1  | 5        | 0.29          |
| (1,1530) | 1:65:A:LEU:HA   | 1:79:A:PHE:HE1  | 8        | 0.29          |
| (1,1529) | 1:65:A:LEU:HA   | 1:79:A:PHE:HD2  | 8        | 0.29          |
| (1,1283) | 1:68:A:ILE:HG21 | 1:79:A:PHE:HE2  | 5        | 0.29          |
| (1,1283) | 1:68:A:ILE:HG22 | 1:79:A:PHE:HE2  | 5        | 0.29          |
| (1,1283) | 1:68:A:ILE:HG23 | 1:79:A:PHE:HE2  | 5        | 0.29          |
| (1,1283) | 1:68:A:ILE:HG21 | 1:79:A:PHE:HE2  | 14       | 0.29          |
| (1,1283) | 1:68:A:ILE:HG22 | 1:79:A:PHE:HE2  | 14       | 0.29          |
| (1,1283) | 1:68:A:ILE:HG23 | 1:79:A:PHE:HE2  | 14       | 0.29          |
| (1,1283) | 1:68:A:ILE:HG21 | 1:79:A:PHE:HE2  | 17       | 0.29          |
| (1,1283) | 1:68:A:ILE:HG22 | 1:79:A:PHE:HE2  | 17       | 0.29          |
| (1,1283) | 1:68:A:ILE:HG23 | 1:79:A:PHE:HE2  | 17       | 0.29          |
| (1,1283) | 1:68:A:ILE:HG21 | 1:79:A:PHE:HE2  | 19       | 0.29          |
| (1,1283) | 1:68:A:ILE:HG22 | 1:79:A:PHE:HE2  | 19       | 0.29          |
| (1,1283) | 1:68:A:ILE:HG23 | 1:79:A:PHE:HE2  | 19       | 0.29          |
| (1,911)  | 1:79:A:PHE:HD2  | 1:80:A:GLU:H    | 9        | 0.29          |
| (1,2196) | 1:61:A:THR:HG21 | 1:63:A:GLU:HB2  | 14       | 0.28          |
| (1,2196) | 1:61:A:THR:HG21 | 1:63:A:GLU:HB3  | 14       | 0.28          |
| (1,2196) | 1:61:A:THR:HG22 | 1:63:A:GLU:HB2  | 14       | 0.28          |
| (1,2196) | 1:61:A:THR:HG22 | 1:63:A:GLU:HB3  | 14       | 0.28          |
| (1,2196) | 1:61:A:THR:HG23 | 1:63:A:GLU:HB2  | 14       | 0.28          |
| (1,2196) | 1:61:A:THR:HG23 | 1:63:A:GLU:HB3  | 14       | 0.28          |
| (1,2118) | 1:57:A:THR:HG21 | 1:79:A:PHE:HD1  | 10       | 0.28          |
| (1,2118) | 1:57:A:THR:HG22 | 1:79:A:PHE:HD1  | 10       | 0.28          |
| (1,2118) | 1:57:A:THR:HG23 | 1:79:A:PHE:HD1  | 10       | 0.28          |
| (1,2011) | 1:56:A:ALA:HB1  | 1:79:A:PHE:HE1  | 5        | 0.28          |
| (1,2011) | 1:56:A:ALA:HB2  | 1:79:A:PHE:HE1  | 5        | 0.28          |
| (1,2011) | 1:56:A:ALA:HB3  | 1:79:A:PHE:HE1  | 5        | 0.28          |
| (1,1876) | 1:56:A:ALA:HB1  | 1:86:A:VAL:HG11 | 4        | 0.28          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1876) | 1:56:A:ALA:HB1  | 1:86:A:VAL:HG12 | 4        | 0.28          |
| (1,1876) | 1:56:A:ALA:HB1  | 1:86:A:VAL:HG13 | 4        | 0.28          |
| (1,1876) | 1:56:A:ALA:HB2  | 1:86:A:VAL:HG11 | 4        | 0.28          |
| (1,1876) | 1:56:A:ALA:HB2  | 1:86:A:VAL:HG12 | 4        | 0.28          |
| (1,1876) | 1:56:A:ALA:HB2  | 1:86:A:VAL:HG13 | 4        | 0.28          |
| (1,1876) | 1:56:A:ALA:HB3  | 1:86:A:VAL:HG11 | 4        | 0.28          |
| (1,1876) | 1:56:A:ALA:HB3  | 1:86:A:VAL:HG12 | 4        | 0.28          |
| (1,1876) | 1:56:A:ALA:HB3  | 1:86:A:VAL:HG13 | 4        | 0.28          |
| (1,1876) | 1:56:A:ALA:HB1  | 1:86:A:VAL:HG11 | 14       | 0.28          |
| (1,1876) | 1:56:A:ALA:HB1  | 1:86:A:VAL:HG12 | 14       | 0.28          |
| (1,1876) | 1:56:A:ALA:HB1  | 1:86:A:VAL:HG13 | 14       | 0.28          |
| (1,1876) | 1:56:A:ALA:HB2  | 1:86:A:VAL:HG11 | 14       | 0.28          |
| (1,1876) | 1:56:A:ALA:HB2  | 1:86:A:VAL:HG12 | 14       | 0.28          |
| (1,1876) | 1:56:A:ALA:HB2  | 1:86:A:VAL:HG13 | 14       | 0.28          |
| (1,1876) | 1:56:A:ALA:HB3  | 1:86:A:VAL:HG11 | 14       | 0.28          |
| (1,1876) | 1:56:A:ALA:HB3  | 1:86:A:VAL:HG12 | 14       | 0.28          |
| (1,1876) | 1:56:A:ALA:HB3  | 1:86:A:VAL:HG13 | 14       | 0.28          |
| (1,1871) | 1:79:A:PHE:HE1  | 1:86:A:VAL:HB   | 9        | 0.28          |
| (1,1871) | 1:79:A:PHE:HE1  | 1:86:A:VAL:HB   | 17       | 0.28          |
| (1,1530) | 1:65:A:LEU:HA   | 1:79:A:PHE:HE1  | 12       | 0.28          |
| (1,1529) | 1:65:A:LEU:HA   | 1:79:A:PHE:HD2  | 12       | 0.28          |
| (1,1283) | 1:68:A:ILE:HG21 | 1:79:A:PHE:HE2  | 9        | 0.28          |
| (1,1283) | 1:68:A:ILE:HG22 | 1:79:A:PHE:HE2  | 9        | 0.28          |
| (1,1283) | 1:68:A:ILE:HG23 | 1:79:A:PHE:HE2  | 9        | 0.28          |
| (1,2271) | 1:9:A:GLU:HG3   | 1:10:A:ALA:HB1  | 19       | 0.27          |
| (1,2271) | 1:9:A:GLU:HG3   | 1:10:A:ALA:HB2  | 19       | 0.27          |
| (1,2271) | 1:9:A:GLU:HG3   | 1:10:A:ALA:HB3  | 19       | 0.27          |
| (1,2270) | 1:103:A:ALA:H   | 1:104:A:GLU:HG2 | 2        | 0.27          |
| (1,2270) | 1:103:A:ALA:H   | 1:104:A:GLU:HG2 | 18       | 0.27          |
| (1,2009) | 1:56:A:ALA:HB1  | 1:79:A:PHE:HD1  | 7        | 0.27          |
| (1,2009) | 1:56:A:ALA:HB2  | 1:79:A:PHE:HD1  | 7        | 0.27          |
| (1,2009) | 1:56:A:ALA:HB3  | 1:79:A:PHE:HD1  | 7        | 0.27          |
| (1,1876) | 1:56:A:ALA:HB1  | 1:86:A:VAL:HG11 | 20       | 0.27          |
| (1,1876) | 1:56:A:ALA:HB1  | 1:86:A:VAL:HG12 | 20       | 0.27          |
| (1,1876) | 1:56:A:ALA:HB1  | 1:86:A:VAL:HG13 | 20       | 0.27          |
| (1,1876) | 1:56:A:ALA:HB2  | 1:86:A:VAL:HG11 | 20       | 0.27          |
| (1,1876) | 1:56:A:ALA:HB2  | 1:86:A:VAL:HG12 | 20       | 0.27          |
| (1,1876) | 1:56:A:ALA:HB2  | 1:86:A:VAL:HG13 | 20       | 0.27          |
| (1,1876) | 1:56:A:ALA:HB3  | 1:86:A:VAL:HG11 | 20       | 0.27          |
| (1,1876) | 1:56:A:ALA:HB3  | 1:86:A:VAL:HG12 | 20       | 0.27          |
| (1,1876) | 1:56:A:ALA:HB3  | 1:86:A:VAL:HG13 | 20       | 0.27          |
| (1,1871) | 1:79:A:PHE:HE1  | 1:86:A:VAL:HB   | 4        | 0.27          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1871) | 1:79:A:PHE:HE1  | 1:86:A:VAL:HB   | 13       | 0.27          |
| (1,1871) | 1:79:A:PHE:HE1  | 1:86:A:VAL:HB   | 16       | 0.27          |
| (1,1871) | 1:79:A:PHE:HE1  | 1:86:A:VAL:HB   | 18       | 0.27          |
| (1,1641) | 1:77:A:VAL:HB   | 1:79:A:PHE:HE2  | 15       | 0.27          |
| (1,1570) | 1:8:A:LEU:HD11  | 1:9:A:GLU:HB2   | 19       | 0.27          |
| (1,1570) | 1:8:A:LEU:HD11  | 1:9:A:GLU:HB3   | 19       | 0.27          |
| (1,1570) | 1:8:A:LEU:HD12  | 1:9:A:GLU:HB2   | 19       | 0.27          |
| (1,1570) | 1:8:A:LEU:HD12  | 1:9:A:GLU:HB3   | 19       | 0.27          |
| (1,1570) | 1:8:A:LEU:HD13  | 1:9:A:GLU:HB2   | 19       | 0.27          |
| (1,1570) | 1:8:A:LEU:HD13  | 1:9:A:GLU:HB3   | 19       | 0.27          |
| (1,1530) | 1:65:A:LEU:HA   | 1:79:A:PHE:HE1  | 15       | 0.27          |
| (1,1530) | 1:65:A:LEU:HA   | 1:79:A:PHE:HE1  | 17       | 0.27          |
| (1,1424) | 1:79:A:PHE:HD1  | 1:82:A:LEU:HD21 | 2        | 0.27          |
| (1,1424) | 1:79:A:PHE:HD1  | 1:82:A:LEU:HD22 | 2        | 0.27          |
| (1,1424) | 1:79:A:PHE:HD1  | 1:82:A:LEU:HD23 | 2        | 0.27          |
| (1,2271) | 1:9:A:GLU:HG3   | 1:10:A:ALA:HB1  | 14       | 0.26          |
| (1,2271) | 1:9:A:GLU:HG3   | 1:10:A:ALA:HB2  | 14       | 0.26          |
| (1,2271) | 1:9:A:GLU:HG3   | 1:10:A:ALA:HB3  | 14       | 0.26          |
| (1,2118) | 1:57:A:THR:HG21 | 1:79:A:PHE:HD1  | 12       | 0.26          |
| (1,2118) | 1:57:A:THR:HG22 | 1:79:A:PHE:HD1  | 12       | 0.26          |
| (1,2118) | 1:57:A:THR:HG23 | 1:79:A:PHE:HD1  | 12       | 0.26          |
| (1,1876) | 1:56:A:ALA:HB1  | 1:86:A:VAL:HG11 | 9        | 0.26          |
| (1,1876) | 1:56:A:ALA:HB1  | 1:86:A:VAL:HG12 | 9        | 0.26          |
| (1,1876) | 1:56:A:ALA:HB1  | 1:86:A:VAL:HG13 | 9        | 0.26          |
| (1,1876) | 1:56:A:ALA:HB2  | 1:86:A:VAL:HG11 | 9        | 0.26          |
| (1,1876) | 1:56:A:ALA:HB2  | 1:86:A:VAL:HG12 | 9        | 0.26          |
| (1,1876) | 1:56:A:ALA:HB2  | 1:86:A:VAL:HG13 | 9        | 0.26          |
| (1,1876) | 1:56:A:ALA:HB3  | 1:86:A:VAL:HG11 | 9        | 0.26          |
| (1,1876) | 1:56:A:ALA:HB3  | 1:86:A:VAL:HG12 | 9        | 0.26          |
| (1,1876) | 1:56:A:ALA:HB3  | 1:86:A:VAL:HG13 | 9        | 0.26          |
| (1,1641) | 1:77:A:VAL:HB   | 1:79:A:PHE:HE2  | 6        | 0.26          |
| (1,1575) | 1:67:A:GLU:HA   | 1:68:A:ILE:HD11 | 11       | 0.26          |
| (1,1575) | 1:67:A:GLU:HA   | 1:68:A:ILE:HD12 | 11       | 0.26          |
| (1,1575) | 1:67:A:GLU:HA   | 1:68:A:ILE:HD13 | 11       | 0.26          |
| (1,1575) | 1:67:A:GLU:HA   | 1:68:A:ILE:HD11 | 14       | 0.26          |
| (1,1575) | 1:67:A:GLU:HA   | 1:68:A:ILE:HD12 | 14       | 0.26          |
| (1,1575) | 1:67:A:GLU:HA   | 1:68:A:ILE:HD13 | 14       | 0.26          |
| (1,1530) | 1:65:A:LEU:HA   | 1:79:A:PHE:HE1  | 9        | 0.26          |
| (1,1530) | 1:65:A:LEU:HA   | 1:79:A:PHE:HE1  | 13       | 0.26          |
| (1,1530) | 1:65:A:LEU:HA   | 1:79:A:PHE:HE1  | 20       | 0.26          |
| (1,1283) | 1:68:A:ILE:HG21 | 1:79:A:PHE:HE2  | 1        | 0.26          |
| (1,1283) | 1:68:A:ILE:HG22 | 1:79:A:PHE:HE2  | 1        | 0.26          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1283) | 1:68:A:ILE:HG23 | 1:79:A:PHE:HE2  | 1        | 0.26          |
| (1,1283) | 1:68:A:ILE:HG21 | 1:79:A:PHE:HE2  | 4        | 0.26          |
| (1,1283) | 1:68:A:ILE:HG22 | 1:79:A:PHE:HE2  | 4        | 0.26          |
| (1,1283) | 1:68:A:ILE:HG23 | 1:79:A:PHE:HE2  | 4        | 0.26          |
| (1,1283) | 1:68:A:ILE:HG21 | 1:79:A:PHE:HE2  | 6        | 0.26          |
| (1,1283) | 1:68:A:ILE:HG22 | 1:79:A:PHE:HE2  | 6        | 0.26          |
| (1,1283) | 1:68:A:ILE:HG23 | 1:79:A:PHE:HE2  | 6        | 0.26          |
| (1,1283) | 1:68:A:ILE:HG21 | 1:79:A:PHE:HE2  | 13       | 0.26          |
| (1,1283) | 1:68:A:ILE:HG22 | 1:79:A:PHE:HE2  | 13       | 0.26          |
| (1,1283) | 1:68:A:ILE:HG23 | 1:79:A:PHE:HE2  | 13       | 0.26          |
| (1,1283) | 1:68:A:ILE:HG21 | 1:79:A:PHE:HE2  | 20       | 0.26          |
| (1,1283) | 1:68:A:ILE:HG22 | 1:79:A:PHE:HE2  | 20       | 0.26          |
| (1,1283) | 1:68:A:ILE:HG23 | 1:79:A:PHE:HE2  | 20       | 0.26          |
| (1,2448) | 1:3:A:VAL:HA    | 1:4:A:SER:HB2   | 6        | 0.25          |
| (1,2448) | 1:3:A:VAL:HA    | 1:4:A:SER:HB3   | 6        | 0.25          |
| (1,2424) | 1:78:A:TYR:HE2  | 1:85:A:ASP:HB3  | 5        | 0.25          |
| (1,2270) | 1:103:A:ALA:H   | 1:104:A:GLU:HG2 | 4        | 0.25          |
| (1,2270) | 1:103:A:ALA:H   | 1:104:A:GLU:HG2 | 19       | 0.25          |
| (1,2196) | 1:61:A:THR:HG21 | 1:63:A:GLU:HB2  | 9        | 0.25          |
| (1,2196) | 1:61:A:THR:HG21 | 1:63:A:GLU:HB3  | 9        | 0.25          |
| (1,2196) | 1:61:A:THR:HG22 | 1:63:A:GLU:HB2  | 9        | 0.25          |
| (1,2196) | 1:61:A:THR:HG22 | 1:63:A:GLU:HB3  | 9        | 0.25          |
| (1,2196) | 1:61:A:THR:HG23 | 1:63:A:GLU:HB2  | 9        | 0.25          |
| (1,2196) | 1:61:A:THR:HG23 | 1:63:A:GLU:HB3  | 9        | 0.25          |
| (1,2118) | 1:57:A:THR:HG21 | 1:79:A:PHE:HD1  | 1        | 0.25          |
| (1,2118) | 1:57:A:THR:HG22 | 1:79:A:PHE:HD1  | 1        | 0.25          |
| (1,2118) | 1:57:A:THR:HG23 | 1:79:A:PHE:HD1  | 1        | 0.25          |
| (1,2118) | 1:57:A:THR:HG21 | 1:79:A:PHE:HD1  | 3        | 0.25          |
| (1,2118) | 1:57:A:THR:HG22 | 1:79:A:PHE:HD1  | 3        | 0.25          |
| (1,2118) | 1:57:A:THR:HG23 | 1:79:A:PHE:HD1  | 3        | 0.25          |
| (1,2118) | 1:57:A:THR:HG21 | 1:79:A:PHE:HD1  | 4        | 0.25          |
| (1,2118) | 1:57:A:THR:HG22 | 1:79:A:PHE:HD1  | 4        | 0.25          |
| (1,2118) | 1:57:A:THR:HG23 | 1:79:A:PHE:HD1  | 4        | 0.25          |
| (1,2118) | 1:57:A:THR:HG21 | 1:79:A:PHE:HD1  | 9        | 0.25          |
| (1,2118) | 1:57:A:THR:HG22 | 1:79:A:PHE:HD1  | 9        | 0.25          |
| (1,2118) | 1:57:A:THR:HG23 | 1:79:A:PHE:HD1  | 9        | 0.25          |
| (1,2118) | 1:57:A:THR:HG21 | 1:79:A:PHE:HD1  | 18       | 0.25          |
| (1,2118) | 1:57:A:THR:HG22 | 1:79:A:PHE:HD1  | 18       | 0.25          |
| (1,2118) | 1:57:A:THR:HG23 | 1:79:A:PHE:HD1  | 18       | 0.25          |
| (1,2009) | 1:56:A:ALA:HB1  | 1:79:A:PHE:HD1  | 3        | 0.25          |
| (1,2009) | 1:56:A:ALA:HB2  | 1:79:A:PHE:HD1  | 3        | 0.25          |
| (1,2009) | 1:56:A:ALA:HB3  | 1:79:A:PHE:HD1  | 3        | 0.25          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2009) | 1:56:A:ALA:HB1  | 1:79:A:PHE:HD1  | 10       | 0.25          |
| (1,2009) | 1:56:A:ALA:HB2  | 1:79:A:PHE:HD1  | 10       | 0.25          |
| (1,2009) | 1:56:A:ALA:HB3  | 1:79:A:PHE:HD1  | 10       | 0.25          |
| (1,1876) | 1:56:A:ALA:HB1  | 1:86:A:VAL:HG11 | 1        | 0.25          |
| (1,1876) | 1:56:A:ALA:HB1  | 1:86:A:VAL:HG12 | 1        | 0.25          |
| (1,1876) | 1:56:A:ALA:HB1  | 1:86:A:VAL:HG13 | 1        | 0.25          |
| (1,1876) | 1:56:A:ALA:HB2  | 1:86:A:VAL:HG11 | 1        | 0.25          |
| (1,1876) | 1:56:A:ALA:HB2  | 1:86:A:VAL:HG12 | 1        | 0.25          |
| (1,1876) | 1:56:A:ALA:HB2  | 1:86:A:VAL:HG13 | 1        | 0.25          |
| (1,1876) | 1:56:A:ALA:HB3  | 1:86:A:VAL:HG11 | 1        | 0.25          |
| (1,1876) | 1:56:A:ALA:HB3  | 1:86:A:VAL:HG12 | 1        | 0.25          |
| (1,1876) | 1:56:A:ALA:HB3  | 1:86:A:VAL:HG13 | 1        | 0.25          |
| (1,1876) | 1:56:A:ALA:HB1  | 1:86:A:VAL:HG11 | 8        | 0.25          |
| (1,1876) | 1:56:A:ALA:HB1  | 1:86:A:VAL:HG12 | 8        | 0.25          |
| (1,1876) | 1:56:A:ALA:HB1  | 1:86:A:VAL:HG13 | 8        | 0.25          |
| (1,1876) | 1:56:A:ALA:HB2  | 1:86:A:VAL:HG11 | 8        | 0.25          |
| (1,1876) | 1:56:A:ALA:HB2  | 1:86:A:VAL:HG12 | 8        | 0.25          |
| (1,1876) | 1:56:A:ALA:HB2  | 1:86:A:VAL:HG13 | 8        | 0.25          |
| (1,1876) | 1:56:A:ALA:HB3  | 1:86:A:VAL:HG11 | 8        | 0.25          |
| (1,1876) | 1:56:A:ALA:HB3  | 1:86:A:VAL:HG12 | 8        | 0.25          |
| (1,1876) | 1:56:A:ALA:HB3  | 1:86:A:VAL:HG13 | 8        | 0.25          |
| (1,1876) | 1:56:A:ALA:HB1  | 1:86:A:VAL:HG11 | 13       | 0.25          |
| (1,1876) | 1:56:A:ALA:HB1  | 1:86:A:VAL:HG12 | 13       | 0.25          |
| (1,1876) | 1:56:A:ALA:HB1  | 1:86:A:VAL:HG13 | 13       | 0.25          |
| (1,1876) | 1:56:A:ALA:HB2  | 1:86:A:VAL:HG11 | 13       | 0.25          |
| (1,1876) | 1:56:A:ALA:HB2  | 1:86:A:VAL:HG12 | 13       | 0.25          |
| (1,1876) | 1:56:A:ALA:HB2  | 1:86:A:VAL:HG13 | 13       | 0.25          |
| (1,1876) | 1:56:A:ALA:HB3  | 1:86:A:VAL:HG11 | 13       | 0.25          |
| (1,1876) | 1:56:A:ALA:HB3  | 1:86:A:VAL:HG12 | 13       | 0.25          |
| (1,1876) | 1:56:A:ALA:HB3  | 1:86:A:VAL:HG13 | 13       | 0.25          |
| (1,1871) | 1:79:A:PHE:HE1  | 1:86:A:VAL:HB   | 10       | 0.25          |
| (1,1871) | 1:79:A:PHE:HE1  | 1:86:A:VAL:HB   | 11       | 0.25          |
| (1,1713) | 1:70:A:ILE:HG21 | 1:74:A:GLY:HA3  | 16       | 0.25          |
| (1,1713) | 1:70:A:ILE:HG22 | 1:74:A:GLY:HA3  | 16       | 0.25          |
| (1,1713) | 1:70:A:ILE:HG23 | 1:74:A:GLY:HA3  | 16       | 0.25          |
| (1,1575) | 1:67:A:GLU:HA   | 1:68:A:ILE:HD11 | 15       | 0.25          |
| (1,1575) | 1:67:A:GLU:HA   | 1:68:A:ILE:HD12 | 15       | 0.25          |
| (1,1575) | 1:67:A:GLU:HA   | 1:68:A:ILE:HD13 | 15       | 0.25          |
| (1,1575) | 1:67:A:GLU:HA   | 1:68:A:ILE:HD11 | 19       | 0.25          |
| (1,1575) | 1:67:A:GLU:HA   | 1:68:A:ILE:HD12 | 19       | 0.25          |
| (1,1575) | 1:67:A:GLU:HA   | 1:68:A:ILE:HD13 | 19       | 0.25          |
| (1,1530) | 1:65:A:LEU:HA   | 1:79:A:PHE:HE1  | 2        | 0.25          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1283) | 1:68:A:ILE:HG21 | 1:79:A:PHE:HE2  | 7        | 0.25          |
| (1,1283) | 1:68:A:ILE:HG22 | 1:79:A:PHE:HE2  | 7        | 0.25          |
| (1,1283) | 1:68:A:ILE:HG23 | 1:79:A:PHE:HE2  | 7        | 0.25          |
| (1,1283) | 1:68:A:ILE:HG21 | 1:79:A:PHE:HE2  | 16       | 0.25          |
| (1,1283) | 1:68:A:ILE:HG22 | 1:79:A:PHE:HE2  | 16       | 0.25          |
| (1,1283) | 1:68:A:ILE:HG23 | 1:79:A:PHE:HE2  | 16       | 0.25          |
| (1,2619) | 1:55:A:GLN:HG2  | 1:101:A:TRP:HE1 | 2        | 0.24          |
| (1,2619) | 1:55:A:GLN:HG3  | 1:101:A:TRP:HE1 | 2        | 0.24          |
| (1,2619) | 1:55:A:GLN:HG2  | 1:101:A:TRP:HE1 | 5        | 0.24          |
| (1,2619) | 1:55:A:GLN:HG3  | 1:101:A:TRP:HE1 | 5        | 0.24          |
| (1,2615) | 1:54:A:LEU:HD21 | 1:96:A:ARG:HG2  | 3        | 0.24          |
| (1,2615) | 1:54:A:LEU:HD21 | 1:96:A:ARG:HG3  | 3        | 0.24          |
| (1,2615) | 1:54:A:LEU:HD22 | 1:96:A:ARG:HG2  | 3        | 0.24          |
| (1,2615) | 1:54:A:LEU:HD22 | 1:96:A:ARG:HG3  | 3        | 0.24          |
| (1,2615) | 1:54:A:LEU:HD23 | 1:96:A:ARG:HG2  | 3        | 0.24          |
| (1,2615) | 1:54:A:LEU:HD23 | 1:96:A:ARG:HG3  | 3        | 0.24          |
| (1,2271) | 1:9:A:GLU:HG3   | 1:10:A:ALA:HB1  | 9        | 0.24          |
| (1,2271) | 1:9:A:GLU:HG3   | 1:10:A:ALA:HB2  | 9        | 0.24          |
| (1,2271) | 1:9:A:GLU:HG3   | 1:10:A:ALA:HB3  | 9        | 0.24          |
| (1,2270) | 1:103:A:ALA:H   | 1:104:A:GLU:HG2 | 1        | 0.24          |
| (1,2270) | 1:103:A:ALA:H   | 1:104:A:GLU:HG2 | 7        | 0.24          |
| (1,2270) | 1:103:A:ALA:H   | 1:104:A:GLU:HG2 | 10       | 0.24          |
| (1,2270) | 1:103:A:ALA:H   | 1:104:A:GLU:HG2 | 20       | 0.24          |
| (1,2225) | 1:47:A:LEU:HD21 | 1:48:A:LYS:HB3  | 18       | 0.24          |
| (1,2225) | 1:47:A:LEU:HD22 | 1:48:A:LYS:HB3  | 18       | 0.24          |
| (1,2225) | 1:47:A:LEU:HD23 | 1:48:A:LYS:HB3  | 18       | 0.24          |
| (1,2118) | 1:57:A:THR:HG21 | 1:79:A:PHE:HD1  | 14       | 0.24          |
| (1,2118) | 1:57:A:THR:HG22 | 1:79:A:PHE:HD1  | 14       | 0.24          |
| (1,2118) | 1:57:A:THR:HG23 | 1:79:A:PHE:HD1  | 14       | 0.24          |
| (1,2009) | 1:56:A:ALA:HB1  | 1:79:A:PHE:HD1  | 13       | 0.24          |
| (1,2009) | 1:56:A:ALA:HB2  | 1:79:A:PHE:HD1  | 13       | 0.24          |
| (1,2009) | 1:56:A:ALA:HB3  | 1:79:A:PHE:HD1  | 13       | 0.24          |
| (1,1876) | 1:56:A:ALA:HB1  | 1:86:A:VAL:HG11 | 11       | 0.24          |
| (1,1876) | 1:56:A:ALA:HB1  | 1:86:A:VAL:HG12 | 11       | 0.24          |
| (1,1876) | 1:56:A:ALA:HB1  | 1:86:A:VAL:HG13 | 11       | 0.24          |
| (1,1876) | 1:56:A:ALA:HB2  | 1:86:A:VAL:HG11 | 11       | 0.24          |
| (1,1876) | 1:56:A:ALA:HB2  | 1:86:A:VAL:HG12 | 11       | 0.24          |
| (1,1876) | 1:56:A:ALA:HB2  | 1:86:A:VAL:HG13 | 11       | 0.24          |
| (1,1876) | 1:56:A:ALA:HB3  | 1:86:A:VAL:HG11 | 11       | 0.24          |
| (1,1876) | 1:56:A:ALA:HB3  | 1:86:A:VAL:HG12 | 11       | 0.24          |
| (1,1876) | 1:56:A:ALA:HB3  | 1:86:A:VAL:HG13 | 11       | 0.24          |
| (1,1871) | 1:79:A:PHE:HE1  | 1:86:A:VAL:HB   | 5        | 0.24          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1871) | 1:79:A:PHE:HE1  | 1:86:A:VAL:HB   | 7        | 0.24          |
| (1,1529) | 1:65:A:LEU:HA   | 1:79:A:PHE:HD2  | 20       | 0.24          |
| (1,1283) | 1:68:A:ILE:HG21 | 1:79:A:PHE:HE2  | 3        | 0.24          |
| (1,1283) | 1:68:A:ILE:HG22 | 1:79:A:PHE:HE2  | 3        | 0.24          |
| (1,1283) | 1:68:A:ILE:HG23 | 1:79:A:PHE:HE2  | 3        | 0.24          |
| (1,1283) | 1:68:A:ILE:HG21 | 1:79:A:PHE:HE2  | 8        | 0.24          |
| (1,1283) | 1:68:A:ILE:HG22 | 1:79:A:PHE:HE2  | 8        | 0.24          |
| (1,1283) | 1:68:A:ILE:HG23 | 1:79:A:PHE:HE2  | 8        | 0.24          |
| (1,1283) | 1:68:A:ILE:HG21 | 1:79:A:PHE:HE2  | 10       | 0.24          |
| (1,1283) | 1:68:A:ILE:HG22 | 1:79:A:PHE:HE2  | 10       | 0.24          |
| (1,1283) | 1:68:A:ILE:HG23 | 1:79:A:PHE:HE2  | 10       | 0.24          |
| (1,1283) | 1:68:A:ILE:HG21 | 1:79:A:PHE:HE2  | 12       | 0.24          |
| (1,1283) | 1:68:A:ILE:HG22 | 1:79:A:PHE:HE2  | 12       | 0.24          |
| (1,1283) | 1:68:A:ILE:HG23 | 1:79:A:PHE:HE2  | 12       | 0.24          |
| (1,932)  | 1:79:A:PHE:H    | 1:82:A:LEU:HB2  | 5        | 0.24          |
| (1,932)  | 1:79:A:PHE:H    | 1:82:A:LEU:HB3  | 5        | 0.24          |
| (1,911)  | 1:79:A:PHE:HD2  | 1:80:A:GLU:H    | 15       | 0.24          |
| (1,2270) | 1:103:A:ALA:H   | 1:104:A:GLU:HG2 | 3        | 0.23          |
| (1,2270) | 1:103:A:ALA:H   | 1:104:A:GLU:HG2 | 12       | 0.23          |
| (1,2270) | 1:103:A:ALA:H   | 1:104:A:GLU:HG2 | 15       | 0.23          |
| (1,2225) | 1:47:A:LEU:HD21 | 1:48:A:LYS:HB3  | 1        | 0.23          |
| (1,2225) | 1:47:A:LEU:HD22 | 1:48:A:LYS:HB3  | 1        | 0.23          |
| (1,2225) | 1:47:A:LEU:HD23 | 1:48:A:LYS:HB3  | 1        | 0.23          |
| (1,2225) | 1:47:A:LEU:HD21 | 1:48:A:LYS:HB3  | 8        | 0.23          |
| (1,2225) | 1:47:A:LEU:HD22 | 1:48:A:LYS:HB3  | 8        | 0.23          |
| (1,2225) | 1:47:A:LEU:HD23 | 1:48:A:LYS:HB3  | 8        | 0.23          |
| (1,2196) | 1:61:A:THR:HG21 | 1:63:A:GLU:HB2  | 1        | 0.23          |
| (1,2196) | 1:61:A:THR:HG21 | 1:63:A:GLU:HB3  | 1        | 0.23          |
| (1,2196) | 1:61:A:THR:HG22 | 1:63:A:GLU:HB2  | 1        | 0.23          |
| (1,2196) | 1:61:A:THR:HG22 | 1:63:A:GLU:HB3  | 1        | 0.23          |
| (1,2196) | 1:61:A:THR:HG23 | 1:63:A:GLU:HB2  | 1        | 0.23          |
| (1,2196) | 1:61:A:THR:HG23 | 1:63:A:GLU:HB3  | 1        | 0.23          |
| (1,2118) | 1:57:A:THR:HG21 | 1:79:A:PHE:HD1  | 2        | 0.23          |
| (1,2118) | 1:57:A:THR:HG22 | 1:79:A:PHE:HD1  | 2        | 0.23          |
| (1,2118) | 1:57:A:THR:HG23 | 1:79:A:PHE:HD1  | 2        | 0.23          |
| (1,2118) | 1:57:A:THR:HG21 | 1:79:A:PHE:HD1  | 8        | 0.23          |
| (1,2118) | 1:57:A:THR:HG22 | 1:79:A:PHE:HD1  | 8        | 0.23          |
| (1,2118) | 1:57:A:THR:HG23 | 1:79:A:PHE:HD1  | 8        | 0.23          |
| (1,2118) | 1:57:A:THR:HG21 | 1:79:A:PHE:HD1  | 11       | 0.23          |
| (1,2118) | 1:57:A:THR:HG22 | 1:79:A:PHE:HD1  | 11       | 0.23          |
| (1,2118) | 1:57:A:THR:HG23 | 1:79:A:PHE:HD1  | 11       | 0.23          |
| (1,2118) | 1:57:A:THR:HG21 | 1:79:A:PHE:HD1  | 13       | 0.23          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2118) | 1:57:A:THR:HG22 | 1:79:A:PHE:HD1  | 13       | 0.23          |
| (1,2118) | 1:57:A:THR:HG23 | 1:79:A:PHE:HD1  | 13       | 0.23          |
| (1,2118) | 1:57:A:THR:HG21 | 1:79:A:PHE:HD1  | 17       | 0.23          |
| (1,2118) | 1:57:A:THR:HG22 | 1:79:A:PHE:HD1  | 17       | 0.23          |
| (1,2118) | 1:57:A:THR:HG23 | 1:79:A:PHE:HD1  | 17       | 0.23          |
| (1,2009) | 1:56:A:ALA:HB1  | 1:79:A:PHE:HD1  | 1        | 0.23          |
| (1,2009) | 1:56:A:ALA:HB2  | 1:79:A:PHE:HD1  | 1        | 0.23          |
| (1,2009) | 1:56:A:ALA:HB3  | 1:79:A:PHE:HD1  | 1        | 0.23          |
| (1,1950) | 1:15:A:MET:HE1  | 1:89:A:ILE:HD11 | 18       | 0.23          |
| (1,1950) | 1:15:A:MET:HE1  | 1:89:A:ILE:HD12 | 18       | 0.23          |
| (1,1950) | 1:15:A:MET:HE1  | 1:89:A:ILE:HD13 | 18       | 0.23          |
| (1,1950) | 1:15:A:MET:HE2  | 1:89:A:ILE:HD11 | 18       | 0.23          |
| (1,1950) | 1:15:A:MET:HE2  | 1:89:A:ILE:HD12 | 18       | 0.23          |
| (1,1950) | 1:15:A:MET:HE2  | 1:89:A:ILE:HD13 | 18       | 0.23          |
| (1,1950) | 1:15:A:MET:HE3  | 1:89:A:ILE:HD11 | 18       | 0.23          |
| (1,1950) | 1:15:A:MET:HE3  | 1:89:A:ILE:HD12 | 18       | 0.23          |
| (1,1950) | 1:15:A:MET:HE3  | 1:89:A:ILE:HD13 | 18       | 0.23          |
| (1,1876) | 1:56:A:ALA:HB1  | 1:86:A:VAL:HG11 | 3        | 0.23          |
| (1,1876) | 1:56:A:ALA:HB1  | 1:86:A:VAL:HG12 | 3        | 0.23          |
| (1,1876) | 1:56:A:ALA:HB1  | 1:86:A:VAL:HG13 | 3        | 0.23          |
| (1,1876) | 1:56:A:ALA:HB2  | 1:86:A:VAL:HG11 | 3        | 0.23          |
| (1,1876) | 1:56:A:ALA:HB2  | 1:86:A:VAL:HG12 | 3        | 0.23          |
| (1,1876) | 1:56:A:ALA:HB2  | 1:86:A:VAL:HG13 | 3        | 0.23          |
| (1,1876) | 1:56:A:ALA:HB3  | 1:86:A:VAL:HG11 | 3        | 0.23          |
| (1,1876) | 1:56:A:ALA:HB3  | 1:86:A:VAL:HG12 | 3        | 0.23          |
| (1,1876) | 1:56:A:ALA:HB3  | 1:86:A:VAL:HG13 | 3        | 0.23          |
| (1,1876) | 1:56:A:ALA:HB1  | 1:86:A:VAL:HG11 | 16       | 0.23          |
| (1,1876) | 1:56:A:ALA:HB1  | 1:86:A:VAL:HG12 | 16       | 0.23          |
| (1,1876) | 1:56:A:ALA:HB1  | 1:86:A:VAL:HG13 | 16       | 0.23          |
| (1,1876) | 1:56:A:ALA:HB2  | 1:86:A:VAL:HG11 | 16       | 0.23          |
| (1,1876) | 1:56:A:ALA:HB2  | 1:86:A:VAL:HG12 | 16       | 0.23          |
| (1,1876) | 1:56:A:ALA:HB2  | 1:86:A:VAL:HG13 | 16       | 0.23          |
| (1,1876) | 1:56:A:ALA:HB3  | 1:86:A:VAL:HG11 | 16       | 0.23          |
| (1,1876) | 1:56:A:ALA:HB3  | 1:86:A:VAL:HG12 | 16       | 0.23          |
| (1,1876) | 1:56:A:ALA:HB3  | 1:86:A:VAL:HG13 | 16       | 0.23          |
| (1,1871) | 1:79:A:PHE:HE1  | 1:86:A:VAL:HB   | 19       | 0.23          |
| (1,1575) | 1:67:A:GLU:HA   | 1:68:A:ILE:HD11 | 8        | 0.23          |
| (1,1575) | 1:67:A:GLU:HA   | 1:68:A:ILE:HD12 | 8        | 0.23          |
| (1,1575) | 1:67:A:GLU:HA   | 1:68:A:ILE:HD13 | 8        | 0.23          |
| (1,1575) | 1:67:A:GLU:HA   | 1:68:A:ILE:HD11 | 13       | 0.23          |
| (1,1575) | 1:67:A:GLU:HA   | 1:68:A:ILE:HD12 | 13       | 0.23          |
| (1,1575) | 1:67:A:GLU:HA   | 1:68:A:ILE:HD13 | 13       | 0.23          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1283) | 1:68:A:ILE:HG21 | 1:79:A:PHE:HE2  | 2        | 0.23          |
| (1,1283) | 1:68:A:ILE:HG22 | 1:79:A:PHE:HE2  | 2        | 0.23          |
| (1,1283) | 1:68:A:ILE:HG23 | 1:79:A:PHE:HE2  | 2        | 0.23          |
| (1,1283) | 1:68:A:ILE:HG21 | 1:79:A:PHE:HE2  | 18       | 0.23          |
| (1,1283) | 1:68:A:ILE:HG22 | 1:79:A:PHE:HE2  | 18       | 0.23          |
| (1,1283) | 1:68:A:ILE:HG23 | 1:79:A:PHE:HE2  | 18       | 0.23          |
| (1,911)  | 1:79:A:PHE:HD2  | 1:80:A:GLU:H    | 4        | 0.23          |
| (1,2615) | 1:54:A:LEU:HD21 | 1:96:A:ARG:HG2  | 15       | 0.22          |
| (1,2615) | 1:54:A:LEU:HD21 | 1:96:A:ARG:HG3  | 15       | 0.22          |
| (1,2615) | 1:54:A:LEU:HD22 | 1:96:A:ARG:HG2  | 15       | 0.22          |
| (1,2615) | 1:54:A:LEU:HD22 | 1:96:A:ARG:HG3  | 15       | 0.22          |
| (1,2615) | 1:54:A:LEU:HD23 | 1:96:A:ARG:HG2  | 15       | 0.22          |
| (1,2615) | 1:54:A:LEU:HD23 | 1:96:A:ARG:HG3  | 15       | 0.22          |
| (1,2456) | 1:8:A:LEU:HB2   | 1:9:A:GLU:H     | 16       | 0.22          |
| (1,2456) | 1:8:A:LEU:HB3   | 1:9:A:GLU:H     | 16       | 0.22          |
| (1,2040) | 1:43:A:ASN:HA   | 1:45:A:ARG:H    | 6        | 0.22          |
| (1,2009) | 1:56:A:ALA:HB1  | 1:79:A:PHE:HD1  | 8        | 0.22          |
| (1,2009) | 1:56:A:ALA:HB2  | 1:79:A:PHE:HD1  | 8        | 0.22          |
| (1,2009) | 1:56:A:ALA:HB3  | 1:79:A:PHE:HD1  | 8        | 0.22          |
| (1,1713) | 1:70:A:ILE:HG21 | 1:74:A:GLY:HA3  | 18       | 0.22          |
| (1,1713) | 1:70:A:ILE:HG22 | 1:74:A:GLY:HA3  | 18       | 0.22          |
| (1,1713) | 1:70:A:ILE:HG23 | 1:74:A:GLY:HA3  | 18       | 0.22          |
| (1,1575) | 1:67:A:GLU:HA   | 1:68:A:ILE:HD11 | 10       | 0.22          |
| (1,1575) | 1:67:A:GLU:HA   | 1:68:A:ILE:HD12 | 10       | 0.22          |
| (1,1575) | 1:67:A:GLU:HA   | 1:68:A:ILE:HD13 | 10       | 0.22          |
| (1,1575) | 1:67:A:GLU:HA   | 1:68:A:ILE:HD11 | 12       | 0.22          |
| (1,1575) | 1:67:A:GLU:HA   | 1:68:A:ILE:HD12 | 12       | 0.22          |
| (1,1575) | 1:67:A:GLU:HA   | 1:68:A:ILE:HD13 | 12       | 0.22          |
| (1,911)  | 1:79:A:PHE:HD2  | 1:80:A:GLU:H    | 14       | 0.22          |
| (1,231)  | 1:106:A:PRO:HB3 | 1:107:A:LEU:H   | 9        | 0.22          |
| (1,231)  | 1:106:A:PRO:HB3 | 1:107:A:LEU:H   | 14       | 0.22          |
| (1,179)  | 1:29:A:GLN:HG2  | 1:30:A:TYR:H    | 11       | 0.22          |
| (1,179)  | 1:29:A:GLN:HG2  | 1:30:A:TYR:H    | 12       | 0.22          |
| (1,179)  | 1:29:A:GLN:HG2  | 1:30:A:TYR:H    | 18       | 0.22          |
| (2,23)   | 1:99:A:ALA:O    | 1:103:A:ALA:H   | 18       | 0.21          |
| (1,2270) | 1:103:A:ALA:H   | 1:104:A:GLU:HG2 | 17       | 0.21          |
| (1,2225) | 1:47:A:LEU:HD21 | 1:48:A:LYS:HB3  | 5        | 0.21          |
| (1,2225) | 1:47:A:LEU:HD22 | 1:48:A:LYS:HB3  | 5        | 0.21          |
| (1,2225) | 1:47:A:LEU:HD23 | 1:48:A:LYS:HB3  | 5        | 0.21          |
| (1,2225) | 1:47:A:LEU:HD21 | 1:48:A:LYS:HB3  | 14       | 0.21          |
| (1,2225) | 1:47:A:LEU:HD22 | 1:48:A:LYS:HB3  | 14       | 0.21          |
| (1,2225) | 1:47:A:LEU:HD23 | 1:48:A:LYS:HB3  | 14       | 0.21          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2133) | 1:57:A:THR:HG21 | 1:84:A:GLU:HB2  | 13       | 0.21          |
| (1,2133) | 1:57:A:THR:HG22 | 1:84:A:GLU:HB2  | 13       | 0.21          |
| (1,2133) | 1:57:A:THR:HG23 | 1:84:A:GLU:HB2  | 13       | 0.21          |
| (1,2118) | 1:57:A:THR:HG21 | 1:79:A:PHE:HD1  | 15       | 0.21          |
| (1,2118) | 1:57:A:THR:HG22 | 1:79:A:PHE:HD1  | 15       | 0.21          |
| (1,2118) | 1:57:A:THR:HG23 | 1:79:A:PHE:HD1  | 15       | 0.21          |
| (1,2118) | 1:57:A:THR:HG21 | 1:79:A:PHE:HD1  | 20       | 0.21          |
| (1,2118) | 1:57:A:THR:HG22 | 1:79:A:PHE:HD1  | 20       | 0.21          |
| (1,2118) | 1:57:A:THR:HG23 | 1:79:A:PHE:HD1  | 20       | 0.21          |
| (1,2009) | 1:56:A:ALA:HB1  | 1:79:A:PHE:HD1  | 20       | 0.21          |
| (1,2009) | 1:56:A:ALA:HB2  | 1:79:A:PHE:HD1  | 20       | 0.21          |
| (1,2009) | 1:56:A:ALA:HB3  | 1:79:A:PHE:HD1  | 20       | 0.21          |
| (1,1960) | 1:33:A:GLU:HA   | 1:34:A:GLU:HG2  | 4        | 0.21          |
| (1,1960) | 1:33:A:GLU:HA   | 1:34:A:GLU:HG2  | 6        | 0.21          |
| (1,1876) | 1:56:A:ALA:HB1  | 1:86:A:VAL:HG11 | 7        | 0.21          |
| (1,1876) | 1:56:A:ALA:HB1  | 1:86:A:VAL:HG12 | 7        | 0.21          |
| (1,1876) | 1:56:A:ALA:HB1  | 1:86:A:VAL:HG13 | 7        | 0.21          |
| (1,1876) | 1:56:A:ALA:HB2  | 1:86:A:VAL:HG11 | 7        | 0.21          |
| (1,1876) | 1:56:A:ALA:HB2  | 1:86:A:VAL:HG12 | 7        | 0.21          |
| (1,1876) | 1:56:A:ALA:HB2  | 1:86:A:VAL:HG13 | 7        | 0.21          |
| (1,1876) | 1:56:A:ALA:HB3  | 1:86:A:VAL:HG11 | 7        | 0.21          |
| (1,1876) | 1:56:A:ALA:HB3  | 1:86:A:VAL:HG12 | 7        | 0.21          |
| (1,1876) | 1:56:A:ALA:HB3  | 1:86:A:VAL:HG13 | 7        | 0.21          |
| (1,1876) | 1:56:A:ALA:HB1  | 1:86:A:VAL:HG11 | 10       | 0.21          |
| (1,1876) | 1:56:A:ALA:HB1  | 1:86:A:VAL:HG12 | 10       | 0.21          |
| (1,1876) | 1:56:A:ALA:HB1  | 1:86:A:VAL:HG13 | 10       | 0.21          |
| (1,1876) | 1:56:A:ALA:HB2  | 1:86:A:VAL:HG11 | 10       | 0.21          |
| (1,1876) | 1:56:A:ALA:HB2  | 1:86:A:VAL:HG12 | 10       | 0.21          |
| (1,1876) | 1:56:A:ALA:HB2  | 1:86:A:VAL:HG13 | 10       | 0.21          |
| (1,1876) | 1:56:A:ALA:HB3  | 1:86:A:VAL:HG11 | 10       | 0.21          |
| (1,1876) | 1:56:A:ALA:HB3  | 1:86:A:VAL:HG12 | 10       | 0.21          |
| (1,1876) | 1:56:A:ALA:HB3  | 1:86:A:VAL:HG13 | 10       | 0.21          |
| (1,1876) | 1:56:A:ALA:HB1  | 1:86:A:VAL:HG11 | 19       | 0.21          |
| (1,1876) | 1:56:A:ALA:HB1  | 1:86:A:VAL:HG12 | 19       | 0.21          |
| (1,1876) | 1:56:A:ALA:HB1  | 1:86:A:VAL:HG13 | 19       | 0.21          |
| (1,1876) | 1:56:A:ALA:HB2  | 1:86:A:VAL:HG11 | 19       | 0.21          |
| (1,1876) | 1:56:A:ALA:HB2  | 1:86:A:VAL:HG12 | 19       | 0.21          |
| (1,1876) | 1:56:A:ALA:HB2  | 1:86:A:VAL:HG13 | 19       | 0.21          |
| (1,1876) | 1:56:A:ALA:HB3  | 1:86:A:VAL:HG11 | 19       | 0.21          |
| (1,1876) | 1:56:A:ALA:HB3  | 1:86:A:VAL:HG12 | 19       | 0.21          |
| (1,1876) | 1:56:A:ALA:HB3  | 1:86:A:VAL:HG13 | 19       | 0.21          |
| (1,1713) | 1:70:A:ILE:HG21 | 1:74:A:GLY:HA3  | 10       | 0.21          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1713) | 1:70:A:ILE:HG22 | 1:74:A:GLY:HA3  | 10       | 0.21          |
| (1,1713) | 1:70:A:ILE:HG23 | 1:74:A:GLY:HA3  | 10       | 0.21          |
| (1,1575) | 1:67:A:GLU:HA   | 1:68:A:ILE:HD11 | 3        | 0.21          |
| (1,1575) | 1:67:A:GLU:HA   | 1:68:A:ILE:HD12 | 3        | 0.21          |
| (1,1575) | 1:67:A:GLU:HA   | 1:68:A:ILE:HD13 | 3        | 0.21          |
| (1,1529) | 1:65:A:LEU:HA   | 1:79:A:PHE:HD2  | 1        | 0.21          |
| (1,932)  | 1:79:A:PHE:H    | 1:82:A:LEU:HB2  | 11       | 0.21          |
| (1,932)  | 1:79:A:PHE:H    | 1:82:A:LEU:HB3  | 11       | 0.21          |
| (1,793)  | 1:67:A:GLU:H    | 1:81:A:THR:HG21 | 18       | 0.21          |
| (1,793)  | 1:67:A:GLU:H    | 1:81:A:THR:HG22 | 18       | 0.21          |
| (1,793)  | 1:67:A:GLU:H    | 1:81:A:THR:HG23 | 18       | 0.21          |
| (1,376)  | 1:65:A:LEU:H    | 1:66:A:ARG:HG2  | 5        | 0.21          |
| (1,179)  | 1:29:A:GLN:HG2  | 1:30:A:TYR:H    | 1        | 0.21          |
| (1,179)  | 1:29:A:GLN:HG2  | 1:30:A:TYR:H    | 8        | 0.21          |
| (2,13)   | 1:16:A:GLU:O    | 1:20:A:ARG:H    | 19       | 0.2           |
| (1,2271) | 1:9:A:GLU:HG3   | 1:10:A:ALA:HB1  | 20       | 0.2           |
| (1,2271) | 1:9:A:GLU:HG3   | 1:10:A:ALA:HB2  | 20       | 0.2           |
| (1,2271) | 1:9:A:GLU:HG3   | 1:10:A:ALA:HB3  | 20       | 0.2           |
| (1,2225) | 1:47:A:LEU:HD21 | 1:48:A:LYS:HB3  | 19       | 0.2           |
| (1,2225) | 1:47:A:LEU:HD22 | 1:48:A:LYS:HB3  | 19       | 0.2           |
| (1,2225) | 1:47:A:LEU:HD23 | 1:48:A:LYS:HB3  | 19       | 0.2           |
| (1,2196) | 1:61:A:THR:HG21 | 1:63:A:GLU:HB2  | 2        | 0.2           |
| (1,2196) | 1:61:A:THR:HG21 | 1:63:A:GLU:HB3  | 2        | 0.2           |
| (1,2196) | 1:61:A:THR:HG22 | 1:63:A:GLU:HB2  | 2        | 0.2           |
| (1,2196) | 1:61:A:THR:HG22 | 1:63:A:GLU:HB3  | 2        | 0.2           |
| (1,2196) | 1:61:A:THR:HG23 | 1:63:A:GLU:HB2  | 2        | 0.2           |
| (1,2196) | 1:61:A:THR:HG23 | 1:63:A:GLU:HB3  | 2        | 0.2           |
| (1,2142) | 1:13:A:SER:HA   | 1:16:A:GLU:HG2  | 14       | 0.2           |
| (1,2142) | 1:13:A:SER:HA   | 1:16:A:GLU:HG3  | 14       | 0.2           |
| (1,2118) | 1:57:A:THR:HG21 | 1:79:A:PHE:HD1  | 7        | 0.2           |
| (1,2118) | 1:57:A:THR:HG22 | 1:79:A:PHE:HD1  | 7        | 0.2           |
| (1,2118) | 1:57:A:THR:HG23 | 1:79:A:PHE:HD1  | 7        | 0.2           |
| (1,2118) | 1:57:A:THR:HG21 | 1:79:A:PHE:HD1  | 16       | 0.2           |
| (1,2118) | 1:57:A:THR:HG22 | 1:79:A:PHE:HD1  | 16       | 0.2           |
| (1,2118) | 1:57:A:THR:HG23 | 1:79:A:PHE:HD1  | 16       | 0.2           |
| (1,1575) | 1:67:A:GLU:HA   | 1:68:A:ILE:HD11 | 2        | 0.2           |
| (1,1575) | 1:67:A:GLU:HA   | 1:68:A:ILE:HD12 | 2        | 0.2           |
| (1,1575) | 1:67:A:GLU:HA   | 1:68:A:ILE:HD13 | 2        | 0.2           |
| (1,1575) | 1:67:A:GLU:HA   | 1:68:A:ILE:HD11 | 4        | 0.2           |
| (1,1575) | 1:67:A:GLU:HA   | 1:68:A:ILE:HD12 | 4        | 0.2           |
| (1,1575) | 1:67:A:GLU:HA   | 1:68:A:ILE:HD13 | 4        | 0.2           |
| (1,1420) | 1:82:A:LEU:HB2  | 1:84:A:GLU:HG3  | 7        | 0.2           |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1420) | 1:82:A:LEU:HB3  | 1:84:A:GLU:HG3   | 7        | 0.2           |
| (1,930)  | 1:105:A:HIS:H   | 1:106:A:PRO:HB3  | 20       | 0.2           |
| (1,528)  | 1:61:A:THR:H    | 1:64:A:GLN:HA    | 20       | 0.2           |
| (1,179)  | 1:29:A:GLN:HG2  | 1:30:A:TYR:H     | 2        | 0.2           |
| (1,179)  | 1:29:A:GLN:HG2  | 1:30:A:TYR:H     | 17       | 0.2           |
| (2,51)   | 1:78:A:TYR:O    | 1:69:A:GLU:H     | 6        | 0.19          |
| (2,13)   | 1:16:A:GLU:O    | 1:20:A:ARG:H     | 1        | 0.19          |
| (1,2437) | 1:104:A:GLU:HB2 | 1:105:A:HIS:HE1  | 11       | 0.19          |
| (1,2437) | 1:104:A:GLU:HB3 | 1:105:A:HIS:HE1  | 11       | 0.19          |
| (1,2270) | 1:103:A:ALA:H   | 1:104:A:GLU:HG2  | 13       | 0.19          |
| (1,2270) | 1:103:A:ALA:H   | 1:104:A:GLU:HG2  | 16       | 0.19          |
| (1,2262) | 1:45:A:ARG:H    | 1:45:A:ARG:HD3   | 13       | 0.19          |
| (1,2225) | 1:47:A:LEU:HD21 | 1:48:A:LYS:HB3   | 4        | 0.19          |
| (1,2225) | 1:47:A:LEU:HD22 | 1:48:A:LYS:HB3   | 4        | 0.19          |
| (1,2225) | 1:47:A:LEU:HD23 | 1:48:A:LYS:HB3   | 4        | 0.19          |
| (1,2225) | 1:47:A:LEU:HD21 | 1:48:A:LYS:HB3   | 15       | 0.19          |
| (1,2225) | 1:47:A:LEU:HD22 | 1:48:A:LYS:HB3   | 15       | 0.19          |
| (1,2225) | 1:47:A:LEU:HD23 | 1:48:A:LYS:HB3   | 15       | 0.19          |
| (1,2078) | 1:53:A:ASP:HB2  | 1:107:A:LEU:HD21 | 12       | 0.19          |
| (1,2078) | 1:53:A:ASP:HB2  | 1:107:A:LEU:HD22 | 12       | 0.19          |
| (1,2078) | 1:53:A:ASP:HB2  | 1:107:A:LEU:HD23 | 12       | 0.19          |
| (1,2009) | 1:56:A:ALA:HB1  | 1:79:A:PHE:HD1   | 14       | 0.19          |
| (1,2009) | 1:56:A:ALA:HB2  | 1:79:A:PHE:HD1   | 14       | 0.19          |
| (1,2009) | 1:56:A:ALA:HB3  | 1:79:A:PHE:HD1   | 14       | 0.19          |
| (1,1950) | 1:15:A:MET:HE1  | 1:89:A:ILE:HD11  | 1        | 0.19          |
| (1,1950) | 1:15:A:MET:HE1  | 1:89:A:ILE:HD12  | 1        | 0.19          |
| (1,1950) | 1:15:A:MET:HE1  | 1:89:A:ILE:HD13  | 1        | 0.19          |
| (1,1950) | 1:15:A:MET:HE2  | 1:89:A:ILE:HD11  | 1        | 0.19          |
| (1,1950) | 1:15:A:MET:HE2  | 1:89:A:ILE:HD12  | 1        | 0.19          |
| (1,1950) | 1:15:A:MET:HE2  | 1:89:A:ILE:HD13  | 1        | 0.19          |
| (1,1950) | 1:15:A:MET:HE3  | 1:89:A:ILE:HD11  | 1        | 0.19          |
| (1,1950) | 1:15:A:MET:HE3  | 1:89:A:ILE:HD12  | 1        | 0.19          |
| (1,1950) | 1:15:A:MET:HE3  | 1:89:A:ILE:HD13  | 1        | 0.19          |
| (1,1575) | 1:67:A:GLU:HA   | 1:68:A:ILE:HD11  | 1        | 0.19          |
| (1,1575) | 1:67:A:GLU:HA   | 1:68:A:ILE:HD12  | 1        | 0.19          |
| (1,1575) | 1:67:A:GLU:HA   | 1:68:A:ILE:HD13  | 1        | 0.19          |
| (1,1572) | 1:8:A:LEU:HD11  | 1:10:A:ALA:HA    | 20       | 0.19          |
| (1,1572) | 1:8:A:LEU:HD12  | 1:10:A:ALA:HA    | 20       | 0.19          |
| (1,1572) | 1:8:A:LEU:HD13  | 1:10:A:ALA:HA    | 20       | 0.19          |
| (1,943)  | 1:23:A:SER:HB2  | 1:43:A:ASN:HD21  | 13       | 0.19          |
| (1,911)  | 1:79:A:PHE:HD2  | 1:80:A:GLU:H     | 10       | 0.19          |
| (1,288)  | 1:47:A:LEU:HD11 | 1:48:A:LYS:H     | 13       | 0.19          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,288)  | 1:47:A:LEU:HD12 | 1:48:A:LYS:H    | 13       | 0.19          |
| (1,288)  | 1:47:A:LEU:HD13 | 1:48:A:LYS:H    | 13       | 0.19          |
| (1,179)  | 1:29:A:GLN:HG2  | 1:30:A:TYR:H    | 4        | 0.19          |
| (2,23)   | 1:99:A:ALA:O    | 1:103:A:ALA:H   | 3        | 0.18          |
| (1,2271) | 1:9:A:GLU:HG3   | 1:10:A:ALA:HB1  | 15       | 0.18          |
| (1,2271) | 1:9:A:GLU:HG3   | 1:10:A:ALA:HB2  | 15       | 0.18          |
| (1,2271) | 1:9:A:GLU:HG3   | 1:10:A:ALA:HB3  | 15       | 0.18          |
| (1,2270) | 1:103:A:ALA:H   | 1:104:A:GLU:HG2 | 5        | 0.18          |
| (1,2270) | 1:103:A:ALA:H   | 1:104:A:GLU:HG2 | 8        | 0.18          |
| (1,2270) | 1:103:A:ALA:H   | 1:104:A:GLU:HG2 | 9        | 0.18          |
| (1,2270) | 1:103:A:ALA:H   | 1:104:A:GLU:HG2 | 11       | 0.18          |
| (1,2118) | 1:57:A:THR:HG21 | 1:79:A:PHE:HD1  | 19       | 0.18          |
| (1,2118) | 1:57:A:THR:HG22 | 1:79:A:PHE:HD1  | 19       | 0.18          |
| (1,2118) | 1:57:A:THR:HG23 | 1:79:A:PHE:HD1  | 19       | 0.18          |
| (1,2009) | 1:56:A:ALA:HB1  | 1:79:A:PHE:HD1  | 5        | 0.18          |
| (1,2009) | 1:56:A:ALA:HB2  | 1:79:A:PHE:HD1  | 5        | 0.18          |
| (1,2009) | 1:56:A:ALA:HB3  | 1:79:A:PHE:HD1  | 5        | 0.18          |
| (1,1993) | 1:72:A:PRO:HB3  | 1:78:A:TYR:HB2  | 19       | 0.18          |
| (1,1960) | 1:33:A:GLU:HA   | 1:34:A:GLU:HG2  | 14       | 0.18          |
| (1,1713) | 1:70:A:ILE:HG21 | 1:74:A:GLY:HA3  | 14       | 0.18          |
| (1,1713) | 1:70:A:ILE:HG22 | 1:74:A:GLY:HA3  | 14       | 0.18          |
| (1,1713) | 1:70:A:ILE:HG23 | 1:74:A:GLY:HA3  | 14       | 0.18          |
| (1,1575) | 1:67:A:GLU:HA   | 1:68:A:ILE:HD11 | 6        | 0.18          |
| (1,1575) | 1:67:A:GLU:HA   | 1:68:A:ILE:HD12 | 6        | 0.18          |
| (1,1575) | 1:67:A:GLU:HA   | 1:68:A:ILE:HD13 | 6        | 0.18          |
| (1,1575) | 1:67:A:GLU:HA   | 1:68:A:ILE:HD11 | 16       | 0.18          |
| (1,1575) | 1:67:A:GLU:HA   | 1:68:A:ILE:HD12 | 16       | 0.18          |
| (1,1575) | 1:67:A:GLU:HA   | 1:68:A:ILE:HD13 | 16       | 0.18          |
| (1,1530) | 1:65:A:LEU:HA   | 1:79:A:PHE:HE1  | 18       | 0.18          |
| (1,1529) | 1:65:A:LEU:HA   | 1:79:A:PHE:HD2  | 17       | 0.18          |
| (1,1500) | 1:36:A:VAL:HG21 | 1:48:A:LYS:HD2  | 14       | 0.18          |
| (1,1500) | 1:36:A:VAL:HG21 | 1:48:A:LYS:HD3  | 14       | 0.18          |
| (1,1500) | 1:36:A:VAL:HG22 | 1:48:A:LYS:HD2  | 14       | 0.18          |
| (1,1500) | 1:36:A:VAL:HG22 | 1:48:A:LYS:HD3  | 14       | 0.18          |
| (1,1500) | 1:36:A:VAL:HG23 | 1:48:A:LYS:HD2  | 14       | 0.18          |
| (1,1500) | 1:36:A:VAL:HG23 | 1:48:A:LYS:HD3  | 14       | 0.18          |
| (1,1312) | 1:7:A:GLU:HG2   | 1:8:A:LEU:HG    | 2        | 0.18          |
| (1,1312) | 1:7:A:GLU:HG3   | 1:8:A:LEU:HG    | 2        | 0.18          |
| (1,943)  | 1:23:A:SER:HB2  | 1:43:A:ASN:HD21 | 11       | 0.18          |
| (1,868)  | 1:55:A:GLN:H    | 1:58:A:TYR:HB2  | 5        | 0.18          |
| (1,288)  | 1:47:A:LEU:HD11 | 1:48:A:LYS:H    | 2        | 0.18          |
| (1,288)  | 1:47:A:LEU:HD12 | 1:48:A:LYS:H    | 2        | 0.18          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,288)  | 1:47:A:LEU:HD13 | 1:48:A:LYS:H    | 2        | 0.18          |
| (1,179)  | 1:29:A:GLN:HG2  | 1:30:A:TYR:H    | 14       | 0.18          |
| (1,2456) | 1:8:A:LEU:HB2   | 1:9:A:GLU:H     | 18       | 0.17          |
| (1,2456) | 1:8:A:LEU:HB3   | 1:9:A:GLU:H     | 18       | 0.17          |
| (1,2335) | 1:41:A:LEU:HB3  | 1:45:A:ARG:HB2  | 17       | 0.17          |
| (1,2335) | 1:41:A:LEU:HB3  | 1:45:A:ARG:HB3  | 17       | 0.17          |
| (1,2271) | 1:9:A:GLU:HG3   | 1:10:A:ALA:HB1  | 5        | 0.17          |
| (1,2271) | 1:9:A:GLU:HG3   | 1:10:A:ALA:HB2  | 5        | 0.17          |
| (1,2271) | 1:9:A:GLU:HG3   | 1:10:A:ALA:HB3  | 5        | 0.17          |
| (1,2271) | 1:9:A:GLU:HG3   | 1:10:A:ALA:HB1  | 16       | 0.17          |
| (1,2271) | 1:9:A:GLU:HG3   | 1:10:A:ALA:HB2  | 16       | 0.17          |
| (1,2271) | 1:9:A:GLU:HG3   | 1:10:A:ALA:HB3  | 16       | 0.17          |
| (1,2225) | 1:47:A:LEU:HD21 | 1:48:A:LYS:HB3  | 13       | 0.17          |
| (1,2225) | 1:47:A:LEU:HD22 | 1:48:A:LYS:HB3  | 13       | 0.17          |
| (1,2225) | 1:47:A:LEU:HD23 | 1:48:A:LYS:HB3  | 13       | 0.17          |
| (1,2133) | 1:57:A:THR:HG21 | 1:84:A:GLU:HB2  | 17       | 0.17          |
| (1,2133) | 1:57:A:THR:HG22 | 1:84:A:GLU:HB2  | 17       | 0.17          |
| (1,2133) | 1:57:A:THR:HG23 | 1:84:A:GLU:HB2  | 17       | 0.17          |
| (1,2040) | 1:43:A:ASN:HA   | 1:45:A:ARG:H    | 20       | 0.17          |
| (1,2009) | 1:56:A:ALA:HB1  | 1:79:A:PHE:HD1  | 4        | 0.17          |
| (1,2009) | 1:56:A:ALA:HB2  | 1:79:A:PHE:HD1  | 4        | 0.17          |
| (1,2009) | 1:56:A:ALA:HB3  | 1:79:A:PHE:HD1  | 4        | 0.17          |
| (1,1993) | 1:72:A:PRO:HB3  | 1:78:A:TYR:HB2  | 3        | 0.17          |
| (1,1713) | 1:70:A:ILE:HG21 | 1:74:A:GLY:HA3  | 13       | 0.17          |
| (1,1713) | 1:70:A:ILE:HG22 | 1:74:A:GLY:HA3  | 13       | 0.17          |
| (1,1713) | 1:70:A:ILE:HG23 | 1:74:A:GLY:HA3  | 13       | 0.17          |
| (1,1572) | 1:8:A:LEU:HD11  | 1:10:A:ALA:HA   | 6        | 0.17          |
| (1,1572) | 1:8:A:LEU:HD12  | 1:10:A:ALA:HA   | 6        | 0.17          |
| (1,1572) | 1:8:A:LEU:HD13  | 1:10:A:ALA:HA   | 6        | 0.17          |
| (1,1529) | 1:65:A:LEU:HA   | 1:79:A:PHE:HD2  | 14       | 0.17          |
| (1,1528) | 1:65:A:LEU:HA   | 1:79:A:PHE:HD1  | 17       | 0.17          |
| (1,1236) | 1:100:A:LYS:HA  | 1:100:A:LYS:HE2 | 11       | 0.17          |
| (1,1236) | 1:100:A:LYS:HA  | 1:100:A:LYS:HE3 | 11       | 0.17          |
| (1,930)  | 1:105:A:HIS:H   | 1:106:A:PRO:HB3 | 16       | 0.17          |
| (1,793)  | 1:67:A:GLU:H    | 1:81:A:THR:HG21 | 15       | 0.17          |
| (1,793)  | 1:67:A:GLU:H    | 1:81:A:THR:HG22 | 15       | 0.17          |
| (1,793)  | 1:67:A:GLU:H    | 1:81:A:THR:HG23 | 15       | 0.17          |
| (1,288)  | 1:47:A:LEU:HD11 | 1:48:A:LYS:H    | 19       | 0.17          |
| (1,288)  | 1:47:A:LEU:HD12 | 1:48:A:LYS:H    | 19       | 0.17          |
| (1,288)  | 1:47:A:LEU:HD13 | 1:48:A:LYS:H    | 19       | 0.17          |
| (1,179)  | 1:29:A:GLN:HG2  | 1:30:A:TYR:H    | 7        | 0.17          |
| (1,179)  | 1:29:A:GLN:HG2  | 1:30:A:TYR:H    | 10       | 0.17          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,179)  | 1:29:A:GLN:HG2  | 1:30:A:TYR:H   | 16       | 0.17          |
| (2,23)   | 1:99:A:ALA:O    | 1:103:A:ALA:H  | 6        | 0.16          |
| (2,13)   | 1:16:A:GLU:O    | 1:20:A:ARG:H   | 15       | 0.16          |
| (1,2615) | 1:54:A:LEU:HD21 | 1:96:A:ARG:HG2 | 1        | 0.16          |
| (1,2615) | 1:54:A:LEU:HD21 | 1:96:A:ARG:HG3 | 1        | 0.16          |
| (1,2615) | 1:54:A:LEU:HD22 | 1:96:A:ARG:HG2 | 1        | 0.16          |
| (1,2615) | 1:54:A:LEU:HD22 | 1:96:A:ARG:HG3 | 1        | 0.16          |
| (1,2615) | 1:54:A:LEU:HD23 | 1:96:A:ARG:HG2 | 1        | 0.16          |
| (1,2615) | 1:54:A:LEU:HD23 | 1:96:A:ARG:HG3 | 1        | 0.16          |
| (1,2576) | 1:45:A:ARG:HD2  | 1:47:A:LEU:HG  | 6        | 0.16          |
| (1,2576) | 1:45:A:ARG:HD3  | 1:47:A:LEU:HG  | 6        | 0.16          |
| (1,2445) | 1:2:A:GLU:HB2   | 1:4:A:SER:H    | 12       | 0.16          |
| (1,2445) | 1:2:A:GLU:HB3   | 1:4:A:SER:H    | 12       | 0.16          |
| (1,2271) | 1:9:A:GLU:HG3   | 1:10:A:ALA:HB1 | 2        | 0.16          |
| (1,2271) | 1:9:A:GLU:HG3   | 1:10:A:ALA:HB2 | 2        | 0.16          |
| (1,2271) | 1:9:A:GLU:HG3   | 1:10:A:ALA:HB3 | 2        | 0.16          |
| (1,2271) | 1:9:A:GLU:HG3   | 1:10:A:ALA:HB1 | 11       | 0.16          |
| (1,2271) | 1:9:A:GLU:HG3   | 1:10:A:ALA:HB2 | 11       | 0.16          |
| (1,2271) | 1:9:A:GLU:HG3   | 1:10:A:ALA:HB3 | 11       | 0.16          |
| (1,2225) | 1:47:A:LEU:HD21 | 1:48:A:LYS:HB3 | 6        | 0.16          |
| (1,2225) | 1:47:A:LEU:HD22 | 1:48:A:LYS:HB3 | 6        | 0.16          |
| (1,2225) | 1:47:A:LEU:HD23 | 1:48:A:LYS:HB3 | 6        | 0.16          |
| (1,2225) | 1:47:A:LEU:HD21 | 1:48:A:LYS:HB3 | 9        | 0.16          |
| (1,2225) | 1:47:A:LEU:HD22 | 1:48:A:LYS:HB3 | 9        | 0.16          |
| (1,2225) | 1:47:A:LEU:HD23 | 1:48:A:LYS:HB3 | 9        | 0.16          |
| (1,2133) | 1:57:A:THR:HG21 | 1:84:A:GLU:HB2 | 8        | 0.16          |
| (1,2133) | 1:57:A:THR:HG22 | 1:84:A:GLU:HB2 | 8        | 0.16          |
| (1,2133) | 1:57:A:THR:HG23 | 1:84:A:GLU:HB2 | 8        | 0.16          |
| (1,2133) | 1:57:A:THR:HG21 | 1:84:A:GLU:HB2 | 15       | 0.16          |
| (1,2133) | 1:57:A:THR:HG22 | 1:84:A:GLU:HB2 | 15       | 0.16          |
| (1,2133) | 1:57:A:THR:HG23 | 1:84:A:GLU:HB2 | 15       | 0.16          |
| (1,2040) | 1:43:A:ASN:HA   | 1:45:A:ARG:H   | 9        | 0.16          |
| (1,2040) | 1:43:A:ASN:HA   | 1:45:A:ARG:H   | 14       | 0.16          |
| (1,2009) | 1:56:A:ALA:HB1  | 1:79:A:PHE:HD1 | 12       | 0.16          |
| (1,2009) | 1:56:A:ALA:HB2  | 1:79:A:PHE:HD1 | 12       | 0.16          |
| (1,2009) | 1:56:A:ALA:HB3  | 1:79:A:PHE:HD1 | 12       | 0.16          |
| (1,1960) | 1:33:A:GLU:HA   | 1:34:A:GLU:HG2 | 11       | 0.16          |
| (1,1920) | 1:39:A:PHE:HB2  | 1:47:A:LEU:HB2 | 14       | 0.16          |
| (1,1713) | 1:70:A:ILE:HG21 | 1:74:A:GLY:HA3 | 3        | 0.16          |
| (1,1713) | 1:70:A:ILE:HG22 | 1:74:A:GLY:HA3 | 3        | 0.16          |
| (1,1713) | 1:70:A:ILE:HG23 | 1:74:A:GLY:HA3 | 3        | 0.16          |
| (1,1713) | 1:70:A:ILE:HG21 | 1:74:A:GLY:HA3 | 4        | 0.16          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1713) | 1:70:A:ILE:HG22 | 1:74:A:GLY:HA3  | 4        | 0.16          |
| (1,1713) | 1:70:A:ILE:HG23 | 1:74:A:GLY:HA3  | 4        | 0.16          |
| (1,1713) | 1:70:A:ILE:HG21 | 1:74:A:GLY:HA3  | 7        | 0.16          |
| (1,1713) | 1:70:A:ILE:HG22 | 1:74:A:GLY:HA3  | 7        | 0.16          |
| (1,1713) | 1:70:A:ILE:HG23 | 1:74:A:GLY:HA3  | 7        | 0.16          |
| (1,1713) | 1:70:A:ILE:HG21 | 1:74:A:GLY:HA3  | 20       | 0.16          |
| (1,1713) | 1:70:A:ILE:HG22 | 1:74:A:GLY:HA3  | 20       | 0.16          |
| (1,1713) | 1:70:A:ILE:HG23 | 1:74:A:GLY:HA3  | 20       | 0.16          |
| (1,1575) | 1:67:A:GLU:HA   | 1:68:A:ILE:HD11 | 9        | 0.16          |
| (1,1575) | 1:67:A:GLU:HA   | 1:68:A:ILE:HD12 | 9        | 0.16          |
| (1,1575) | 1:67:A:GLU:HA   | 1:68:A:ILE:HD13 | 9        | 0.16          |
| (1,1530) | 1:65:A:LEU:HA   | 1:79:A:PHE:HE1  | 6        | 0.16          |
| (1,1528) | 1:65:A:LEU:HA   | 1:79:A:PHE:HD1  | 7        | 0.16          |
| (1,1528) | 1:65:A:LEU:HA   | 1:79:A:PHE:HD1  | 12       | 0.16          |
| (1,1489) | 1:39:A:PHE:HE2  | 1:48:A:LYS:HA   | 10       | 0.16          |
| (1,1489) | 1:39:A:PHE:HE2  | 1:48:A:LYS:HA   | 19       | 0.16          |
| (1,1434) | 1:65:A:LEU:HG   | 1:82:A:LEU:HD11 | 19       | 0.16          |
| (1,1434) | 1:65:A:LEU:HG   | 1:82:A:LEU:HD12 | 19       | 0.16          |
| (1,1434) | 1:65:A:LEU:HG   | 1:82:A:LEU:HD13 | 19       | 0.16          |
| (1,1416) | 1:7:A:GLU:HG2   | 1:8:A:LEU:HD21  | 18       | 0.16          |
| (1,1416) | 1:7:A:GLU:HG2   | 1:8:A:LEU:HD22  | 18       | 0.16          |
| (1,1416) | 1:7:A:GLU:HG2   | 1:8:A:LEU:HD23  | 18       | 0.16          |
| (1,1416) | 1:7:A:GLU:HG3   | 1:8:A:LEU:HD21  | 18       | 0.16          |
| (1,1416) | 1:7:A:GLU:HG3   | 1:8:A:LEU:HD22  | 18       | 0.16          |
| (1,1416) | 1:7:A:GLU:HG3   | 1:8:A:LEU:HD23  | 18       | 0.16          |
| (1,1312) | 1:7:A:GLU:HG2   | 1:8:A:LEU:HG    | 17       | 0.16          |
| (1,1312) | 1:7:A:GLU:HG3   | 1:8:A:LEU:HG    | 17       | 0.16          |
| (1,1298) | 1:68:A:ILE:HG13 | 1:79:A:PHE:HD2  | 20       | 0.16          |
| (1,911)  | 1:79:A:PHE:HD2  | 1:80:A:GLU:H    | 11       | 0.16          |
| (1,288)  | 1:47:A:LEU:HD11 | 1:48:A:LYS:H    | 8        | 0.16          |
| (1,288)  | 1:47:A:LEU:HD12 | 1:48:A:LYS:H    | 8        | 0.16          |
| (1,288)  | 1:47:A:LEU:HD13 | 1:48:A:LYS:H    | 8        | 0.16          |
| (1,231)  | 1:106:A:PRO:HB3 | 1:107:A:LEU:H   | 17       | 0.16          |
| (1,179)  | 1:29:A:GLN:HG2  | 1:30:A:TYR:H    | 15       | 0.16          |
| (2,51)   | 1:78:A:TYR:O    | 1:69:A:GLU:H    | 12       | 0.15          |
| (2,13)   | 1:16:A:GLU:O    | 1:20:A:ARG:H    | 16       | 0.15          |
| (1,2615) | 1:54:A:LEU:HD21 | 1:96:A:ARG:HG2  | 7        | 0.15          |
| (1,2615) | 1:54:A:LEU:HD21 | 1:96:A:ARG:HG3  | 7        | 0.15          |
| (1,2615) | 1:54:A:LEU:HD22 | 1:96:A:ARG:HG2  | 7        | 0.15          |
| (1,2615) | 1:54:A:LEU:HD22 | 1:96:A:ARG:HG3  | 7        | 0.15          |
| (1,2615) | 1:54:A:LEU:HD23 | 1:96:A:ARG:HG2  | 7        | 0.15          |
| (1,2615) | 1:54:A:LEU:HD23 | 1:96:A:ARG:HG3  | 7        | 0.15          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2591) | 1:49:A:PHE:HE1  | 1:96:A:ARG:HD2   | 3        | 0.15          |
| (1,2591) | 1:49:A:PHE:HE1  | 1:96:A:ARG:HD3   | 3        | 0.15          |
| (1,2225) | 1:47:A:LEU:HD21 | 1:48:A:LYS:HB3   | 2        | 0.15          |
| (1,2225) | 1:47:A:LEU:HD22 | 1:48:A:LYS:HB3   | 2        | 0.15          |
| (1,2225) | 1:47:A:LEU:HD23 | 1:48:A:LYS:HB3   | 2        | 0.15          |
| (1,2225) | 1:47:A:LEU:HD21 | 1:48:A:LYS:HB3   | 20       | 0.15          |
| (1,2225) | 1:47:A:LEU:HD22 | 1:48:A:LYS:HB3   | 20       | 0.15          |
| (1,2225) | 1:47:A:LEU:HD23 | 1:48:A:LYS:HB3   | 20       | 0.15          |
| (1,2133) | 1:57:A:THR:HG21 | 1:84:A:GLU:HB2   | 14       | 0.15          |
| (1,2133) | 1:57:A:THR:HG22 | 1:84:A:GLU:HB2   | 14       | 0.15          |
| (1,2133) | 1:57:A:THR:HG23 | 1:84:A:GLU:HB2   | 14       | 0.15          |
| (1,2120) | 1:57:A:THR:HG21 | 1:79:A:PHE:HE1   | 18       | 0.15          |
| (1,2120) | 1:57:A:THR:HG22 | 1:79:A:PHE:HE1   | 18       | 0.15          |
| (1,2120) | 1:57:A:THR:HG23 | 1:79:A:PHE:HE1   | 18       | 0.15          |
| (1,2120) | 1:57:A:THR:HG21 | 1:79:A:PHE:HE1   | 19       | 0.15          |
| (1,2120) | 1:57:A:THR:HG22 | 1:79:A:PHE:HE1   | 19       | 0.15          |
| (1,2120) | 1:57:A:THR:HG23 | 1:79:A:PHE:HE1   | 19       | 0.15          |
| (1,2079) | 1:53:A:ASP:HB3  | 1:107:A:LEU:HD21 | 14       | 0.15          |
| (1,2079) | 1:53:A:ASP:HB3  | 1:107:A:LEU:HD22 | 14       | 0.15          |
| (1,2079) | 1:53:A:ASP:HB3  | 1:107:A:LEU:HD23 | 14       | 0.15          |
| (1,2079) | 1:53:A:ASP:HB3  | 1:107:A:LEU:HD21 | 16       | 0.15          |
| (1,2079) | 1:53:A:ASP:HB3  | 1:107:A:LEU:HD22 | 16       | 0.15          |
| (1,2079) | 1:53:A:ASP:HB3  | 1:107:A:LEU:HD23 | 16       | 0.15          |
| (1,2078) | 1:53:A:ASP:HB2  | 1:107:A:LEU:HD21 | 8        | 0.15          |
| (1,2078) | 1:53:A:ASP:HB2  | 1:107:A:LEU:HD22 | 8        | 0.15          |
| (1,2078) | 1:53:A:ASP:HB2  | 1:107:A:LEU:HD23 | 8        | 0.15          |
| (1,2040) | 1:43:A:ASN:HA   | 1:45:A:ARG:H     | 15       | 0.15          |
| (1,2009) | 1:56:A:ALA:HB1  | 1:79:A:PHE:HD1   | 2        | 0.15          |
| (1,2009) | 1:56:A:ALA:HB2  | 1:79:A:PHE:HD1   | 2        | 0.15          |
| (1,2009) | 1:56:A:ALA:HB3  | 1:79:A:PHE:HD1   | 2        | 0.15          |
| (1,2009) | 1:56:A:ALA:HB1  | 1:79:A:PHE:HD1   | 17       | 0.15          |
| (1,2009) | 1:56:A:ALA:HB2  | 1:79:A:PHE:HD1   | 17       | 0.15          |
| (1,2009) | 1:56:A:ALA:HB3  | 1:79:A:PHE:HD1   | 17       | 0.15          |
| (1,1993) | 1:72:A:PRO:HB3  | 1:78:A:TYR:HB2   | 17       | 0.15          |
| (1,1960) | 1:33:A:GLU:HA   | 1:34:A:GLU:HG2   | 13       | 0.15          |
| (1,1960) | 1:33:A:GLU:HA   | 1:34:A:GLU:HG2   | 15       | 0.15          |
| (1,1726) | 1:11:A:ALA:HA   | 1:15:A:MET:HE1   | 12       | 0.15          |
| (1,1726) | 1:11:A:ALA:HA   | 1:15:A:MET:HE2   | 12       | 0.15          |
| (1,1726) | 1:11:A:ALA:HA   | 1:15:A:MET:HE3   | 12       | 0.15          |
| (1,1713) | 1:70:A:ILE:HG21 | 1:74:A:GLY:HA3   | 2        | 0.15          |
| (1,1713) | 1:70:A:ILE:HG22 | 1:74:A:GLY:HA3   | 2        | 0.15          |
| (1,1713) | 1:70:A:ILE:HG23 | 1:74:A:GLY:HA3   | 2        | 0.15          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1599) | 1:54:A:LEU:HD21 | 1:96:A:ARG:HD2  | 3        | 0.15          |
| (1,1599) | 1:54:A:LEU:HD22 | 1:96:A:ARG:HD2  | 3        | 0.15          |
| (1,1599) | 1:54:A:LEU:HD23 | 1:96:A:ARG:HD2  | 3        | 0.15          |
| (1,1575) | 1:67:A:GLU:HA   | 1:68:A:ILE:HD11 | 20       | 0.15          |
| (1,1575) | 1:67:A:GLU:HA   | 1:68:A:ILE:HD12 | 20       | 0.15          |
| (1,1575) | 1:67:A:GLU:HA   | 1:68:A:ILE:HD13 | 20       | 0.15          |
| (1,1553) | 1:65:A:LEU:HD21 | 1:79:A:PHE:HE1  | 13       | 0.15          |
| (1,1553) | 1:65:A:LEU:HD22 | 1:79:A:PHE:HE1  | 13       | 0.15          |
| (1,1553) | 1:65:A:LEU:HD23 | 1:79:A:PHE:HE1  | 13       | 0.15          |
| (1,1528) | 1:65:A:LEU:HA   | 1:79:A:PHE:HD1  | 6        | 0.15          |
| (1,1528) | 1:65:A:LEU:HA   | 1:79:A:PHE:HD1  | 20       | 0.15          |
| (1,1500) | 1:36:A:VAL:HG21 | 1:48:A:LYS:HD2  | 11       | 0.15          |
| (1,1500) | 1:36:A:VAL:HG21 | 1:48:A:LYS:HD3  | 11       | 0.15          |
| (1,1500) | 1:36:A:VAL:HG22 | 1:48:A:LYS:HD2  | 11       | 0.15          |
| (1,1500) | 1:36:A:VAL:HG22 | 1:48:A:LYS:HD3  | 11       | 0.15          |
| (1,1500) | 1:36:A:VAL:HG23 | 1:48:A:LYS:HD2  | 11       | 0.15          |
| (1,1500) | 1:36:A:VAL:HG23 | 1:48:A:LYS:HD3  | 11       | 0.15          |
| (1,1298) | 1:68:A:ILE:HG13 | 1:79:A:PHE:HD2  | 2        | 0.15          |
| (1,1298) | 1:68:A:ILE:HG13 | 1:79:A:PHE:HD2  | 13       | 0.15          |
| (1,1298) | 1:68:A:ILE:HG13 | 1:79:A:PHE:HD2  | 17       | 0.15          |
| (1,1293) | 1:68:A:ILE:HD11 | 1:79:A:PHE:HD2  | 15       | 0.15          |
| (1,1293) | 1:68:A:ILE:HD12 | 1:79:A:PHE:HD2  | 15       | 0.15          |
| (1,1293) | 1:68:A:ILE:HD13 | 1:79:A:PHE:HD2  | 15       | 0.15          |
| (1,1277) | 1:67:A:GLU:HG2  | 1:68:A:ILE:HA   | 15       | 0.15          |
| (1,1277) | 1:67:A:GLU:HG3  | 1:68:A:ILE:HA   | 15       | 0.15          |
| (1,1236) | 1:100:A:LYS:HA  | 1:100:A:LYS:HE2 | 7        | 0.15          |
| (1,1236) | 1:100:A:LYS:HA  | 1:100:A:LYS:HE3 | 7        | 0.15          |
| (1,1236) | 1:100:A:LYS:HA  | 1:100:A:LYS:HE2 | 12       | 0.15          |
| (1,1236) | 1:100:A:LYS:HA  | 1:100:A:LYS:HE3 | 12       | 0.15          |
| (1,932)  | 1:79:A:PHE:H    | 1:82:A:LEU:HB2  | 16       | 0.15          |
| (1,932)  | 1:79:A:PHE:H    | 1:82:A:LEU:HB3  | 16       | 0.15          |
| (1,928)  | 1:52:A:ASP:H    | 1:58:A:TYR:HE1  | 20       | 0.15          |
| (1,918)  | 1:65:A:LEU:H    | 1:66:A:ARG:HG3  | 12       | 0.15          |
| (1,793)  | 1:67:A:GLU:H    | 1:81:A:THR:HG21 | 11       | 0.15          |
| (1,793)  | 1:67:A:GLU:H    | 1:81:A:THR:HG22 | 11       | 0.15          |
| (1,793)  | 1:67:A:GLU:H    | 1:81:A:THR:HG23 | 11       | 0.15          |
| (1,633)  | 1:36:A:VAL:H    | 1:50:A:ARG:HG2  | 15       | 0.15          |
| (1,633)  | 1:36:A:VAL:H    | 1:50:A:ARG:HG3  | 15       | 0.15          |
| (1,528)  | 1:61:A:THR:H    | 1:64:A:GLN:HA   | 8        | 0.15          |
| (1,456)  | 1:25:A:LEU:H    | 1:88:A:LEU:HG   | 6        | 0.15          |
| (1,288)  | 1:47:A:LEU:HD11 | 1:48:A:LYS:H    | 3        | 0.15          |
| (1,288)  | 1:47:A:LEU:HD12 | 1:48:A:LYS:H    | 3        | 0.15          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,288)  | 1:47:A:LEU:HD13 | 1:48:A:LYS:H    | 3        | 0.15          |
| (1,288)  | 1:47:A:LEU:HD11 | 1:48:A:LYS:H    | 4        | 0.15          |
| (1,288)  | 1:47:A:LEU:HD12 | 1:48:A:LYS:H    | 4        | 0.15          |
| (1,288)  | 1:47:A:LEU:HD13 | 1:48:A:LYS:H    | 4        | 0.15          |
| (1,288)  | 1:47:A:LEU:HD11 | 1:48:A:LYS:H    | 10       | 0.15          |
| (1,288)  | 1:47:A:LEU:HD12 | 1:48:A:LYS:H    | 10       | 0.15          |
| (1,288)  | 1:47:A:LEU:HD13 | 1:48:A:LYS:H    | 10       | 0.15          |
| (1,288)  | 1:47:A:LEU:HD11 | 1:48:A:LYS:H    | 16       | 0.15          |
| (1,288)  | 1:47:A:LEU:HD12 | 1:48:A:LYS:H    | 16       | 0.15          |
| (1,288)  | 1:47:A:LEU:HD13 | 1:48:A:LYS:H    | 16       | 0.15          |
| (1,231)  | 1:106:A:PRO:HB3 | 1:107:A:LEU:H   | 12       | 0.15          |
| (1,231)  | 1:106:A:PRO:HB3 | 1:107:A:LEU:H   | 15       | 0.15          |
| (1,99)   | 1:102:A:MET:HG3 | 1:103:A:ALA:H   | 19       | 0.15          |
| (2,23)   | 1:99:A:ALA:O    | 1:103:A:ALA:H   | 17       | 0.14          |
| (2,14)   | 1:16:A:GLU:O    | 1:20:A:ARG:N    | 1        | 0.14          |
| (2,14)   | 1:16:A:GLU:O    | 1:20:A:ARG:N    | 19       | 0.14          |
| (1,2606) | 1:52:A:ASP:HB2  | 1:59:A:GLY:H    | 4        | 0.14          |
| (1,2606) | 1:52:A:ASP:HB3  | 1:59:A:GLY:H    | 4        | 0.14          |
| (1,2576) | 1:45:A:ARG:HD2  | 1:47:A:LEU:HG   | 5        | 0.14          |
| (1,2576) | 1:45:A:ARG:HD3  | 1:47:A:LEU:HG   | 5        | 0.14          |
| (1,2335) | 1:41:A:LEU:HB3  | 1:45:A:ARG:HB2  | 7        | 0.14          |
| (1,2335) | 1:41:A:LEU:HB3  | 1:45:A:ARG:HB3  | 7        | 0.14          |
| (1,2335) | 1:41:A:LEU:HB3  | 1:45:A:ARG:HB2  | 18       | 0.14          |
| (1,2335) | 1:41:A:LEU:HB3  | 1:45:A:ARG:HB3  | 18       | 0.14          |
| (1,2320) | 1:25:A:LEU:HB3  | 1:70:A:ILE:HG12 | 13       | 0.14          |
| (1,2271) | 1:9:A:GLU:HG3   | 1:10:A:ALA:HB1  | 18       | 0.14          |
| (1,2271) | 1:9:A:GLU:HG3   | 1:10:A:ALA:HB2  | 18       | 0.14          |
| (1,2271) | 1:9:A:GLU:HG3   | 1:10:A:ALA:HB3  | 18       | 0.14          |
| (1,2267) | 1:43:A:ASN:HD21 | 1:45:A:ARG:HD3  | 1        | 0.14          |
| (1,2267) | 1:43:A:ASN:HD21 | 1:45:A:ARG:HD3  | 12       | 0.14          |
| (1,2229) | 1:39:A:PHE:HD2  | 1:47:A:LEU:HD21 | 3        | 0.14          |
| (1,2229) | 1:39:A:PHE:HD2  | 1:47:A:LEU:HD22 | 3        | 0.14          |
| (1,2229) | 1:39:A:PHE:HD2  | 1:47:A:LEU:HD23 | 3        | 0.14          |
| (1,2225) | 1:47:A:LEU:HD21 | 1:48:A:LYS:HB3  | 16       | 0.14          |
| (1,2225) | 1:47:A:LEU:HD22 | 1:48:A:LYS:HB3  | 16       | 0.14          |
| (1,2225) | 1:47:A:LEU:HD23 | 1:48:A:LYS:HB3  | 16       | 0.14          |
| (1,2196) | 1:61:A:THR:HG21 | 1:63:A:GLU:HB2  | 5        | 0.14          |
| (1,2196) | 1:61:A:THR:HG21 | 1:63:A:GLU:HB3  | 5        | 0.14          |
| (1,2196) | 1:61:A:THR:HG22 | 1:63:A:GLU:HB2  | 5        | 0.14          |
| (1,2196) | 1:61:A:THR:HG22 | 1:63:A:GLU:HB3  | 5        | 0.14          |
| (1,2196) | 1:61:A:THR:HG23 | 1:63:A:GLU:HB2  | 5        | 0.14          |
| (1,2196) | 1:61:A:THR:HG23 | 1:63:A:GLU:HB3  | 5        | 0.14          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2133) | 1:57:A:THR:HG21 | 1:84:A:GLU:HB2  | 12       | 0.14          |
| (1,2133) | 1:57:A:THR:HG22 | 1:84:A:GLU:HB2  | 12       | 0.14          |
| (1,2133) | 1:57:A:THR:HG23 | 1:84:A:GLU:HB2  | 12       | 0.14          |
| (1,2120) | 1:57:A:THR:HG21 | 1:79:A:PHE:HE1  | 16       | 0.14          |
| (1,2120) | 1:57:A:THR:HG22 | 1:79:A:PHE:HE1  | 16       | 0.14          |
| (1,2120) | 1:57:A:THR:HG23 | 1:79:A:PHE:HE1  | 16       | 0.14          |
| (1,2034) | 1:104:A:GLU:HA  | 1:106:A:PRO:HD2 | 17       | 0.14          |
| (1,2009) | 1:56:A:ALA:HB1  | 1:79:A:PHE:HD1  | 18       | 0.14          |
| (1,2009) | 1:56:A:ALA:HB2  | 1:79:A:PHE:HD1  | 18       | 0.14          |
| (1,2009) | 1:56:A:ALA:HB3  | 1:79:A:PHE:HD1  | 18       | 0.14          |
| (1,1996) | 1:78:A:TYR:HA   | 1:79:A:PHE:HD2  | 14       | 0.14          |
| (1,1993) | 1:72:A:PRO:HB3  | 1:78:A:TYR:HB2  | 5        | 0.14          |
| (1,1993) | 1:72:A:PRO:HB3  | 1:78:A:TYR:HB2  | 9        | 0.14          |
| (1,1993) | 1:72:A:PRO:HB3  | 1:78:A:TYR:HB2  | 12       | 0.14          |
| (1,1993) | 1:72:A:PRO:HB3  | 1:78:A:TYR:HB2  | 13       | 0.14          |
| (1,1993) | 1:72:A:PRO:HB3  | 1:78:A:TYR:HB2  | 20       | 0.14          |
| (1,1950) | 1:15:A:MET:HE1  | 1:89:A:ILE:HD11 | 2        | 0.14          |
| (1,1950) | 1:15:A:MET:HE1  | 1:89:A:ILE:HD12 | 2        | 0.14          |
| (1,1950) | 1:15:A:MET:HE1  | 1:89:A:ILE:HD13 | 2        | 0.14          |
| (1,1950) | 1:15:A:MET:HE2  | 1:89:A:ILE:HD11 | 2        | 0.14          |
| (1,1950) | 1:15:A:MET:HE2  | 1:89:A:ILE:HD12 | 2        | 0.14          |
| (1,1950) | 1:15:A:MET:HE2  | 1:89:A:ILE:HD13 | 2        | 0.14          |
| (1,1950) | 1:15:A:MET:HE3  | 1:89:A:ILE:HD11 | 2        | 0.14          |
| (1,1950) | 1:15:A:MET:HE3  | 1:89:A:ILE:HD12 | 2        | 0.14          |
| (1,1950) | 1:15:A:MET:HE3  | 1:89:A:ILE:HD13 | 2        | 0.14          |
| (1,1950) | 1:15:A:MET:HE1  | 1:89:A:ILE:HD11 | 20       | 0.14          |
| (1,1950) | 1:15:A:MET:HE1  | 1:89:A:ILE:HD12 | 20       | 0.14          |
| (1,1950) | 1:15:A:MET:HE1  | 1:89:A:ILE:HD13 | 20       | 0.14          |
| (1,1950) | 1:15:A:MET:HE2  | 1:89:A:ILE:HD11 | 20       | 0.14          |
| (1,1950) | 1:15:A:MET:HE2  | 1:89:A:ILE:HD12 | 20       | 0.14          |
| (1,1950) | 1:15:A:MET:HE2  | 1:89:A:ILE:HD13 | 20       | 0.14          |
| (1,1950) | 1:15:A:MET:HE3  | 1:89:A:ILE:HD11 | 20       | 0.14          |
| (1,1950) | 1:15:A:MET:HE3  | 1:89:A:ILE:HD12 | 20       | 0.14          |
| (1,1950) | 1:15:A:MET:HE3  | 1:89:A:ILE:HD13 | 20       | 0.14          |
| (1,1713) | 1:70:A:ILE:HG21 | 1:74:A:GLY:HA3  | 5        | 0.14          |
| (1,1713) | 1:70:A:ILE:HG22 | 1:74:A:GLY:HA3  | 5        | 0.14          |
| (1,1713) | 1:70:A:ILE:HG23 | 1:74:A:GLY:HA3  | 5        | 0.14          |
| (1,1713) | 1:70:A:ILE:HG21 | 1:74:A:GLY:HA3  | 17       | 0.14          |
| (1,1713) | 1:70:A:ILE:HG22 | 1:74:A:GLY:HA3  | 17       | 0.14          |
| (1,1713) | 1:70:A:ILE:HG23 | 1:74:A:GLY:HA3  | 17       | 0.14          |
| (1,1671) | 1:71:A:SER:HA   | 1:77:A:VAL:HG11 | 6        | 0.14          |
| (1,1671) | 1:71:A:SER:HA   | 1:77:A:VAL:HG12 | 6        | 0.14          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1671) | 1:71:A:SER:HA   | 1:77:A:VAL:HG13 | 6        | 0.14          |
| (1,1599) | 1:54:A:LEU:HD21 | 1:96:A:ARG:HD2  | 14       | 0.14          |
| (1,1599) | 1:54:A:LEU:HD22 | 1:96:A:ARG:HD2  | 14       | 0.14          |
| (1,1599) | 1:54:A:LEU:HD23 | 1:96:A:ARG:HD2  | 14       | 0.14          |
| (1,1575) | 1:67:A:GLU:HA   | 1:68:A:ILE:HD11 | 7        | 0.14          |
| (1,1575) | 1:67:A:GLU:HA   | 1:68:A:ILE:HD12 | 7        | 0.14          |
| (1,1575) | 1:67:A:GLU:HA   | 1:68:A:ILE:HD13 | 7        | 0.14          |
| (1,1553) | 1:65:A:LEU:HD21 | 1:79:A:PHE:HE1  | 15       | 0.14          |
| (1,1553) | 1:65:A:LEU:HD22 | 1:79:A:PHE:HE1  | 15       | 0.14          |
| (1,1553) | 1:65:A:LEU:HD23 | 1:79:A:PHE:HE1  | 15       | 0.14          |
| (1,1553) | 1:65:A:LEU:HD21 | 1:79:A:PHE:HE1  | 20       | 0.14          |
| (1,1553) | 1:65:A:LEU:HD22 | 1:79:A:PHE:HE1  | 20       | 0.14          |
| (1,1553) | 1:65:A:LEU:HD23 | 1:79:A:PHE:HE1  | 20       | 0.14          |
| (1,1528) | 1:65:A:LEU:HA   | 1:79:A:PHE:HD1  | 3        | 0.14          |
| (1,1528) | 1:65:A:LEU:HA   | 1:79:A:PHE:HD1  | 8        | 0.14          |
| (1,928)  | 1:52:A:ASP:H    | 1:58:A:TYR:HE1  | 6        | 0.14          |
| (1,918)  | 1:65:A:LEU:H    | 1:66:A:ARG:HG3  | 13       | 0.14          |
| (1,376)  | 1:65:A:LEU:H    | 1:66:A:ARG:HG2  | 14       | 0.14          |
| (1,288)  | 1:47:A:LEU:HD11 | 1:48:A:LYS:H    | 15       | 0.14          |
| (1,288)  | 1:47:A:LEU:HD12 | 1:48:A:LYS:H    | 15       | 0.14          |
| (1,288)  | 1:47:A:LEU:HD13 | 1:48:A:LYS:H    | 15       | 0.14          |
| (2,59)   | 1:77:A:VAL:O    | 1:86:A:VAL:H    | 19       | 0.13          |
| (2,13)   | 1:16:A:GLU:O    | 1:20:A:ARG:H    | 2        | 0.13          |
| (2,13)   | 1:16:A:GLU:O    | 1:20:A:ARG:H    | 14       | 0.13          |
| (2,5)    | 1:12:A:SER:O    | 1:16:A:GLU:H    | 12       | 0.13          |
| (1,2722) | 1:103:A:ALA:HB1 | 1:104:A:GLU:HG2 | 14       | 0.13          |
| (1,2722) | 1:103:A:ALA:HB1 | 1:104:A:GLU:HG3 | 14       | 0.13          |
| (1,2722) | 1:103:A:ALA:HB2 | 1:104:A:GLU:HG2 | 14       | 0.13          |
| (1,2722) | 1:103:A:ALA:HB2 | 1:104:A:GLU:HG3 | 14       | 0.13          |
| (1,2722) | 1:103:A:ALA:HB3 | 1:104:A:GLU:HG2 | 14       | 0.13          |
| (1,2722) | 1:103:A:ALA:HB3 | 1:104:A:GLU:HG3 | 14       | 0.13          |
| (1,2606) | 1:52:A:ASP:HB2  | 1:59:A:GLY:H    | 17       | 0.13          |
| (1,2606) | 1:52:A:ASP:HB3  | 1:59:A:GLY:H    | 17       | 0.13          |
| (1,2320) | 1:25:A:LEU:HB3  | 1:70:A:ILE:HG12 | 12       | 0.13          |
| (1,2307) | 1:19:A:GLN:HA   | 1:75:A:LEU:HD11 | 6        | 0.13          |
| (1,2307) | 1:19:A:GLN:HA   | 1:75:A:LEU:HD12 | 6        | 0.13          |
| (1,2307) | 1:19:A:GLN:HA   | 1:75:A:LEU:HD13 | 6        | 0.13          |
| (1,2294) | 1:11:A:ALA:HB1  | 1:15:A:MET:HE1  | 18       | 0.13          |
| (1,2294) | 1:11:A:ALA:HB1  | 1:15:A:MET:HE2  | 18       | 0.13          |
| (1,2294) | 1:11:A:ALA:HB1  | 1:15:A:MET:HE3  | 18       | 0.13          |
| (1,2294) | 1:11:A:ALA:HB2  | 1:15:A:MET:HE1  | 18       | 0.13          |
| (1,2294) | 1:11:A:ALA:HB2  | 1:15:A:MET:HE2  | 18       | 0.13          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2294) | 1:11:A:ALA:HB2  | 1:15:A:MET:HE3   | 18       | 0.13          |
| (1,2294) | 1:11:A:ALA:HB3  | 1:15:A:MET:HE1   | 18       | 0.13          |
| (1,2294) | 1:11:A:ALA:HB3  | 1:15:A:MET:HE2   | 18       | 0.13          |
| (1,2294) | 1:11:A:ALA:HB3  | 1:15:A:MET:HE3   | 18       | 0.13          |
| (1,2282) | 1:97:A:GLY:HA2  | 1:102:A:MET:HE1  | 11       | 0.13          |
| (1,2282) | 1:97:A:GLY:HA2  | 1:102:A:MET:HE2  | 11       | 0.13          |
| (1,2282) | 1:97:A:GLY:HA2  | 1:102:A:MET:HE3  | 11       | 0.13          |
| (1,2282) | 1:97:A:GLY:HA3  | 1:102:A:MET:HE1  | 11       | 0.13          |
| (1,2282) | 1:97:A:GLY:HA3  | 1:102:A:MET:HE2  | 11       | 0.13          |
| (1,2282) | 1:97:A:GLY:HA3  | 1:102:A:MET:HE3  | 11       | 0.13          |
| (1,2216) | 1:47:A:LEU:HD11 | 1:92:A:LEU:HB2   | 13       | 0.13          |
| (1,2216) | 1:47:A:LEU:HD12 | 1:92:A:LEU:HB2   | 13       | 0.13          |
| (1,2216) | 1:47:A:LEU:HD13 | 1:92:A:LEU:HB2   | 13       | 0.13          |
| (1,2121) | 1:57:A:THR:HG21 | 1:79:A:PHE:HE2   | 6        | 0.13          |
| (1,2121) | 1:57:A:THR:HG22 | 1:79:A:PHE:HE2   | 6        | 0.13          |
| (1,2121) | 1:57:A:THR:HG23 | 1:79:A:PHE:HE2   | 6        | 0.13          |
| (1,2120) | 1:57:A:THR:HG21 | 1:79:A:PHE:HE1   | 4        | 0.13          |
| (1,2120) | 1:57:A:THR:HG22 | 1:79:A:PHE:HE1   | 4        | 0.13          |
| (1,2120) | 1:57:A:THR:HG23 | 1:79:A:PHE:HE1   | 4        | 0.13          |
| (1,2079) | 1:53:A:ASP:HB3  | 1:107:A:LEU:HD21 | 6        | 0.13          |
| (1,2079) | 1:53:A:ASP:HB3  | 1:107:A:LEU:HD22 | 6        | 0.13          |
| (1,2079) | 1:53:A:ASP:HB3  | 1:107:A:LEU:HD23 | 6        | 0.13          |
| (1,2057) | 1:25:A:LEU:HD11 | 1:88:A:LEU:H     | 14       | 0.13          |
| (1,2057) | 1:25:A:LEU:HD12 | 1:88:A:LEU:H     | 14       | 0.13          |
| (1,2057) | 1:25:A:LEU:HD13 | 1:88:A:LEU:H     | 14       | 0.13          |
| (1,2009) | 1:56:A:ALA:HB1  | 1:79:A:PHE:HD1   | 15       | 0.13          |
| (1,2009) | 1:56:A:ALA:HB2  | 1:79:A:PHE:HD1   | 15       | 0.13          |
| (1,2009) | 1:56:A:ALA:HB3  | 1:79:A:PHE:HD1   | 15       | 0.13          |
| (1,1993) | 1:72:A:PRO:HB3  | 1:78:A:TYR:HB2   | 10       | 0.13          |
| (1,1993) | 1:72:A:PRO:HB3  | 1:78:A:TYR:HB2   | 16       | 0.13          |
| (1,1903) | 1:15:A:MET:HE1  | 1:75:A:LEU:HD21  | 15       | 0.13          |
| (1,1903) | 1:15:A:MET:HE1  | 1:75:A:LEU:HD22  | 15       | 0.13          |
| (1,1903) | 1:15:A:MET:HE1  | 1:75:A:LEU:HD23  | 15       | 0.13          |
| (1,1903) | 1:15:A:MET:HE2  | 1:75:A:LEU:HD21  | 15       | 0.13          |
| (1,1903) | 1:15:A:MET:HE2  | 1:75:A:LEU:HD22  | 15       | 0.13          |
| (1,1903) | 1:15:A:MET:HE2  | 1:75:A:LEU:HD23  | 15       | 0.13          |
| (1,1903) | 1:15:A:MET:HE3  | 1:75:A:LEU:HD21  | 15       | 0.13          |
| (1,1903) | 1:15:A:MET:HE3  | 1:75:A:LEU:HD22  | 15       | 0.13          |
| (1,1903) | 1:15:A:MET:HE3  | 1:75:A:LEU:HD23  | 15       | 0.13          |
| (1,1894) | 1:84:A:GLU:HB3  | 1:86:A:VAL:HG21  | 19       | 0.13          |
| (1,1894) | 1:84:A:GLU:HB3  | 1:86:A:VAL:HG22  | 19       | 0.13          |
| (1,1894) | 1:84:A:GLU:HB3  | 1:86:A:VAL:HG23  | 19       | 0.13          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1756) | 1:38:A:VAL:HG11 | 1:39:A:PHE:HD2  | 3        | 0.13          |
| (1,1756) | 1:38:A:VAL:HG12 | 1:39:A:PHE:HD2  | 3        | 0.13          |
| (1,1756) | 1:38:A:VAL:HG13 | 1:39:A:PHE:HD2  | 3        | 0.13          |
| (1,1713) | 1:70:A:ILE:HG21 | 1:74:A:GLY:HA3  | 1        | 0.13          |
| (1,1713) | 1:70:A:ILE:HG22 | 1:74:A:GLY:HA3  | 1        | 0.13          |
| (1,1713) | 1:70:A:ILE:HG23 | 1:74:A:GLY:HA3  | 1        | 0.13          |
| (1,1713) | 1:70:A:ILE:HG21 | 1:74:A:GLY:HA3  | 6        | 0.13          |
| (1,1713) | 1:70:A:ILE:HG22 | 1:74:A:GLY:HA3  | 6        | 0.13          |
| (1,1713) | 1:70:A:ILE:HG23 | 1:74:A:GLY:HA3  | 6        | 0.13          |
| (1,1713) | 1:70:A:ILE:HG21 | 1:74:A:GLY:HA3  | 11       | 0.13          |
| (1,1713) | 1:70:A:ILE:HG22 | 1:74:A:GLY:HA3  | 11       | 0.13          |
| (1,1713) | 1:70:A:ILE:HG23 | 1:74:A:GLY:HA3  | 11       | 0.13          |
| (1,1529) | 1:65:A:LEU:HA   | 1:79:A:PHE:HD2  | 7        | 0.13          |
| (1,1528) | 1:65:A:LEU:HA   | 1:79:A:PHE:HD1  | 13       | 0.13          |
| (1,1293) | 1:68:A:ILE:HD11 | 1:79:A:PHE:HD2  | 6        | 0.13          |
| (1,1293) | 1:68:A:ILE:HD12 | 1:79:A:PHE:HD2  | 6        | 0.13          |
| (1,1293) | 1:68:A:ILE:HD13 | 1:79:A:PHE:HD2  | 6        | 0.13          |
| (1,1277) | 1:67:A:GLU:HG2  | 1:68:A:ILE:HA   | 10       | 0.13          |
| (1,1277) | 1:67:A:GLU:HG3  | 1:68:A:ILE:HA   | 10       | 0.13          |
| (1,1277) | 1:67:A:GLU:HG2  | 1:68:A:ILE:HA   | 14       | 0.13          |
| (1,1277) | 1:67:A:GLU:HG3  | 1:68:A:ILE:HA   | 14       | 0.13          |
| (1,911)  | 1:79:A:PHE:HD2  | 1:80:A:GLU:H    | 19       | 0.13          |
| (1,443)  | 1:24:A:THR:H    | 1:41:A:LEU:HB3  | 7        | 0.13          |
| (1,231)  | 1:106:A:PRO:HB3 | 1:107:A:LEU:H   | 13       | 0.13          |
| (2,23)   | 1:99:A:ALA:O    | 1:103:A:ALA:H   | 10       | 0.12          |
| (2,13)   | 1:16:A:GLU:O    | 1:20:A:ARG:H    | 3        | 0.12          |
| (2,13)   | 1:16:A:GLU:O    | 1:20:A:ARG:H    | 13       | 0.12          |
| (1,2619) | 1:55:A:GLN:HG2  | 1:101:A:TRP:HE1 | 18       | 0.12          |
| (1,2619) | 1:55:A:GLN:HG3  | 1:101:A:TRP:HE1 | 18       | 0.12          |
| (1,2606) | 1:52:A:ASP:HB2  | 1:59:A:GLY:H    | 12       | 0.12          |
| (1,2606) | 1:52:A:ASP:HB3  | 1:59:A:GLY:H    | 12       | 0.12          |
| (1,2456) | 1:8:A:LEU:HB2   | 1:9:A:GLU:H     | 5        | 0.12          |
| (1,2456) | 1:8:A:LEU:HB3   | 1:9:A:GLU:H     | 5        | 0.12          |
| (1,2271) | 1:9:A:GLU:HG3   | 1:10:A:ALA:HB1  | 8        | 0.12          |
| (1,2271) | 1:9:A:GLU:HG3   | 1:10:A:ALA:HB2  | 8        | 0.12          |
| (1,2271) | 1:9:A:GLU:HG3   | 1:10:A:ALA:HB3  | 8        | 0.12          |
| (1,2229) | 1:39:A:PHE:HD2  | 1:47:A:LEU:HD21 | 5        | 0.12          |
| (1,2229) | 1:39:A:PHE:HD2  | 1:47:A:LEU:HD22 | 5        | 0.12          |
| (1,2229) | 1:39:A:PHE:HD2  | 1:47:A:LEU:HD23 | 5        | 0.12          |
| (1,2225) | 1:47:A:LEU:HD21 | 1:48:A:LYS:HB3  | 3        | 0.12          |
| (1,2225) | 1:47:A:LEU:HD22 | 1:48:A:LYS:HB3  | 3        | 0.12          |
| (1,2225) | 1:47:A:LEU:HD23 | 1:48:A:LYS:HB3  | 3        | 0.12          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2225) | 1:47:A:LEU:HD21 | 1:48:A:LYS:HB3  | 7        | 0.12          |
| (1,2225) | 1:47:A:LEU:HD22 | 1:48:A:LYS:HB3  | 7        | 0.12          |
| (1,2225) | 1:47:A:LEU:HD23 | 1:48:A:LYS:HB3  | 7        | 0.12          |
| (1,2225) | 1:47:A:LEU:HD21 | 1:48:A:LYS:HB3  | 10       | 0.12          |
| (1,2225) | 1:47:A:LEU:HD22 | 1:48:A:LYS:HB3  | 10       | 0.12          |
| (1,2225) | 1:47:A:LEU:HD23 | 1:48:A:LYS:HB3  | 10       | 0.12          |
| (1,2225) | 1:47:A:LEU:HD21 | 1:48:A:LYS:HB3  | 17       | 0.12          |
| (1,2225) | 1:47:A:LEU:HD22 | 1:48:A:LYS:HB3  | 17       | 0.12          |
| (1,2225) | 1:47:A:LEU:HD23 | 1:48:A:LYS:HB3  | 17       | 0.12          |
| (1,2194) | 1:61:A:THR:HG21 | 1:62:A:PRO:HG2  | 13       | 0.12          |
| (1,2194) | 1:61:A:THR:HG22 | 1:62:A:PRO:HG2  | 13       | 0.12          |
| (1,2194) | 1:61:A:THR:HG23 | 1:62:A:PRO:HG2  | 13       | 0.12          |
| (1,2134) | 1:57:A:THR:HG21 | 1:82:A:LEU:HB2  | 5        | 0.12          |
| (1,2134) | 1:57:A:THR:HG21 | 1:82:A:LEU:HB3  | 5        | 0.12          |
| (1,2134) | 1:57:A:THR:HG22 | 1:82:A:LEU:HB2  | 5        | 0.12          |
| (1,2134) | 1:57:A:THR:HG22 | 1:82:A:LEU:HB3  | 5        | 0.12          |
| (1,2134) | 1:57:A:THR:HG23 | 1:82:A:LEU:HB2  | 5        | 0.12          |
| (1,2134) | 1:57:A:THR:HG23 | 1:82:A:LEU:HB3  | 5        | 0.12          |
| (1,2120) | 1:57:A:THR:HG21 | 1:79:A:PHE:HE1  | 7        | 0.12          |
| (1,2120) | 1:57:A:THR:HG22 | 1:79:A:PHE:HE1  | 7        | 0.12          |
| (1,2120) | 1:57:A:THR:HG23 | 1:79:A:PHE:HE1  | 7        | 0.12          |
| (1,2057) | 1:25:A:LEU:HD11 | 1:88:A:LEU:H    | 4        | 0.12          |
| (1,2057) | 1:25:A:LEU:HD12 | 1:88:A:LEU:H    | 4        | 0.12          |
| (1,2057) | 1:25:A:LEU:HD13 | 1:88:A:LEU:H    | 4        | 0.12          |
| (1,2040) | 1:43:A:ASN:HA   | 1:45:A:ARG:H    | 13       | 0.12          |
| (1,2034) | 1:104:A:GLU:HA  | 1:106:A:PRO:HD2 | 4        | 0.12          |
| (1,2034) | 1:104:A:GLU:HA  | 1:106:A:PRO:HD2 | 11       | 0.12          |
| (1,2034) | 1:104:A:GLU:HA  | 1:106:A:PRO:HD2 | 12       | 0.12          |
| (1,2034) | 1:104:A:GLU:HA  | 1:106:A:PRO:HD2 | 16       | 0.12          |
| (1,1950) | 1:15:A:MET:HE1  | 1:89:A:ILE:HD11 | 4        | 0.12          |
| (1,1950) | 1:15:A:MET:HE1  | 1:89:A:ILE:HD12 | 4        | 0.12          |
| (1,1950) | 1:15:A:MET:HE1  | 1:89:A:ILE:HD13 | 4        | 0.12          |
| (1,1950) | 1:15:A:MET:HE2  | 1:89:A:ILE:HD11 | 4        | 0.12          |
| (1,1950) | 1:15:A:MET:HE2  | 1:89:A:ILE:HD12 | 4        | 0.12          |
| (1,1950) | 1:15:A:MET:HE2  | 1:89:A:ILE:HD13 | 4        | 0.12          |
| (1,1950) | 1:15:A:MET:HE3  | 1:89:A:ILE:HD11 | 4        | 0.12          |
| (1,1950) | 1:15:A:MET:HE3  | 1:89:A:ILE:HD12 | 4        | 0.12          |
| (1,1950) | 1:15:A:MET:HE3  | 1:89:A:ILE:HD13 | 4        | 0.12          |
| (1,1950) | 1:15:A:MET:HE1  | 1:89:A:ILE:HD11 | 10       | 0.12          |
| (1,1950) | 1:15:A:MET:HE1  | 1:89:A:ILE:HD12 | 10       | 0.12          |
| (1,1950) | 1:15:A:MET:HE1  | 1:89:A:ILE:HD13 | 10       | 0.12          |
| (1,1950) | 1:15:A:MET:HE2  | 1:89:A:ILE:HD11 | 10       | 0.12          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1950) | 1:15:A:MET:HE2  | 1:89:A:ILE:HD12 | 10       | 0.12          |
| (1,1950) | 1:15:A:MET:HE2  | 1:89:A:ILE:HD13 | 10       | 0.12          |
| (1,1950) | 1:15:A:MET:HE3  | 1:89:A:ILE:HD11 | 10       | 0.12          |
| (1,1950) | 1:15:A:MET:HE3  | 1:89:A:ILE:HD12 | 10       | 0.12          |
| (1,1950) | 1:15:A:MET:HE3  | 1:89:A:ILE:HD13 | 10       | 0.12          |
| (1,1950) | 1:15:A:MET:HE1  | 1:89:A:ILE:HD11 | 16       | 0.12          |
| (1,1950) | 1:15:A:MET:HE1  | 1:89:A:ILE:HD12 | 16       | 0.12          |
| (1,1950) | 1:15:A:MET:HE1  | 1:89:A:ILE:HD13 | 16       | 0.12          |
| (1,1950) | 1:15:A:MET:HE2  | 1:89:A:ILE:HD11 | 16       | 0.12          |
| (1,1950) | 1:15:A:MET:HE2  | 1:89:A:ILE:HD12 | 16       | 0.12          |
| (1,1950) | 1:15:A:MET:HE2  | 1:89:A:ILE:HD13 | 16       | 0.12          |
| (1,1950) | 1:15:A:MET:HE3  | 1:89:A:ILE:HD11 | 16       | 0.12          |
| (1,1950) | 1:15:A:MET:HE3  | 1:89:A:ILE:HD12 | 16       | 0.12          |
| (1,1950) | 1:15:A:MET:HE3  | 1:89:A:ILE:HD13 | 16       | 0.12          |
| (1,1945) | 1:89:A:ILE:HG21 | 1:93:A:GLU:HB3  | 17       | 0.12          |
| (1,1945) | 1:89:A:ILE:HG22 | 1:93:A:GLU:HB3  | 17       | 0.12          |
| (1,1945) | 1:89:A:ILE:HG23 | 1:93:A:GLU:HB3  | 17       | 0.12          |
| (1,1903) | 1:15:A:MET:HE1  | 1:75:A:LEU:HD21 | 2        | 0.12          |
| (1,1903) | 1:15:A:MET:HE1  | 1:75:A:LEU:HD22 | 2        | 0.12          |
| (1,1903) | 1:15:A:MET:HE1  | 1:75:A:LEU:HD23 | 2        | 0.12          |
| (1,1903) | 1:15:A:MET:HE2  | 1:75:A:LEU:HD21 | 2        | 0.12          |
| (1,1903) | 1:15:A:MET:HE2  | 1:75:A:LEU:HD22 | 2        | 0.12          |
| (1,1903) | 1:15:A:MET:HE2  | 1:75:A:LEU:HD23 | 2        | 0.12          |
| (1,1903) | 1:15:A:MET:HE3  | 1:75:A:LEU:HD21 | 2        | 0.12          |
| (1,1903) | 1:15:A:MET:HE3  | 1:75:A:LEU:HD22 | 2        | 0.12          |
| (1,1903) | 1:15:A:MET:HE3  | 1:75:A:LEU:HD23 | 2        | 0.12          |
| (1,1903) | 1:15:A:MET:HE1  | 1:75:A:LEU:HD21 | 13       | 0.12          |
| (1,1903) | 1:15:A:MET:HE1  | 1:75:A:LEU:HD22 | 13       | 0.12          |
| (1,1903) | 1:15:A:MET:HE1  | 1:75:A:LEU:HD23 | 13       | 0.12          |
| (1,1903) | 1:15:A:MET:HE2  | 1:75:A:LEU:HD21 | 13       | 0.12          |
| (1,1903) | 1:15:A:MET:HE2  | 1:75:A:LEU:HD22 | 13       | 0.12          |
| (1,1903) | 1:15:A:MET:HE2  | 1:75:A:LEU:HD23 | 13       | 0.12          |
| (1,1903) | 1:15:A:MET:HE3  | 1:75:A:LEU:HD21 | 13       | 0.12          |
| (1,1903) | 1:15:A:MET:HE3  | 1:75:A:LEU:HD22 | 13       | 0.12          |
| (1,1903) | 1:15:A:MET:HE3  | 1:75:A:LEU:HD23 | 13       | 0.12          |
| (1,1894) | 1:84:A:GLU:HB3  | 1:86:A:VAL:HG21 | 7        | 0.12          |
| (1,1894) | 1:84:A:GLU:HB3  | 1:86:A:VAL:HG22 | 7        | 0.12          |
| (1,1894) | 1:84:A:GLU:HB3  | 1:86:A:VAL:HG23 | 7        | 0.12          |
| (1,1713) | 1:70:A:ILE:HG21 | 1:74:A:GLY:HA3  | 8        | 0.12          |
| (1,1713) | 1:70:A:ILE:HG22 | 1:74:A:GLY:HA3  | 8        | 0.12          |
| (1,1713) | 1:70:A:ILE:HG23 | 1:74:A:GLY:HA3  | 8        | 0.12          |
| (1,1713) | 1:70:A:ILE:HG21 | 1:74:A:GLY:HA3  | 9        | 0.12          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1713) | 1:70:A:ILE:HG22 | 1:74:A:GLY:HA3  | 9        | 0.12          |
| (1,1713) | 1:70:A:ILE:HG23 | 1:74:A:GLY:HA3  | 9        | 0.12          |
| (1,1671) | 1:71:A:SER:HA   | 1:77:A:VAL:HG11 | 8        | 0.12          |
| (1,1671) | 1:71:A:SER:HA   | 1:77:A:VAL:HG12 | 8        | 0.12          |
| (1,1671) | 1:71:A:SER:HA   | 1:77:A:VAL:HG13 | 8        | 0.12          |
| (1,1671) | 1:71:A:SER:HA   | 1:77:A:VAL:HG11 | 12       | 0.12          |
| (1,1671) | 1:71:A:SER:HA   | 1:77:A:VAL:HG12 | 12       | 0.12          |
| (1,1671) | 1:71:A:SER:HA   | 1:77:A:VAL:HG13 | 12       | 0.12          |
| (1,1593) | 1:49:A:PHE:HE1  | 1:54:A:LEU:HD21 | 19       | 0.12          |
| (1,1593) | 1:49:A:PHE:HE1  | 1:54:A:LEU:HD22 | 19       | 0.12          |
| (1,1593) | 1:49:A:PHE:HE1  | 1:54:A:LEU:HD23 | 19       | 0.12          |
| (1,1528) | 1:65:A:LEU:HA   | 1:79:A:PHE:HD1  | 1        | 0.12          |
| (1,1528) | 1:65:A:LEU:HA   | 1:79:A:PHE:HD1  | 16       | 0.12          |
| (1,1528) | 1:65:A:LEU:HA   | 1:79:A:PHE:HD1  | 19       | 0.12          |
| (1,1444) | 1:79:A:PHE:HD1  | 1:82:A:LEU:HD11 | 5        | 0.12          |
| (1,1444) | 1:79:A:PHE:HD1  | 1:82:A:LEU:HD12 | 5        | 0.12          |
| (1,1444) | 1:79:A:PHE:HD1  | 1:82:A:LEU:HD13 | 5        | 0.12          |
| (1,1444) | 1:79:A:PHE:HD1  | 1:82:A:LEU:HD11 | 18       | 0.12          |
| (1,1444) | 1:79:A:PHE:HD1  | 1:82:A:LEU:HD12 | 18       | 0.12          |
| (1,1444) | 1:79:A:PHE:HD1  | 1:82:A:LEU:HD13 | 18       | 0.12          |
| (1,1434) | 1:65:A:LEU:HG   | 1:82:A:LEU:HD11 | 7        | 0.12          |
| (1,1434) | 1:65:A:LEU:HG   | 1:82:A:LEU:HD12 | 7        | 0.12          |
| (1,1434) | 1:65:A:LEU:HG   | 1:82:A:LEU:HD13 | 7        | 0.12          |
| (1,1420) | 1:82:A:LEU:HB2  | 1:84:A:GLU:HG3  | 10       | 0.12          |
| (1,1420) | 1:82:A:LEU:HB3  | 1:84:A:GLU:HG3  | 10       | 0.12          |
| (1,1298) | 1:68:A:ILE:HG13 | 1:79:A:PHE:HD2  | 1        | 0.12          |
| (1,1298) | 1:68:A:ILE:HG13 | 1:79:A:PHE:HD2  | 18       | 0.12          |
| (1,930)  | 1:105:A:HIS:H   | 1:106:A:PRO:HB3 | 4        | 0.12          |
| (1,928)  | 1:52:A:ASP:H    | 1:58:A:TYR:HE1  | 15       | 0.12          |
| (1,864)  | 1:25:A:LEU:HD21 | 1:28:A:VAL:H    | 20       | 0.12          |
| (1,864)  | 1:25:A:LEU:HD22 | 1:28:A:VAL:H    | 20       | 0.12          |
| (1,864)  | 1:25:A:LEU:HD23 | 1:28:A:VAL:H    | 20       | 0.12          |
| (1,793)  | 1:67:A:GLU:H    | 1:81:A:THR:HG21 | 7        | 0.12          |
| (1,793)  | 1:67:A:GLU:H    | 1:81:A:THR:HG22 | 7        | 0.12          |
| (1,793)  | 1:67:A:GLU:H    | 1:81:A:THR:HG23 | 7        | 0.12          |
| (1,618)  | 1:60:A:ALA:H    | 1:82:A:LEU:HD11 | 14       | 0.12          |
| (1,618)  | 1:60:A:ALA:H    | 1:82:A:LEU:HD12 | 14       | 0.12          |
| (1,618)  | 1:60:A:ALA:H    | 1:82:A:LEU:HD13 | 14       | 0.12          |
| (1,528)  | 1:61:A:THR:H    | 1:64:A:GLN:HA   | 7        | 0.12          |
| (1,528)  | 1:61:A:THR:H    | 1:64:A:GLN:HA   | 17       | 0.12          |
| (1,521)  | 1:18:A:LEU:HD21 | 1:21:A:GLU:H    | 18       | 0.12          |
| (1,521)  | 1:18:A:LEU:HD22 | 1:21:A:GLU:H    | 18       | 0.12          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,521)  | 1:18:A:LEU:HD23 | 1:21:A:GLU:H    | 18       | 0.12          |
| (1,456)  | 1:25:A:LEU:H    | 1:88:A:LEU:HG   | 2        | 0.12          |
| (1,288)  | 1:47:A:LEU:HD11 | 1:48:A:LYS:H    | 12       | 0.12          |
| (1,288)  | 1:47:A:LEU:HD12 | 1:48:A:LYS:H    | 12       | 0.12          |
| (1,288)  | 1:47:A:LEU:HD13 | 1:48:A:LYS:H    | 12       | 0.12          |
| (1,288)  | 1:47:A:LEU:HD11 | 1:48:A:LYS:H    | 18       | 0.12          |
| (1,288)  | 1:47:A:LEU:HD12 | 1:48:A:LYS:H    | 18       | 0.12          |
| (1,288)  | 1:47:A:LEU:HD13 | 1:48:A:LYS:H    | 18       | 0.12          |
| (1,179)  | 1:29:A:GLN:HG2  | 1:30:A:TYR:H    | 19       | 0.12          |
| (2,55)   | 1:79:A:PHE:O    | 1:84:A:GLU:H    | 16       | 0.11          |
| (2,51)   | 1:78:A:TYR:O    | 1:69:A:GLU:H    | 17       | 0.11          |
| (2,23)   | 1:99:A:ALA:O    | 1:103:A:ALA:H   | 12       | 0.11          |
| (2,23)   | 1:99:A:ALA:O    | 1:103:A:ALA:H   | 19       | 0.11          |
| (2,13)   | 1:16:A:GLU:O    | 1:20:A:ARG:H    | 8        | 0.11          |
| (2,13)   | 1:16:A:GLU:O    | 1:20:A:ARG:H    | 12       | 0.11          |
| (2,13)   | 1:16:A:GLU:O    | 1:20:A:ARG:H    | 20       | 0.11          |
| (1,2615) | 1:54:A:LEU:HD21 | 1:96:A:ARG:HG2  | 9        | 0.11          |
| (1,2615) | 1:54:A:LEU:HD21 | 1:96:A:ARG:HG3  | 9        | 0.11          |
| (1,2615) | 1:54:A:LEU:HD22 | 1:96:A:ARG:HG2  | 9        | 0.11          |
| (1,2615) | 1:54:A:LEU:HD22 | 1:96:A:ARG:HG3  | 9        | 0.11          |
| (1,2615) | 1:54:A:LEU:HD23 | 1:96:A:ARG:HG2  | 9        | 0.11          |
| (1,2615) | 1:54:A:LEU:HD23 | 1:96:A:ARG:HG3  | 9        | 0.11          |
| (1,2335) | 1:41:A:LEU:HB3  | 1:45:A:ARG:HB2  | 8        | 0.11          |
| (1,2335) | 1:41:A:LEU:HB3  | 1:45:A:ARG:HB3  | 8        | 0.11          |
| (1,2320) | 1:25:A:LEU:HB3  | 1:70:A:ILE:HG12 | 15       | 0.11          |
| (1,2267) | 1:43:A:ASN:HD21 | 1:45:A:ARG:HD3  | 15       | 0.11          |
| (1,2216) | 1:47:A:LEU:HD11 | 1:92:A:LEU:HB2  | 7        | 0.11          |
| (1,2216) | 1:47:A:LEU:HD12 | 1:92:A:LEU:HB2  | 7        | 0.11          |
| (1,2216) | 1:47:A:LEU:HD13 | 1:92:A:LEU:HB2  | 7        | 0.11          |
| (1,2202) | 1:61:A:THR:HB   | 1:62:A:PRO:HG3  | 13       | 0.11          |
| (1,2196) | 1:61:A:THR:HG21 | 1:63:A:GLU:HB2  | 6        | 0.11          |
| (1,2196) | 1:61:A:THR:HG21 | 1:63:A:GLU:HB3  | 6        | 0.11          |
| (1,2196) | 1:61:A:THR:HG22 | 1:63:A:GLU:HB2  | 6        | 0.11          |
| (1,2196) | 1:61:A:THR:HG22 | 1:63:A:GLU:HB3  | 6        | 0.11          |
| (1,2196) | 1:61:A:THR:HG23 | 1:63:A:GLU:HB2  | 6        | 0.11          |
| (1,2196) | 1:61:A:THR:HG23 | 1:63:A:GLU:HB3  | 6        | 0.11          |
| (1,2194) | 1:61:A:THR:HG21 | 1:62:A:PRO:HG2  | 2        | 0.11          |
| (1,2194) | 1:61:A:THR:HG22 | 1:62:A:PRO:HG2  | 2        | 0.11          |
| (1,2194) | 1:61:A:THR:HG23 | 1:62:A:PRO:HG2  | 2        | 0.11          |
| (1,2139) | 1:9:A:GLU:HA    | 1:12:A:SER:HB2  | 8        | 0.11          |
| (1,2139) | 1:9:A:GLU:HA    | 1:12:A:SER:HB3  | 8        | 0.11          |
| (1,2133) | 1:57:A:THR:HG21 | 1:84:A:GLU:HB2  | 9        | 0.11          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2133) | 1:57:A:THR:HG22 | 1:84:A:GLU:HB2  | 9        | 0.11          |
| (1,2133) | 1:57:A:THR:HG23 | 1:84:A:GLU:HB2  | 9        | 0.11          |
| (1,2120) | 1:57:A:THR:HG21 | 1:79:A:PHE:HE1  | 10       | 0.11          |
| (1,2120) | 1:57:A:THR:HG22 | 1:79:A:PHE:HE1  | 10       | 0.11          |
| (1,2120) | 1:57:A:THR:HG23 | 1:79:A:PHE:HE1  | 10       | 0.11          |
| (1,2057) | 1:25:A:LEU:HD11 | 1:88:A:LEU:H    | 10       | 0.11          |
| (1,2057) | 1:25:A:LEU:HD12 | 1:88:A:LEU:H    | 10       | 0.11          |
| (1,2057) | 1:25:A:LEU:HD13 | 1:88:A:LEU:H    | 10       | 0.11          |
| (1,2034) | 1:104:A:GLU:HA  | 1:106:A:PRO:HD2 | 2        | 0.11          |
| (1,1996) | 1:78:A:TYR:HA   | 1:79:A:PHE:HD2  | 12       | 0.11          |
| (1,1996) | 1:78:A:TYR:HA   | 1:79:A:PHE:HD2  | 13       | 0.11          |
| (1,1996) | 1:78:A:TYR:HA   | 1:79:A:PHE:HD2  | 16       | 0.11          |
| (1,1993) | 1:72:A:PRO:HB3  | 1:78:A:TYR:HB2  | 11       | 0.11          |
| (1,1960) | 1:33:A:GLU:HA   | 1:34:A:GLU:HG2  | 5        | 0.11          |
| (1,1950) | 1:15:A:MET:HE1  | 1:89:A:ILE:HD11 | 8        | 0.11          |
| (1,1950) | 1:15:A:MET:HE1  | 1:89:A:ILE:HD12 | 8        | 0.11          |
| (1,1950) | 1:15:A:MET:HE1  | 1:89:A:ILE:HD13 | 8        | 0.11          |
| (1,1950) | 1:15:A:MET:HE2  | 1:89:A:ILE:HD11 | 8        | 0.11          |
| (1,1950) | 1:15:A:MET:HE2  | 1:89:A:ILE:HD12 | 8        | 0.11          |
| (1,1950) | 1:15:A:MET:HE2  | 1:89:A:ILE:HD13 | 8        | 0.11          |
| (1,1950) | 1:15:A:MET:HE3  | 1:89:A:ILE:HD11 | 8        | 0.11          |
| (1,1950) | 1:15:A:MET:HE3  | 1:89:A:ILE:HD12 | 8        | 0.11          |
| (1,1950) | 1:15:A:MET:HE3  | 1:89:A:ILE:HD13 | 8        | 0.11          |
| (1,1872) | 1:79:A:PHE:HE2  | 1:86:A:VAL:HB   | 18       | 0.11          |
| (1,1806) | 1:28:A:VAL:HG21 | 1:79:A:PHE:HE2  | 5        | 0.11          |
| (1,1806) | 1:28:A:VAL:HG22 | 1:79:A:PHE:HE2  | 5        | 0.11          |
| (1,1806) | 1:28:A:VAL:HG23 | 1:79:A:PHE:HE2  | 5        | 0.11          |
| (1,1756) | 1:38:A:VAL:HG11 | 1:39:A:PHE:HD2  | 15       | 0.11          |
| (1,1756) | 1:38:A:VAL:HG12 | 1:39:A:PHE:HD2  | 15       | 0.11          |
| (1,1756) | 1:38:A:VAL:HG13 | 1:39:A:PHE:HD2  | 15       | 0.11          |
| (1,1726) | 1:11:A:ALA:HA   | 1:15:A:MET:HE1  | 19       | 0.11          |
| (1,1726) | 1:11:A:ALA:HA   | 1:15:A:MET:HE2  | 19       | 0.11          |
| (1,1726) | 1:11:A:ALA:HA   | 1:15:A:MET:HE3  | 19       | 0.11          |
| (1,1671) | 1:71:A:SER:HA   | 1:77:A:VAL:HG11 | 5        | 0.11          |
| (1,1671) | 1:71:A:SER:HA   | 1:77:A:VAL:HG12 | 5        | 0.11          |
| (1,1671) | 1:71:A:SER:HA   | 1:77:A:VAL:HG13 | 5        | 0.11          |
| (1,1652) | 1:71:A:SER:HA   | 1:77:A:VAL:HG21 | 11       | 0.11          |
| (1,1652) | 1:71:A:SER:HA   | 1:77:A:VAL:HG22 | 11       | 0.11          |
| (1,1652) | 1:71:A:SER:HA   | 1:77:A:VAL:HG23 | 11       | 0.11          |
| (1,1529) | 1:65:A:LEU:HA   | 1:79:A:PHE:HD2  | 3        | 0.11          |
| (1,1528) | 1:65:A:LEU:HA   | 1:79:A:PHE:HD1  | 9        | 0.11          |
| (1,1434) | 1:65:A:LEU:HG   | 1:82:A:LEU:HD11 | 18       | 0.11          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1434) | 1:65:A:LEU:HG   | 1:82:A:LEU:HD12 | 18       | 0.11          |
| (1,1434) | 1:65:A:LEU:HG   | 1:82:A:LEU:HD13 | 18       | 0.11          |
| (1,1420) | 1:82:A:LEU:HB2  | 1:84:A:GLU:HG3  | 4        | 0.11          |
| (1,1420) | 1:82:A:LEU:HB3  | 1:84:A:GLU:HG3  | 4        | 0.11          |
| (1,1420) | 1:82:A:LEU:HB2  | 1:84:A:GLU:HG3  | 19       | 0.11          |
| (1,1420) | 1:82:A:LEU:HB3  | 1:84:A:GLU:HG3  | 19       | 0.11          |
| (1,1416) | 1:7:A:GLU:HG2   | 1:8:A:LEU:HD21  | 1        | 0.11          |
| (1,1416) | 1:7:A:GLU:HG2   | 1:8:A:LEU:HD22  | 1        | 0.11          |
| (1,1416) | 1:7:A:GLU:HG2   | 1:8:A:LEU:HD23  | 1        | 0.11          |
| (1,1416) | 1:7:A:GLU:HG3   | 1:8:A:LEU:HD21  | 1        | 0.11          |
| (1,1416) | 1:7:A:GLU:HG3   | 1:8:A:LEU:HD22  | 1        | 0.11          |
| (1,1416) | 1:7:A:GLU:HG3   | 1:8:A:LEU:HD23  | 1        | 0.11          |
| (1,1330) | 1:41:A:LEU:HD21 | 1:43:A:ASN:HD21 | 20       | 0.11          |
| (1,1330) | 1:41:A:LEU:HD22 | 1:43:A:ASN:HD21 | 20       | 0.11          |
| (1,1330) | 1:41:A:LEU:HD23 | 1:43:A:ASN:HD21 | 20       | 0.11          |
| (1,1322) | 1:26:A:ARG:HB3  | 1:41:A:LEU:HA   | 18       | 0.11          |
| (1,1298) | 1:68:A:ILE:HG13 | 1:79:A:PHE:HD2  | 3        | 0.11          |
| (1,1298) | 1:68:A:ILE:HG13 | 1:79:A:PHE:HD2  | 6        | 0.11          |
| (1,1298) | 1:68:A:ILE:HG13 | 1:79:A:PHE:HD2  | 9        | 0.11          |
| (1,1298) | 1:68:A:ILE:HG13 | 1:79:A:PHE:HD2  | 12       | 0.11          |
| (1,1293) | 1:68:A:ILE:HD11 | 1:79:A:PHE:HD2  | 5        | 0.11          |
| (1,1293) | 1:68:A:ILE:HD12 | 1:79:A:PHE:HD2  | 5        | 0.11          |
| (1,1293) | 1:68:A:ILE:HD13 | 1:79:A:PHE:HD2  | 5        | 0.11          |
| (1,1293) | 1:68:A:ILE:HD11 | 1:79:A:PHE:HD2  | 19       | 0.11          |
| (1,1293) | 1:68:A:ILE:HD12 | 1:79:A:PHE:HD2  | 19       | 0.11          |
| (1,1293) | 1:68:A:ILE:HD13 | 1:79:A:PHE:HD2  | 19       | 0.11          |
| (1,868)  | 1:55:A:GLN:H    | 1:58:A:TYR:HB2  | 19       | 0.11          |
| (1,864)  | 1:25:A:LEU:HD21 | 1:28:A:VAL:H    | 4        | 0.11          |
| (1,864)  | 1:25:A:LEU:HD22 | 1:28:A:VAL:H    | 4        | 0.11          |
| (1,864)  | 1:25:A:LEU:HD23 | 1:28:A:VAL:H    | 4        | 0.11          |
| (1,864)  | 1:25:A:LEU:HD21 | 1:28:A:VAL:H    | 13       | 0.11          |
| (1,864)  | 1:25:A:LEU:HD22 | 1:28:A:VAL:H    | 13       | 0.11          |
| (1,864)  | 1:25:A:LEU:HD23 | 1:28:A:VAL:H    | 13       | 0.11          |
| (1,864)  | 1:25:A:LEU:HD21 | 1:28:A:VAL:H    | 16       | 0.11          |
| (1,864)  | 1:25:A:LEU:HD22 | 1:28:A:VAL:H    | 16       | 0.11          |
| (1,864)  | 1:25:A:LEU:HD23 | 1:28:A:VAL:H    | 16       | 0.11          |
| (1,793)  | 1:67:A:GLU:H    | 1:81:A:THR:HG21 | 8        | 0.11          |
| (1,793)  | 1:67:A:GLU:H    | 1:81:A:THR:HG22 | 8        | 0.11          |
| (1,793)  | 1:67:A:GLU:H    | 1:81:A:THR:HG23 | 8        | 0.11          |
| (1,528)  | 1:61:A:THR:H    | 1:64:A:GLN:HA   | 1        | 0.11          |
| (1,521)  | 1:18:A:LEU:HD21 | 1:21:A:GLU:H    | 10       | 0.11          |
| (1,521)  | 1:18:A:LEU:HD22 | 1:21:A:GLU:H    | 10       | 0.11          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,521)  | 1:18:A:LEU:HD23 | 1:21:A:GLU:H    | 10       | 0.11          |
| (1,456)  | 1:25:A:LEU:H    | 1:88:A:LEU:HG   | 17       | 0.11          |
| (1,443)  | 1:24:A:THR:H    | 1:41:A:LEU:HB3  | 18       | 0.11          |
| (1,376)  | 1:65:A:LEU:H    | 1:66:A:ARG:HG2  | 6        | 0.11          |
| (1,376)  | 1:65:A:LEU:H    | 1:66:A:ARG:HG2  | 15       | 0.11          |
| (1,376)  | 1:65:A:LEU:H    | 1:66:A:ARG:HG2  | 19       | 0.11          |
| (1,288)  | 1:47:A:LEU:HD11 | 1:48:A:LYS:H    | 1        | 0.11          |
| (1,288)  | 1:47:A:LEU:HD12 | 1:48:A:LYS:H    | 1        | 0.11          |
| (1,288)  | 1:47:A:LEU:HD13 | 1:48:A:LYS:H    | 1        | 0.11          |
| (1,259)  | 1:107:A:LEU:HG  | 1:108:A:ALA:H   | 19       | 0.11          |
| (1,179)  | 1:29:A:GLN:HG2  | 1:30:A:TYR:H    | 3        | 0.11          |
| (1,179)  | 1:29:A:GLN:HG2  | 1:30:A:TYR:H    | 9        | 0.11          |
| (2,55)   | 1:79:A:PHE:O    | 1:84:A:GLU:H    | 19       | 0.1           |
| (2,25)   | 1:100:A:LYS:O   | 1:104:A:GLU:H   | 11       | 0.1           |
| (2,13)   | 1:16:A:GLU:O    | 1:20:A:ARG:H    | 6        | 0.1           |
| (2,5)    | 1:12:A:SER:O    | 1:16:A:GLU:H    | 5        | 0.1           |
| (1,2426) | 1:69:A:GLU:HB2  | 1:78:A:TYR:HE1  | 3        | 0.1           |
| (1,2426) | 1:69:A:GLU:HB3  | 1:78:A:TYR:HE1  | 3        | 0.1           |
| (1,2291) | 1:15:A:MET:HE1  | 1:73:A:SER:HB2  | 5        | 0.1           |
| (1,2291) | 1:15:A:MET:HE1  | 1:73:A:SER:HB3  | 5        | 0.1           |
| (1,2291) | 1:15:A:MET:HE2  | 1:73:A:SER:HB2  | 5        | 0.1           |
| (1,2291) | 1:15:A:MET:HE2  | 1:73:A:SER:HB3  | 5        | 0.1           |
| (1,2291) | 1:15:A:MET:HE3  | 1:73:A:SER:HB2  | 5        | 0.1           |
| (1,2291) | 1:15:A:MET:HE3  | 1:73:A:SER:HB3  | 5        | 0.1           |
| (1,2281) | 1:99:A:ALA:HA   | 1:102:A:MET:HE1 | 20       | 0.1           |
| (1,2281) | 1:99:A:ALA:HA   | 1:102:A:MET:HE2 | 20       | 0.1           |
| (1,2281) | 1:99:A:ALA:HA   | 1:102:A:MET:HE3 | 20       | 0.1           |
| (1,2194) | 1:61:A:THR:HG21 | 1:62:A:PRO:HG2  | 4        | 0.1           |
| (1,2194) | 1:61:A:THR:HG22 | 1:62:A:PRO:HG2  | 4        | 0.1           |
| (1,2194) | 1:61:A:THR:HG23 | 1:62:A:PRO:HG2  | 4        | 0.1           |
| (1,2057) | 1:25:A:LEU:HD11 | 1:88:A:LEU:H    | 15       | 0.1           |
| (1,2057) | 1:25:A:LEU:HD12 | 1:88:A:LEU:H    | 15       | 0.1           |
| (1,2057) | 1:25:A:LEU:HD13 | 1:88:A:LEU:H    | 15       | 0.1           |
| (1,2034) | 1:104:A:GLU:HA  | 1:106:A:PRO:HD2 | 9        | 0.1           |
| (1,1993) | 1:72:A:PRO:HB3  | 1:78:A:TYR:HB2  | 1        | 0.1           |
| (1,1575) | 1:67:A:GLU:HA   | 1:68:A:ILE:HD11 | 17       | 0.1           |
| (1,1575) | 1:67:A:GLU:HA   | 1:68:A:ILE:HD12 | 17       | 0.1           |
| (1,1575) | 1:67:A:GLU:HA   | 1:68:A:ILE:HD13 | 17       | 0.1           |
| (1,1528) | 1:65:A:LEU:HA   | 1:79:A:PHE:HD1  | 10       | 0.1           |
| (1,1528) | 1:65:A:LEU:HA   | 1:79:A:PHE:HD1  | 15       | 0.1           |
| (1,1528) | 1:65:A:LEU:HA   | 1:79:A:PHE:HD1  | 18       | 0.1           |
| (1,1293) | 1:68:A:ILE:HD11 | 1:79:A:PHE:HD2  | 3        | 0.1           |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1293) | 1:68:A:ILE:HD12 | 1:79:A:PHE:HD2 | 3        | 0.1           |
| (1,1293) | 1:68:A:ILE:HD13 | 1:79:A:PHE:HD2 | 3        | 0.1           |
| (1,932)  | 1:79:A:PHE:H    | 1:82:A:LEU:HB2 | 4        | 0.1           |
| (1,932)  | 1:79:A:PHE:H    | 1:82:A:LEU:HB3 | 4        | 0.1           |
| (1,932)  | 1:79:A:PHE:H    | 1:82:A:LEU:HB2 | 18       | 0.1           |
| (1,932)  | 1:79:A:PHE:H    | 1:82:A:LEU:HB3 | 18       | 0.1           |
| (1,928)  | 1:52:A:ASP:H    | 1:58:A:TYR:HE1 | 4        | 0.1           |
| (1,911)  | 1:79:A:PHE:HD2  | 1:80:A:GLU:H   | 16       | 0.1           |
| (1,869)  | 1:55:A:GLN:H    | 1:96:A:ARG:HB3 | 7        | 0.1           |
| (1,868)  | 1:55:A:GLN:H    | 1:58:A:TYR:HB2 | 8        | 0.1           |
| (1,864)  | 1:25:A:LEU:HD21 | 1:28:A:VAL:H   | 3        | 0.1           |
| (1,864)  | 1:25:A:LEU:HD22 | 1:28:A:VAL:H   | 3        | 0.1           |
| (1,864)  | 1:25:A:LEU:HD23 | 1:28:A:VAL:H   | 3        | 0.1           |
| (1,864)  | 1:25:A:LEU:HD21 | 1:28:A:VAL:H   | 5        | 0.1           |
| (1,864)  | 1:25:A:LEU:HD22 | 1:28:A:VAL:H   | 5        | 0.1           |
| (1,864)  | 1:25:A:LEU:HD23 | 1:28:A:VAL:H   | 5        | 0.1           |
| (1,791)  | 1:67:A:GLU:H    | 1:67:A:GLU:HG2 | 17       | 0.1           |
| (1,791)  | 1:67:A:GLU:H    | 1:67:A:GLU:HG3 | 17       | 0.1           |
| (1,669)  | 1:50:A:ARG:HG2  | 1:52:A:ASP:H   | 20       | 0.1           |
| (1,669)  | 1:50:A:ARG:HG3  | 1:52:A:ASP:H   | 20       | 0.1           |
| (1,528)  | 1:61:A:THR:H    | 1:64:A:GLN:HA  | 3        | 0.1           |
| (1,528)  | 1:61:A:THR:H    | 1:64:A:GLN:HA  | 9        | 0.1           |
| (1,456)  | 1:25:A:LEU:H    | 1:88:A:LEU:HG  | 15       | 0.1           |
| (1,288)  | 1:47:A:LEU:HD11 | 1:48:A:LYS:H   | 6        | 0.1           |
| (1,288)  | 1:47:A:LEU:HD12 | 1:48:A:LYS:H   | 6        | 0.1           |
| (1,288)  | 1:47:A:LEU:HD13 | 1:48:A:LYS:H   | 6        | 0.1           |
| (1,231)  | 1:106:A:PRO:HB3 | 1:107:A:LEU:H  | 19       | 0.1           |
| (1,231)  | 1:106:A:PRO:HB3 | 1:107:A:LEU:H  | 20       | 0.1           |
| (1,201)  | 1:33:A:GLU:HB2  | 1:34:A:GLU:H   | 13       | 0.1           |
| (1,201)  | 1:33:A:GLU:HB3  | 1:34:A:GLU:H   | 13       | 0.1           |
| (1,50)   | 1:3:A:VAL:HA    | 1:4:A:SER:H    | 3        | 0.1           |

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

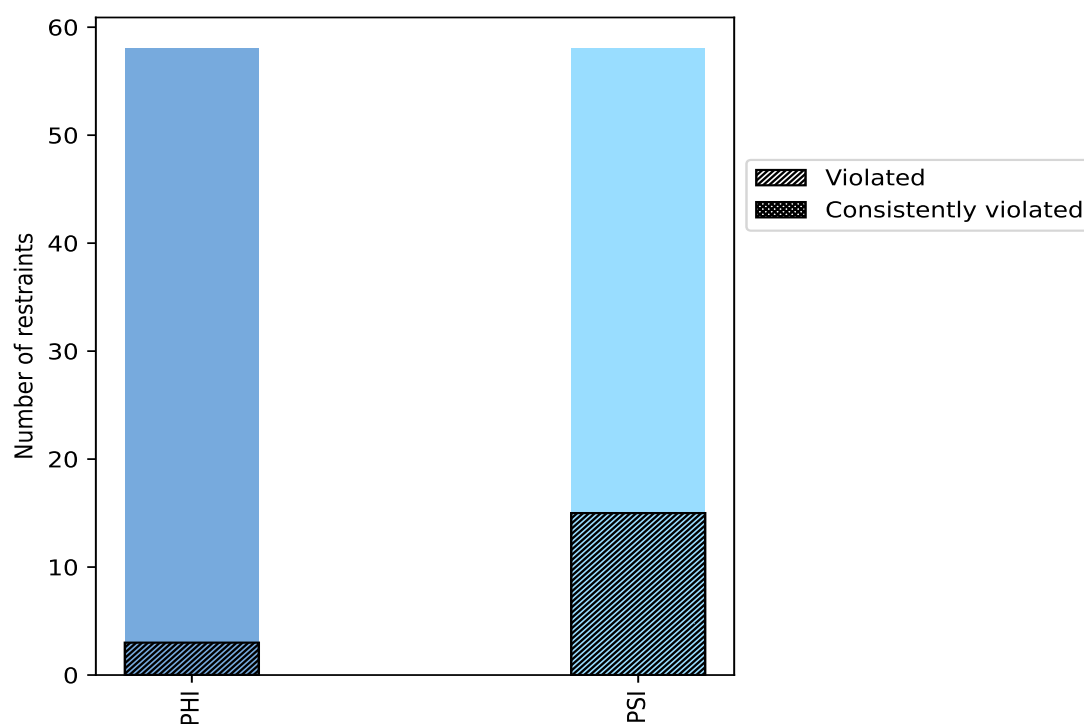
### 10.1 Summary of dihedral-angle violations [i](#)

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

| Angle type | Count | % <sup>1</sup> | Violated <sup>3</sup> |                |                | Consistently Violated <sup>4</sup> |                |                |
|------------|-------|----------------|-----------------------|----------------|----------------|------------------------------------|----------------|----------------|
|            |       |                | Count                 | % <sup>2</sup> | % <sup>1</sup> | Count                              | % <sup>2</sup> | % <sup>1</sup> |
| PHI        | 58    | 50.0           | 3                     | 5.2            | 2.6            | 0                                  | 0.0            | 0.0            |
| PSI        | 58    | 50.0           | 15                    | 25.9           | 12.9           | 0                                  | 0.0            | 0.0            |
| Total      | 116   | 100.0          | 18                    | 15.5           | 15.5           | 0                                  | 0.0            | 0.0            |

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

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



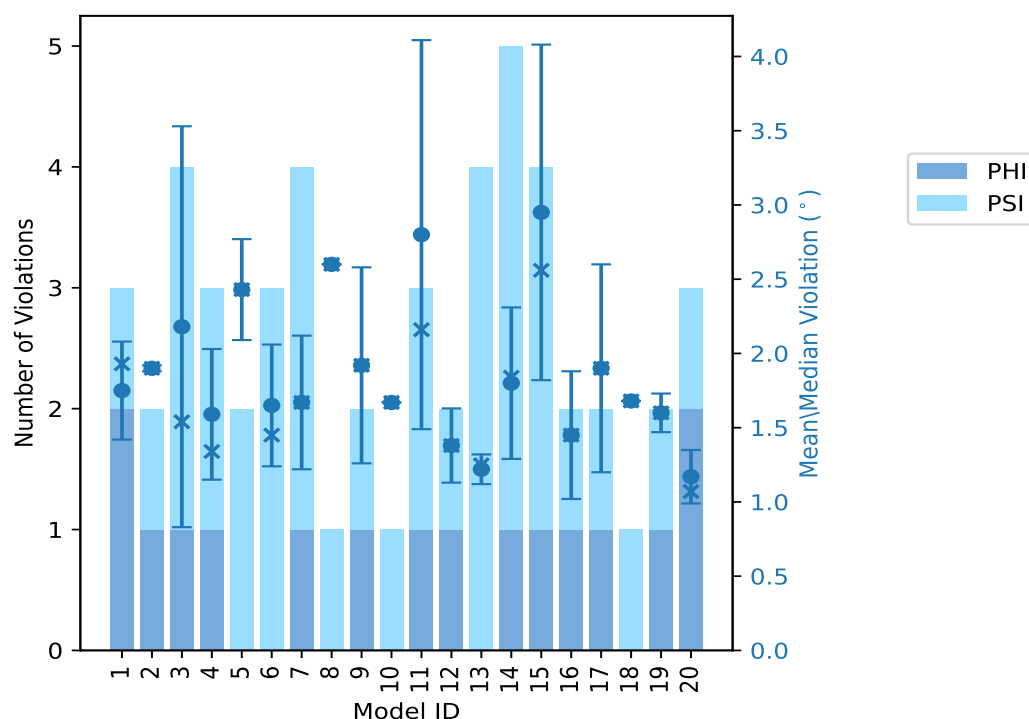
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

## 10.2 Dihedral-angle violation statistics for each model

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

| Model ID | Number of violations |     |       | Mean (°) | Max (°) | SD (°) | Median (°) |
|----------|----------------------|-----|-------|----------|---------|--------|------------|
|          | PHI                  | PSI | Total |          |         |        |            |
| 1        | 2                    | 1   | 3     | 1.75     | 2.04    | 0.33   | 1.93       |
| 2        | 1                    | 1   | 2     | 1.9      | 1.91    | 0.02   | 1.9        |
| 3        | 1                    | 3   | 4     | 2.18     | 4.5     | 1.35   | 1.54       |
| 4        | 1                    | 2   | 3     | 1.59     | 2.21    | 0.44   | 1.34       |
| 5        | 0                    | 2   | 2     | 2.43     | 2.77    | 0.34   | 2.43       |
| 6        | 0                    | 3   | 3     | 1.65     | 2.23    | 0.41   | 1.45       |
| 7        | 1                    | 3   | 4     | 1.67     | 2.3     | 0.45   | 1.67       |
| 8        | 0                    | 1   | 1     | 2.6      | 2.6     | 0.0    | 2.6        |
| 9        | 1                    | 1   | 2     | 1.92     | 2.58    | 0.66   | 1.92       |
| 10       | 0                    | 1   | 1     | 1.67     | 1.67    | 0.0    | 1.67       |
| 11       | 1                    | 2   | 3     | 2.8      | 4.62    | 1.31   | 2.16       |
| 12       | 1                    | 1   | 2     | 1.38     | 1.62    | 0.25   | 1.38       |
| 13       | 0                    | 4   | 4     | 1.22     | 1.33    | 0.1    | 1.25       |
| 14       | 1                    | 4   | 5     | 1.8      | 2.55    | 0.51   | 1.84       |
| 15       | 1                    | 3   | 4     | 2.95     | 4.74    | 1.13   | 2.56       |
| 16       | 1                    | 1   | 2     | 1.45     | 1.88    | 0.43   | 1.45       |
| 17       | 1                    | 1   | 2     | 1.9      | 2.59    | 0.7    | 1.9        |
| 18       | 0                    | 1   | 1     | 1.68     | 1.68    | 0.0    | 1.68       |
| 19       | 1                    | 1   | 2     | 1.6      | 1.73    | 0.13   | 1.6        |
| 20       | 2                    | 1   | 3     | 1.17     | 1.43    | 0.18   | 1.07       |

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



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

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

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

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

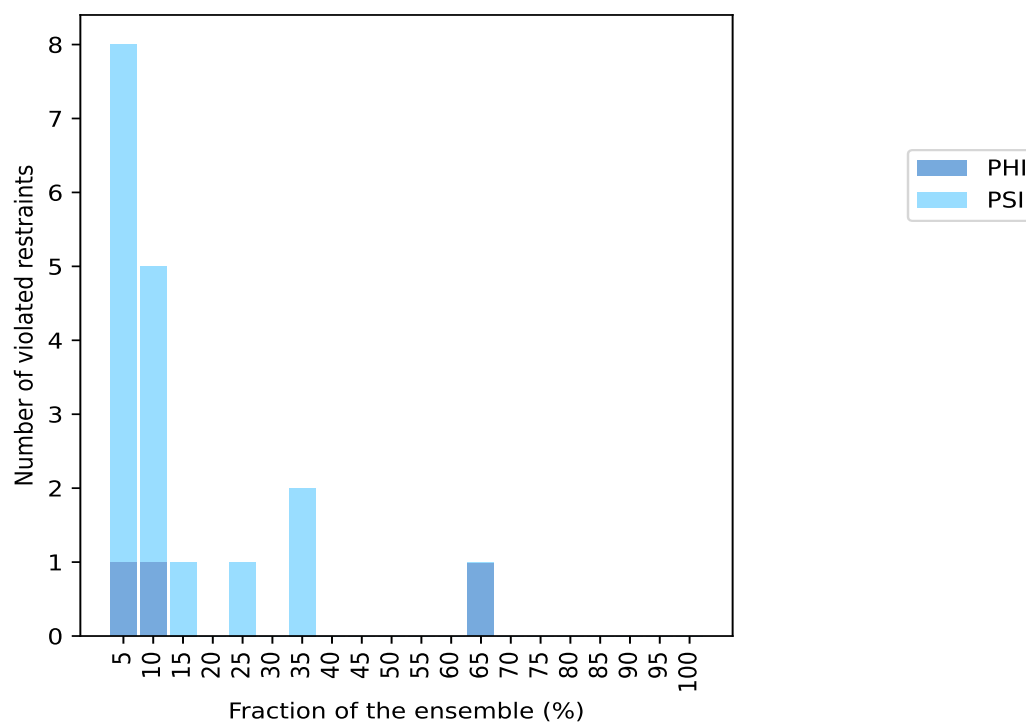
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| Number of violated restraints |     |       | Fraction of the ensemble |       |
|-------------------------------|-----|-------|--------------------------|-------|
| PHI                           | PSI | Total | Count <sup>1</sup>       | %     |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

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

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

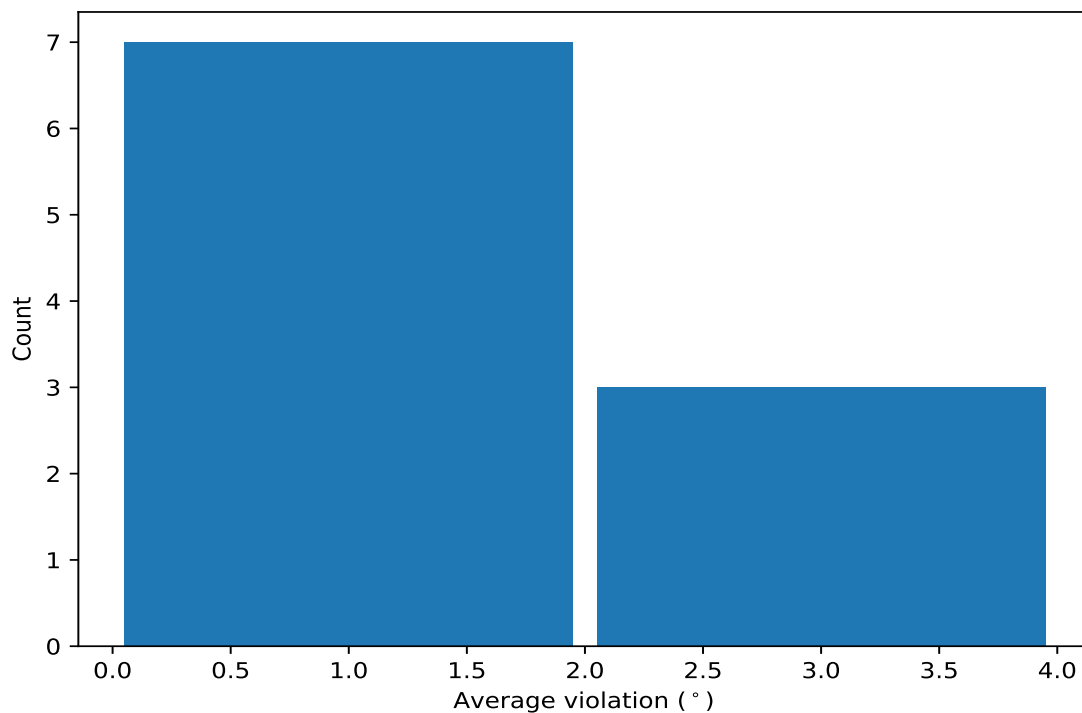


## 10.4 Most violated dihedral-angle restraints in the ensemble [i](#)

### 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.

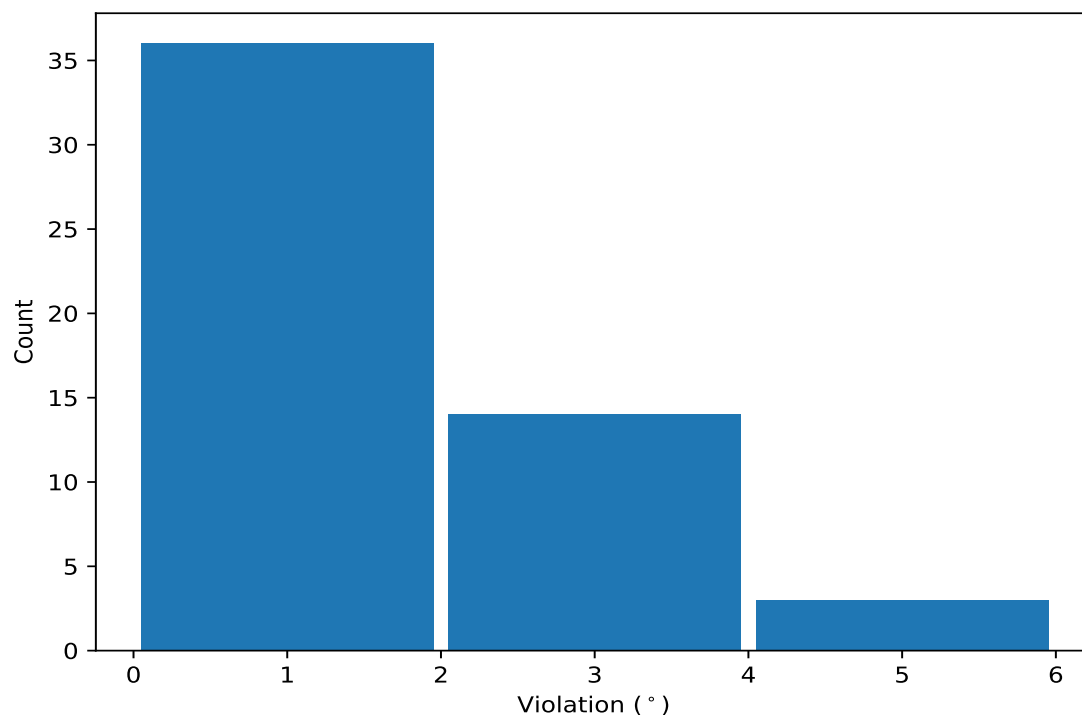
| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Models <sup>1</sup> | Mean | SD <sup>2</sup> | Median |
|---------|---------------|----------------|----------------|---------------|---------------------|------|-----------------|--------|
| (1,53)  | 1:46:A:GLU:C  | 1:47:A:LEU:N   | 1:47:A:LEU:CA  | 1:47:A:LEU:C  | 13                  | 2.17 | 0.9             | 1.91   |
| (1,88)  | 1:82:A:LEU:N  | 1:82:A:LEU:CA  | 1:82:A:LEU:C   | 1:83:A:GLU:N  | 7                   | 2.76 | 1.24            | 2.23   |
| (1,114) | 1:103:A:ALA:N | 1:103:A:ALA:CA | 1:103:A:ALA:C  | 1:104:A:GLU:N | 7                   | 1.81 | 0.61            | 1.77   |
| (1,90)  | 1:83:A:GLU:N  | 1:83:A:GLU:CA  | 1:83:A:GLU:C   | 1:84:A:GLU:N  | 5                   | 1.29 | 0.28            | 1.13   |
| (1,102) | 1:90:A:GLY:N  | 1:90:A:GLY:CA  | 1:90:A:GLY:C   | 1:91:A:LEU:N  | 3                   | 1.36 | 0.22            | 1.21   |
| (1,84)  | 1:80:A:GLU:N  | 1:80:A:GLU:CA  | 1:80:A:GLU:C   | 1:81:A:THR:N  | 2                   | 2.08 | 0.08            | 2.08   |
| (1,113) | 1:102:A:MET:C | 1:103:A:ALA:N  | 1:103:A:ALA:CA | 1:103:A:ALA:C | 2                   | 1.96 | 0.08            | 1.96   |
| (1,116) | 1:104:A:GLU:N | 1:104:A:GLU:CA | 1:104:A:GLU:C  | 1:105:A:HIS:N | 2                   | 1.64 | 0.31            | 1.64   |
| (1,22)  | 1:20:A:ARG:N  | 1:20:A:ARG:CA  | 1:20:A:ARG:C   | 1:21:A:GLU:N  | 2                   | 1.44 | 0.3             | 1.44   |
| (1,112) | 1:102:A:MET:N | 1:102:A:MET:CA | 1:102:A:MET:C  | 1:103:A:ALA:N | 2                   | 1.4  | 0.12            | 1.4    |

<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 (°) |
|---------|---------------|----------------|---------------|---------------|----------|---------------|
| (1,88)  | 1:82:A:LEU:N  | 1:82:A:LEU:CA  | 1:82:A:LEU:C  | 1:83:A:GLU:N  | 15       | 4.74          |
| (1,53)  | 1:46:A:GLU:C  | 1:47:A:LEU:N   | 1:47:A:LEU:CA | 1:47:A:LEU:C  | 11       | 4.62          |
| (1,88)  | 1:82:A:LEU:N  | 1:82:A:LEU:CA  | 1:82:A:LEU:C  | 1:83:A:GLU:N  | 3        | 4.5           |
| (1,53)  | 1:46:A:GLU:C  | 1:47:A:LEU:N   | 1:47:A:LEU:CA | 1:47:A:LEU:C  | 15       | 3.11          |
| (1,114) | 1:103:A:ALA:N | 1:103:A:ALA:CA | 1:103:A:ALA:C | 1:104:A:GLU:N | 5        | 2.77          |
| (1,88)  | 1:82:A:LEU:N  | 1:82:A:LEU:CA  | 1:82:A:LEU:C  | 1:83:A:GLU:N  | 8        | 2.6           |
| (1,53)  | 1:46:A:GLU:C  | 1:47:A:LEU:N   | 1:47:A:LEU:CA | 1:47:A:LEU:C  | 17       | 2.59          |
| (1,53)  | 1:46:A:GLU:C  | 1:47:A:LEU:N   | 1:47:A:LEU:CA | 1:47:A:LEU:C  | 9        | 2.58          |
| (1,114) | 1:103:A:ALA:N | 1:103:A:ALA:CA | 1:103:A:ALA:C | 1:104:A:GLU:N | 14       | 2.55          |
| (1,53)  | 1:46:A:GLU:C  | 1:47:A:LEU:N   | 1:47:A:LEU:CA | 1:47:A:LEU:C  | 7        | 2.3           |
| (1,88)  | 1:82:A:LEU:N  | 1:82:A:LEU:CA  | 1:82:A:LEU:C  | 1:83:A:GLU:N  | 6        | 2.23          |
| (1,53)  | 1:46:A:GLU:C  | 1:47:A:LEU:N   | 1:47:A:LEU:CA | 1:47:A:LEU:C  | 4        | 2.21          |
| (1,84)  | 1:80:A:GLU:N  | 1:80:A:GLU:CA  | 1:80:A:GLU:C  | 1:81:A:THR:N  | 11       | 2.16          |
| (1,88)  | 1:82:A:LEU:N  | 1:82:A:LEU:CA  | 1:82:A:LEU:C  | 1:83:A:GLU:N  | 14       | 2.09          |

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| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,74)  | 1:73:A:SER:N  | 1:73:A:SER:CA  | 1:73:A:SER:C   | 1:74:A:GLY:N  | 5        | 2.09          |
| (1,113) | 1:102:A:MET:C | 1:103:A:ALA:N  | 1:103:A:ALA:CA | 1:103:A:ALA:C | 1        | 2.04          |
| (1,84)  | 1:80:A:GLU:N  | 1:80:A:GLU:CA  | 1:80:A:GLU:C   | 1:81:A:THR:N  | 15       | 2.01          |
| (1,116) | 1:104:A:GLU:N | 1:104:A:GLU:CA | 1:104:A:GLU:C  | 1:105:A:HIS:N | 15       | 1.95          |
| (1,114) | 1:103:A:ALA:N | 1:103:A:ALA:CA | 1:103:A:ALA:C  | 1:104:A:GLU:N | 1        | 1.93          |
| (1,53)  | 1:46:A:GLU:C  | 1:47:A:LEU:N   | 1:47:A:LEU:CA  | 1:47:A:LEU:C  | 2        | 1.91          |
| (1,113) | 1:102:A:MET:C | 1:103:A:ALA:N  | 1:103:A:ALA:CA | 1:103:A:ALA:C | 16       | 1.88          |
| (1,88)  | 1:82:A:LEU:N  | 1:82:A:LEU:CA  | 1:82:A:LEU:C   | 1:83:A:GLU:N  | 2        | 1.88          |
| (1,53)  | 1:46:A:GLU:C  | 1:47:A:LEU:N   | 1:47:A:LEU:CA  | 1:47:A:LEU:C  | 14       | 1.84          |
| (1,114) | 1:103:A:ALA:N | 1:103:A:ALA:CA | 1:103:A:ALA:C  | 1:104:A:GLU:N | 7        | 1.77          |
| (1,22)  | 1:20:A:ARG:N  | 1:20:A:ARG:CA  | 1:20:A:ARG:C   | 1:21:A:GLU:N  | 19       | 1.73          |
| (1,90)  | 1:83:A:GLU:N  | 1:83:A:GLU:CA  | 1:83:A:GLU:C   | 1:84:A:GLU:N  | 18       | 1.68          |
| (1,102) | 1:90:A:GLY:N  | 1:90:A:GLY:CA  | 1:90:A:GLY:C   | 1:91:A:LEU:N  | 10       | 1.67          |
| (1,53)  | 1:46:A:GLU:C  | 1:47:A:LEU:N   | 1:47:A:LEU:CA  | 1:47:A:LEU:C  | 12       | 1.62          |
| (1,8)   | 1:11:A:ALA:N  | 1:11:A:ALA:CA  | 1:11:A:ALA:C   | 1:12:A:SER:N  | 11       | 1.62          |
| (1,53)  | 1:46:A:GLU:C  | 1:47:A:LEU:N   | 1:47:A:LEU:CA  | 1:47:A:LEU:C  | 3        | 1.58          |
| (1,90)  | 1:83:A:GLU:N  | 1:83:A:GLU:CA  | 1:83:A:GLU:C   | 1:84:A:GLU:N  | 7        | 1.57          |
| (1,112) | 1:102:A:MET:N | 1:102:A:MET:CA | 1:102:A:MET:C  | 1:103:A:ALA:N | 3        | 1.51          |
| (1,53)  | 1:46:A:GLU:C  | 1:47:A:LEU:N   | 1:47:A:LEU:CA  | 1:47:A:LEU:C  | 19       | 1.47          |
| (1,58)  | 1:49:A:PHE:N  | 1:49:A:PHE:CA  | 1:49:A:PHE:C   | 1:50:A:ARG:N  | 6        | 1.45          |
| (1,18)  | 1:18:A:LEU:N  | 1:18:A:LEU:CA  | 1:18:A:LEU:C   | 1:19:A:GLN:N  | 14       | 1.44          |
| (1,41)  | 1:38:A:VAL:C  | 1:39:A:PHE:N   | 1:39:A:PHE:CA  | 1:39:A:PHE:C  | 20       | 1.43          |
| (1,114) | 1:103:A:ALA:N | 1:103:A:ALA:CA | 1:103:A:ALA:C  | 1:104:A:GLU:N | 4        | 1.34          |
| (1,116) | 1:104:A:GLU:N | 1:104:A:GLU:CA | 1:104:A:GLU:C  | 1:105:A:HIS:N | 13       | 1.33          |
| (1,53)  | 1:46:A:GLU:C  | 1:47:A:LEU:N   | 1:47:A:LEU:CA  | 1:47:A:LEU:C  | 1        | 1.29          |
| (1,112) | 1:102:A:MET:N | 1:102:A:MET:CA | 1:102:A:MET:C  | 1:103:A:ALA:N | 6        | 1.28          |
| (1,114) | 1:103:A:ALA:N | 1:103:A:ALA:CA | 1:103:A:ALA:C  | 1:104:A:GLU:N | 13       | 1.27          |
| (1,88)  | 1:82:A:LEU:N  | 1:82:A:LEU:CA  | 1:82:A:LEU:C   | 1:83:A:GLU:N  | 9        | 1.25          |
| (1,6)   | 1:10:A:ALA:N  | 1:10:A:ALA:CA  | 1:10:A:ALA:C   | 1:11:A:ALA:N  | 13       | 1.23          |
| (1,102) | 1:90:A:GLY:N  | 1:90:A:GLY:CA  | 1:90:A:GLY:C   | 1:91:A:LEU:N  | 4        | 1.21          |
| (1,102) | 1:90:A:GLY:N  | 1:90:A:GLY:CA  | 1:90:A:GLY:C   | 1:91:A:LEU:N  | 17       | 1.2           |
| (1,22)  | 1:20:A:ARG:N  | 1:20:A:ARG:CA  | 1:20:A:ARG:C   | 1:21:A:GLU:N  | 3        | 1.14          |
| (1,90)  | 1:83:A:GLU:N  | 1:83:A:GLU:CA  | 1:83:A:GLU:C   | 1:84:A:GLU:N  | 12       | 1.13          |
| (1,80)  | 1:78:A:TYR:N  | 1:78:A:TYR:CA  | 1:78:A:TYR:C   | 1:79:A:PHE:N  | 14       | 1.08          |
| (1,53)  | 1:46:A:GLU:C  | 1:47:A:LEU:N   | 1:47:A:LEU:CA  | 1:47:A:LEU:C  | 20       | 1.07          |
| (1,90)  | 1:83:A:GLU:N  | 1:83:A:GLU:CA  | 1:83:A:GLU:C   | 1:84:A:GLU:N  | 13       | 1.06          |
| (1,104) | 1:93:A:GLU:N  | 1:93:A:GLU:CA  | 1:93:A:GLU:C   | 1:94:A:GLY:N  | 7        | 1.04          |
| (1,114) | 1:103:A:ALA:N | 1:103:A:ALA:CA | 1:103:A:ALA:C  | 1:104:A:GLU:N | 16       | 1.02          |
| (1,90)  | 1:83:A:GLU:N  | 1:83:A:GLU:CA  | 1:83:A:GLU:C   | 1:84:A:GLU:N  | 20       | 1.02          |