



# Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2026 – 11:01 PM UTC

PDB ID : 6PRJ / pdb\_00006prj  
BMRB ID : 30635  
Title : Structural Basis for Client Recognition and Activity of Hsp40 Chaperones  
Authors : Jiang, Y.; Rossi, P.; Kalodimos, C.G.  
Deposited on : 2019-07-10

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

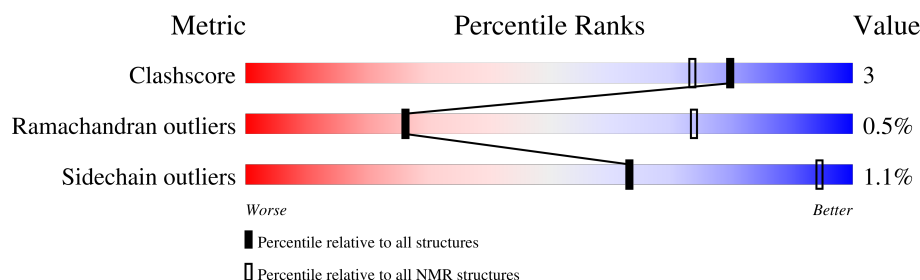
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 82%.

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



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

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 89     |                  |

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 3 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

| Well-defined (core) protein residues |                                  |                   |              |
|--------------------------------------|----------------------------------|-------------------|--------------|
| Well-defined core                    | Residue range (total)            | Backbone RMSD (Å) | Medoid model |
| 1                                    | A:172-A:180, A:191-A:256<br>(75) | 0.53              | 3            |

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

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

The models can be grouped into 2 clusters and 15 single-model clusters were found.

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

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1301 atoms, of which 661 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Alkaline phosphatase,Chaperone protein DnaJ 2 fusion.

| Mol | Chain | Residues | Atoms |     |     |     |     |   | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|-------|
| 1   | A     | 89       | Total | C   | H   | N   | O   | S | 0     |
|     |       |          | 1301  | 402 | 661 | 115 | 120 | 3 |       |

There are 12 discrepancies between the modelled and reference sequences:

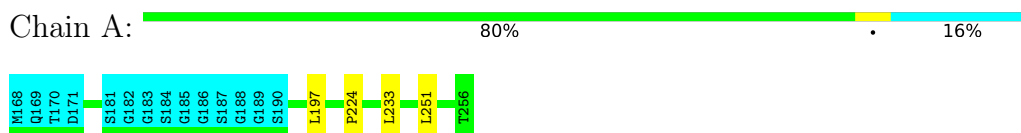
| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| A     | 168     | MET      | -      | initiating methionine | UNP P00634 |
| A     | 180     | GLY      | -      | linker                | UNP P00634 |
| A     | 181     | SER      | -      | linker                | UNP P00634 |
| A     | 182     | GLY      | -      | linker                | UNP P00634 |
| A     | 183     | GLY      | -      | linker                | UNP P00634 |
| A     | 184     | SER      | -      | linker                | UNP P00634 |
| A     | 185     | GLY      | -      | linker                | UNP P00634 |
| A     | 186     | GLY      | -      | linker                | UNP P00634 |
| A     | 187     | SER      | -      | linker                | UNP P00634 |
| A     | 188     | GLY      | -      | linker                | UNP P00634 |
| A     | 189     | GLY      | -      | linker                | UNP P00634 |
| A     | 190     | SER      | -      | linker                | UNP P00634 |

## 4 Residue-property plots

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

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

- Molecule 1: Alkaline phosphatase,Chaperone protein DnaJ 2 fusion

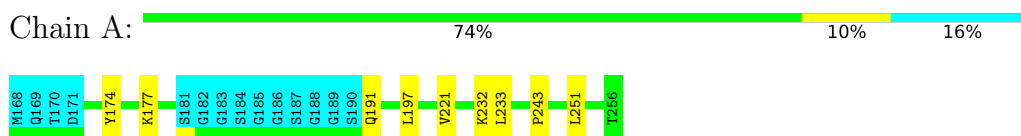


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

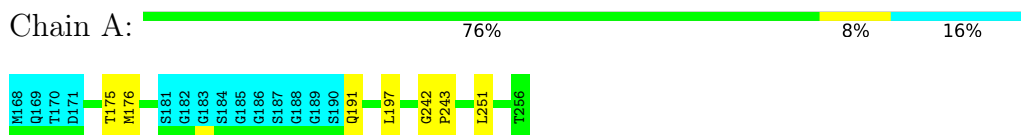
#### 4.2.1 Score per residue for model 1

- Molecule 1: Alkaline phosphatase,Chaperone protein DnaJ 2 fusion



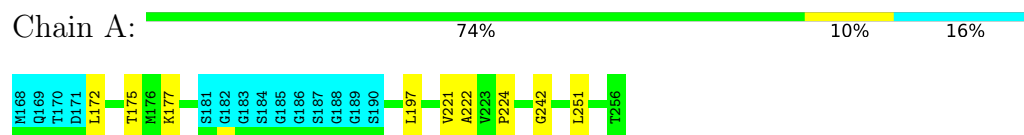
#### 4.2.2 Score per residue for model 2

- Molecule 1: Alkaline phosphatase,Chaperone protein DnaJ 2 fusion



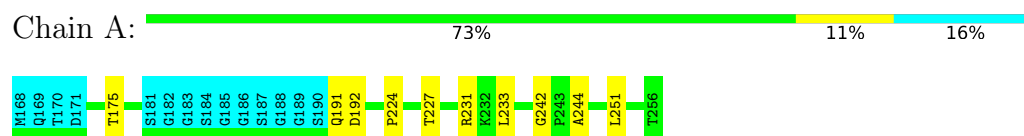
### 4.2.3 Score per residue for model 3 (medoid)

- Molecule 1: Alkaline phosphatase,Chaperone protein DnaJ 2 fusion



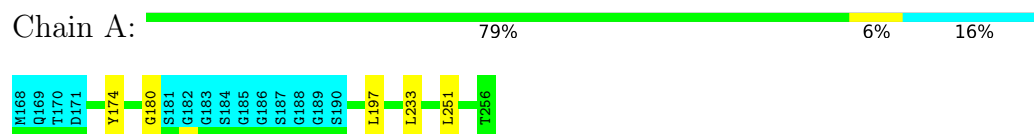
### 4.2.4 Score per residue for model 4

- Molecule 1: Alkaline phosphatase,Chaperone protein DnaJ 2 fusion



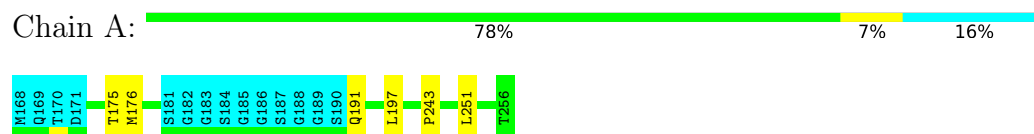
### 4.2.5 Score per residue for model 5

- Molecule 1: Alkaline phosphatase,Chaperone protein DnaJ 2 fusion



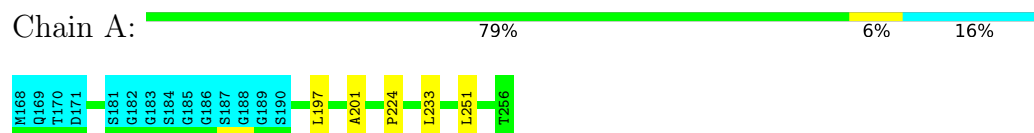
### 4.2.6 Score per residue for model 6

- Molecule 1: Alkaline phosphatase,Chaperone protein DnaJ 2 fusion



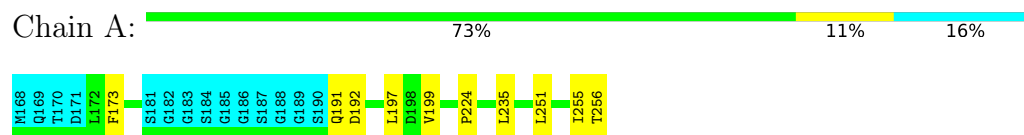
### 4.2.7 Score per residue for model 7

- Molecule 1: Alkaline phosphatase,Chaperone protein DnaJ 2 fusion



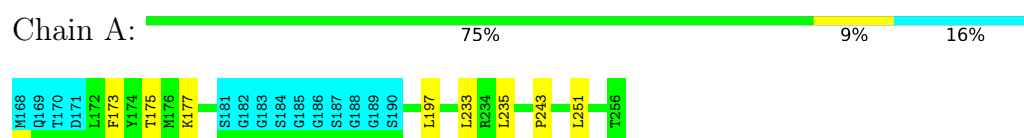
### 4.2.8 Score per residue for model 8

- Molecule 1: Alkaline phosphatase,Chaperone protein DnaJ 2 fusion



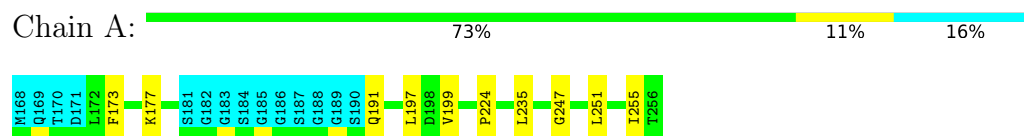
### 4.2.9 Score per residue for model 9

- Molecule 1: Alkaline phosphatase,Chaperone protein DnaJ 2 fusion



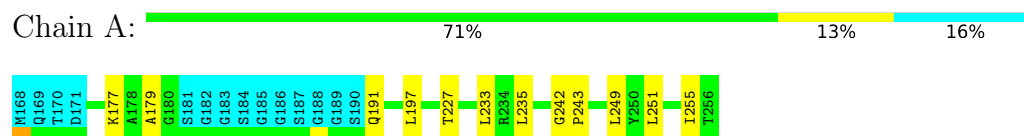
### 4.2.10 Score per residue for model 10

- Molecule 1: Alkaline phosphatase,Chaperone protein DnaJ 2 fusion



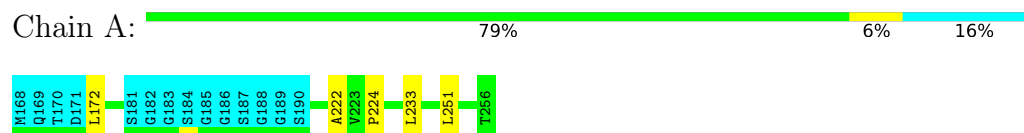
### 4.2.11 Score per residue for model 11

- Molecule 1: Alkaline phosphatase,Chaperone protein DnaJ 2 fusion



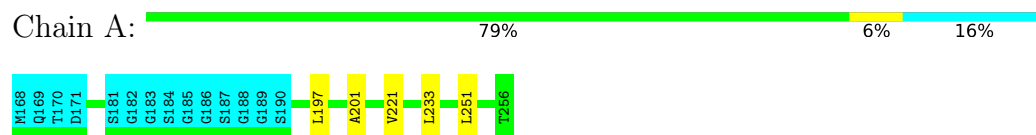
### 4.2.12 Score per residue for model 12

- Molecule 1: Alkaline phosphatase,Chaperone protein DnaJ 2 fusion



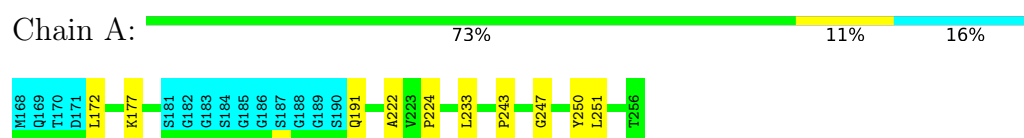
### 4.2.13 Score per residue for model 13

- Molecule 1: Alkaline phosphatase,Chaperone protein DnaJ 2 fusion



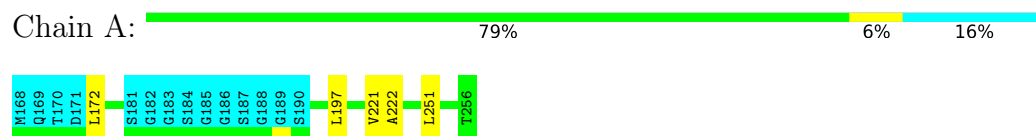
### 4.2.14 Score per residue for model 14

- Molecule 1: Alkaline phosphatase,Chaperone protein DnaJ 2 fusion



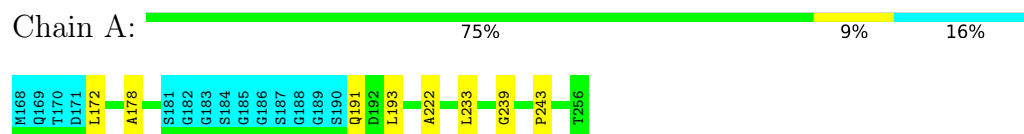
### 4.2.15 Score per residue for model 15

- Molecule 1: Alkaline phosphatase,Chaperone protein DnaJ 2 fusion



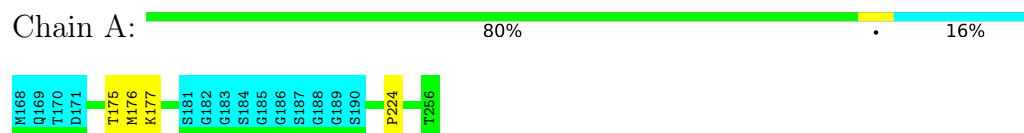
### 4.2.16 Score per residue for model 16

- Molecule 1: Alkaline phosphatase,Chaperone protein DnaJ 2 fusion



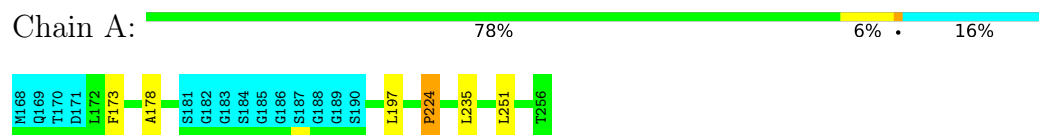
### 4.2.17 Score per residue for model 17

- Molecule 1: Alkaline phosphatase,Chaperone protein DnaJ 2 fusion



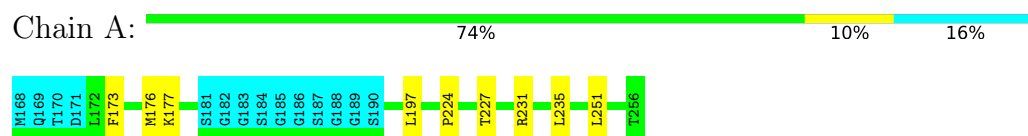
#### 4.2.18 Score per residue for model 18

- Molecule 1: Alkaline phosphatase,Chaperone protein DnaJ 2 fusion



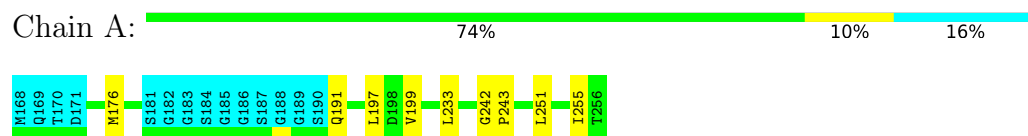
#### 4.2.19 Score per residue for model 19

- Molecule 1: Alkaline phosphatase,Chaperone protein DnaJ 2 fusion



#### 4.2.20 Score per residue for model 20

- Molecule 1: Alkaline phosphatase,Chaperone protein DnaJ 2 fusion



## 5 Refinement protocol and experimental data overview

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

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

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

| Software name | Classification        | Version |
|---------------|-----------------------|---------|
| CNS           | refinement            |         |
| CYANA         | structure calculation |         |
| TALOS         | geometry optimization |         |

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

|                                              |                |
|----------------------------------------------|----------------|
| Chemical shift file(s)                       | working_cs.cif |
| Number of chemical shift lists               | 1              |
| Total number of shifts                       | 910            |
| Number of shifts mapped to atoms             | 910            |
| Number of unparsed shifts                    | 0              |
| Number of shifts with mapping errors         | 0              |
| Number of shifts with mapping warnings       | 0              |
| Assignment completeness (well-defined parts) | 82%            |

## 6 Model quality [i](#)

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

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

| Mol | Chain | Bond lengths |                      | Bond angles |                      |
|-----|-------|--------------|----------------------|-------------|----------------------|
|     |       | RMSZ         | #Z>5                 | RMSZ        | #Z>5                 |
| 1   | A     | 1.24±0.03    | 1±1/571 ( 0.1± 0.1%) | 0.86±0.03   | 0±1/772 ( 0.1± 0.1%) |
| All | All   | 1.24         | 16/11420 ( 0.1%)     | 0.86        | 10/15440 ( 0.1%)     |

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

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) | Models |       |
|-----|-------|-----|------|-------|------|-------------|----------|--------|-------|
|     |       |     |      |       |      |             |          | Worst  | Total |
| 1   | A     | 224 | PRO  | CA-C  | 7.69 | 1.56        | 1.51     | 17     | 10    |
| 1   | A     | 201 | ALA  | C-N   | 5.50 | 1.40        | 1.34     | 7      | 2     |
| 1   | A     | 221 | VAL  | CA-CB | 5.20 | 1.60        | 1.54     | 3      | 4     |

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

| Mol | Chain | Res | Type | Atoms  | Z    | Observed(°) | Ideal(°) | Models |       |
|-----|-------|-----|------|--------|------|-------------|----------|--------|-------|
|     |       |     |      |        |      |             |          | Worst  | Total |
| 1   | A     | 242 | GLY  | CA-C-N | 6.15 | 125.36      | 118.97   | 4      | 5     |
| 1   | A     | 242 | GLY  | C-N-CA | 6.15 | 125.36      | 118.97   | 4      | 5     |

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     | 560   | 593      | 593      | 3±1     |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes |
|-----|-------|-------|----------|----------|---------|
| All | All   | 11200 | 11860    | 11860    | 63      |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

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

| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:233:LEU:HB2  | 1:A:251:LEU:HB2  | 0.57     | 1.75        | 4      | 10    |
| 1:A:197:LEU:HD22 | 1:A:251:LEU:HD13 | 0.54     | 1.79        | 18     | 15    |
| 1:A:172:LEU:HD21 | 1:A:222:ALA:H    | 0.52     | 1.63        | 14     | 5     |
| 1:A:176:MET:SD   | 1:A:177:LYS:N    | 0.51     | 2.84        | 17     | 1     |
| 1:A:191:GLN:HB3  | 1:A:243:PRO:HD2  | 0.50     | 1.81        | 1      | 7     |
| 1:A:191:GLN:HB2  | 1:A:247:GLY:HA2  | 0.50     | 1.82        | 14     | 2     |
| 1:A:191:GLN:HE22 | 1:A:244:ALA:HB3  | 0.47     | 1.68        | 4      | 1     |
| 1:A:193:LEU:HD12 | 1:A:239:GLY:HA2  | 0.45     | 1.88        | 16     | 1     |
| 1:A:172:LEU:HD13 | 1:A:175:THR:HG21 | 0.44     | 1.88        | 3      | 1     |
| 1:A:191:GLN:HG3  | 1:A:192:ASP:N    | 0.44     | 2.28        | 4      | 2     |
| 1:A:173:PHE:CD1  | 1:A:235:LEU:HD22 | 0.44     | 2.48        | 10     | 5     |
| 1:A:227:THR:HA   | 1:A:231:ARG:HE   | 0.43     | 1.73        | 4      | 1     |
| 1:A:199:VAL:O    | 1:A:255:ILE:HA   | 0.43     | 2.13        | 8      | 3     |
| 1:A:235:LEU:HB2  | 1:A:249:LEU:HB3  | 0.42     | 1.92        | 11     | 1     |
| 1:A:178:ALA:HB1  | 1:A:224:PRO:HB3  | 0.42     | 1.92        | 18     | 1     |
| 1:A:174:TYR:CD2  | 1:A:233:LEU:HB3  | 0.42     | 2.50        | 1      | 2     |
| 1:A:178:ALA:HB1  | 1:A:233:LEU:HD22 | 0.41     | 1.92        | 16     | 1     |
| 1:A:227:THR:O    | 1:A:255:ILE:HD11 | 0.41     | 2.16        | 11     | 1     |
| 1:A:233:LEU:O    | 1:A:250:TYR:HA   | 0.41     | 2.16        | 14     | 1     |
| 1:A:227:THR:HA   | 1:A:231:ARG:HH11 | 0.40     | 1.77        | 19     | 1     |
| 1:A:227:THR:HA   | 1:A:231:ARG:NH1  | 0.40     | 2.31        | 19     | 1     |

## 6.3 Torsion angles [i](#)

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

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

| Mol | Chain | Analysed    | Favoured     | Allowed    | Outliers   | Percentiles |    |
|-----|-------|-------------|--------------|------------|------------|-------------|----|
| 1   | A     | 74/89 (83%) | 67±2 (91±3%) | 6±2 (9±3%) | 0±1 (1±1%) | 26          | 74 |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |
|-----|-------|-----------------|------------|----------|----------|-------------|
| All | All   | 1480/1780 (83%) | 1346 (91%) | 126 (9%) | 8 (1%)   | 26 74       |

All 5 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     | 176 | MET  | 3              |
| 1   | A     | 177 | LYS  | 2              |
| 1   | A     | 180 | GLY  | 1              |
| 1   | A     | 243 | PRO  | 1              |
| 1   | A     | 179 | ALA  | 1              |

### 6.3.2 Protein sidechains ⓘ

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

| Mol | Chain | Analysed        | Rotameric    | Outliers   | Percentiles |
|-----|-------|-----------------|--------------|------------|-------------|
| 1   | A     | 56/64 (88%)     | 55±1 (99±1%) | 1±1 (1±1%) | 63 94       |
| All | All   | 1120/1280 (88%) | 1108 (99%)   | 12 (1%)    | 63 94       |

All 5 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     | 175 | THR  | 5              |
| 1   | A     | 177 | LYS  | 4              |
| 1   | A     | 232 | LYS  | 1              |
| 1   | A     | 176 | MET  | 1              |
| 1   | A     | 256 | THR  | 1              |

### 6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 6.7 Other polymers [i](#)

There are no such molecules in this entry.

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

There are no chain breaks in this entry.

## 7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 82% for the well-defined parts and 80% for the entire structure.

### 7.1 Chemical shift list 1

File name: working\_cs.cif

Chemical shift list name: *G\_CBD2rev2.bmrB*

#### 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                  | 910 |
| Number of shifts mapped to atoms        | 910 |
| Number of unparsed shifts               | 0   |
| Number of shifts with mapping errors    | 0   |
| Number of shifts with mapping warnings  | 0   |
| Number of shift outliers (ShiftChecker) | 0   |

#### 7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

| Nucleus                | # values | Correction $\pm$ precision, ppm | Suggested action           |
|------------------------|----------|---------------------------------|----------------------------|
| $^{13}\text{C}_\alpha$ | 81       | $-0.01 \pm 0.23$                | None needed ( $< 0.5$ ppm) |
| $^{13}\text{C}_\beta$  | 71       | $0.27 \pm 0.21$                 | None needed ( $< 0.5$ ppm) |
| $^{13}\text{C}'$       | 60       | $-0.03 \pm 0.18$                | None needed ( $< 0.5$ ppm) |
| $^{15}\text{N}$        | 76       | $-0.63 \pm 0.67$                | None needed (imprecise)    |

#### 7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 82%, i.e. 835 atoms were assigned a chemical shift out of a possible 1018. 0 out of 16 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total         | $^1\text{H}$  | $^{13}\text{C}$ | $^{15}\text{N}$ |
|-----------|---------------|---------------|-----------------|-----------------|
| Backbone  | 327/371 (88%) | 137/153 (90%) | 123/150 (82%)   | 67/68 (99%)     |
| Sidechain | 466/600 (78%) | 310/395 (78%) | 156/180 (87%)   | 0/25 (0%)       |

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|          | Total          | <sup>1</sup> H | <sup>13</sup> C | <sup>15</sup> N |
|----------|----------------|----------------|-----------------|-----------------|
| Aromatic | 42/47 (89%)    | 21/22 (95%)    | 21/25 (84%)     | 0/0 (—%)        |
| Overall  | 835/1018 (82%) | 468/570 (82%)  | 300/355 (85%)   | 67/93 (72%)     |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 80%, i.e. 910 atoms were assigned a chemical shift out of a possible 1136. 0 out of 16 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total          | <sup>1</sup> H | <sup>13</sup> C | <sup>15</sup> N |
|-----------|----------------|----------------|-----------------|-----------------|
| Backbone  | 375/447 (84%)  | 158/187 (84%)  | 141/178 (79%)   | 76/82 (93%)     |
| Sidechain | 493/642 (77%)  | 327/422 (77%)  | 166/194 (86%)   | 0/26 (0%)       |
| Aromatic  | 42/47 (89%)    | 21/22 (95%)    | 21/25 (84%)     | 0/0 (—%)        |
| Overall   | 910/1136 (80%) | 506/631 (80%)  | 328/397 (83%)   | 76/108 (70%)    |

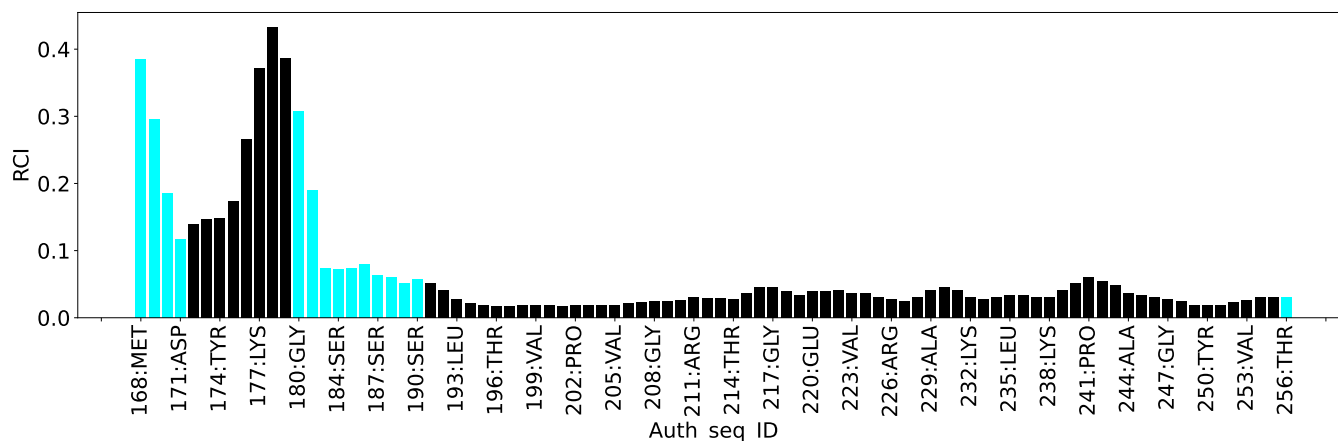
#### 7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

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

Random coil index (RCI) for chain A:



## 8 NMR restraints analysis

### 8.1 Conformationally restricting restraints

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

| Description                                              | Value |
|----------------------------------------------------------|-------|
| Total distance restraints                                | 1753  |
| Intra-residue ( $ i-j =0$ )                              | 294   |
| Sequential ( $ i-j =1$ )                                 | 459   |
| Medium range ( $ i-j >1$ and $ i-j <5$ )                 | 208   |
| Long range ( $ i-j \geq 5$ )                             | 736   |
| Inter-chain                                              | 0     |
| Hydrogen bond restraints                                 | 56    |
| Disulfide bond restraints                                | 0     |
| Total dihedral-angle restraints                          | 156   |
| Number of unmapped restraints                            | 0     |
| Number of restraints per residue                         | 21.4  |
| Number of long range restraints per residue <sup>1</sup> | 8.8   |

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

### 8.2 Residual restraint violations

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

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

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

| Bins (Å)         | Average number of violations per model | Max (Å) |
|------------------|----------------------------------------|---------|
| 0.1-0.2 (Small)  | 18.1                                   | 0.2     |
| 0.2-0.5 (Medium) | 6.1                                    | 0.46    |
| >0.5 (Large)     | 0.1                                    | 0.59    |

### 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)   | 17.2                                   | 9.62    |
| 10.0-20.0 (Medium) | None                                   | None    |
| >20.0 (Large)      | None                                   | None    |

## 9 Distance violation analysis ⓘ

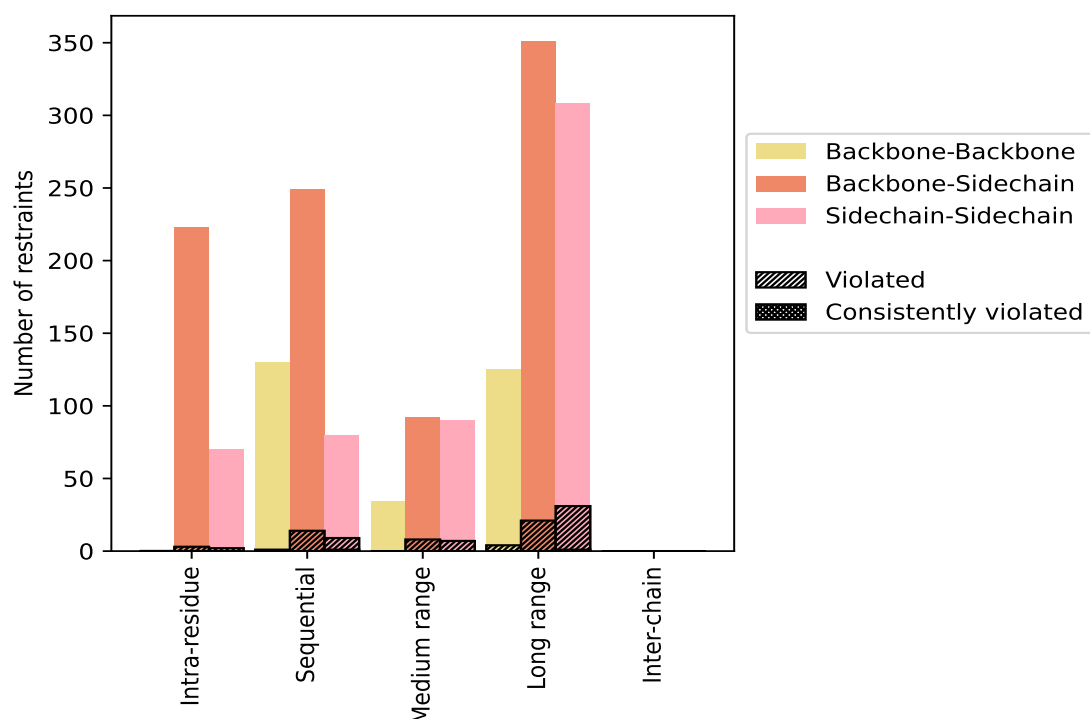
### 9.1 Summary of distance violations ⓘ

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

| Restrains type                                                              | Count       | % <sup>1</sup> | Violated <sup>3</sup> |                |                | Consistently Violated <sup>4</sup> |                |                |
|-----------------------------------------------------------------------------|-------------|----------------|-----------------------|----------------|----------------|------------------------------------|----------------|----------------|
|                                                                             |             |                | Count                 | % <sup>2</sup> | % <sup>1</sup> | Count                              | % <sup>2</sup> | % <sup>1</sup> |
| <b>Intra-residue (<math> i-j =0</math>)</b>                                 | <b>294</b>  | <b>16.8</b>    | <b>5</b>              | <b>1.7</b>     | <b>0.3</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| Backbone-Backbone                                                           | 1           | 0.1            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 223         | 12.7           | 3                     | 1.3            | 0.2            | 0                                  | 0.0            | 0.0            |
| Sidechain-Sidechain                                                         | 70          | 4.0            | 2                     | 2.9            | 0.1            | 0                                  | 0.0            | 0.0            |
| <b>Sequential (<math> i-j =1</math>)</b>                                    | <b>459</b>  | <b>26.2</b>    | <b>24</b>             | <b>5.2</b>     | <b>1.4</b>     | <b>1</b>                           | <b>0.2</b>     | <b>0.1</b>     |
| Backbone-Backbone                                                           | 130         | 7.4            | 1                     | 0.8            | 0.1            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 249         | 14.2           | 14                    | 5.6            | 0.8            | 0                                  | 0.0            | 0.0            |
| Sidechain-Sidechain                                                         | 80          | 4.6            | 9                     | 11.2           | 0.5            | 1                                  | 1.2            | 0.1            |
| <b>Medium range (<math> i-j &gt;1</math> &amp; <math> i-j &lt;5</math>)</b> | <b>208</b>  | <b>11.9</b>    | <b>15</b>             | <b>7.2</b>     | <b>0.9</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| Backbone-Backbone                                                           | 34          | 1.9            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 84          | 4.8            | 8                     | 9.5            | 0.5            | 0                                  | 0.0            | 0.0            |
| Sidechain-Sidechain                                                         | 90          | 5.1            | 7                     | 7.8            | 0.4            | 0                                  | 0.0            | 0.0            |
| <b>Long range (<math> i-j \geq 5</math>)</b>                                | <b>736</b>  | <b>42.0</b>    | <b>54</b>             | <b>7.3</b>     | <b>3.1</b>     | <b>1</b>                           | <b>0.1</b>     | <b>0.1</b>     |
| Backbone-Backbone                                                           | 125         | 7.1            | 4                     | 3.2            | 0.2            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 303         | 17.3           | 19                    | 6.3            | 1.1            | 0                                  | 0.0            | 0.0            |
| Sidechain-Sidechain                                                         | 308         | 17.6           | 31                    | 10.1           | 1.8            | 1                                  | 0.3            | 0.1            |
| <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>56</b>   | <b>3.2</b>     | <b>2</b>              | <b>3.6</b>     | <b>0.1</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>1753</b> | <b>100.0</b>   | <b>100</b>            | <b>5.7</b>     | <b>5.7</b>     | <b>2</b>                           | <b>0.1</b>     | <b>0.1</b>     |
| Backbone-Backbone                                                           | 290         | 16.5           | 5                     | 1.7            | 0.3            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 915         | 52.2           | 46                    | 5.0            | 2.6            | 0                                  | 0.0            | 0.0            |
| Sidechain-Sidechain                                                         | 548         | 31.3           | 49                    | 8.9            | 2.8            | 2                                  | 0.4            | 0.1            |

<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 disulfide 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                    | 3               | 4               | 13              | 0               | 20    | 0.17     | 0.35    | 0.06                | 0.18       |
| 2        | 0                    | 3               | 4               | 22              | 0               | 29    | 0.18     | 0.46    | 0.07                | 0.17       |
| 3        | 2                    | 6               | 5               | 12              | 0               | 25    | 0.19     | 0.46    | 0.09                | 0.17       |
| 4        | 1                    | 7               | 6               | 11              | 0               | 25    | 0.19     | 0.42    | 0.09                | 0.17       |
| 5        | 2                    | 8               | 3               | 14              | 0               | 27    | 0.18     | 0.44    | 0.08                | 0.15       |
| 6        | 1                    | 5               | 4               | 19              | 0               | 29    | 0.17     | 0.34    | 0.06                | 0.16       |
| 7        | 2                    | 7               | 6               | 14              | 0               | 29    | 0.16     | 0.59    | 0.09                | 0.14       |
| 8        | 0                    | 4               | 4               | 14              | 0               | 22    | 0.17     | 0.29    | 0.05                | 0.16       |
| 9        | 1                    | 6               | 4               | 13              | 0               | 24    | 0.19     | 0.34    | 0.07                | 0.16       |
| 10       | 1                    | 7               | 2               | 14              | 0               | 24    | 0.19     | 0.45    | 0.08                | 0.18       |

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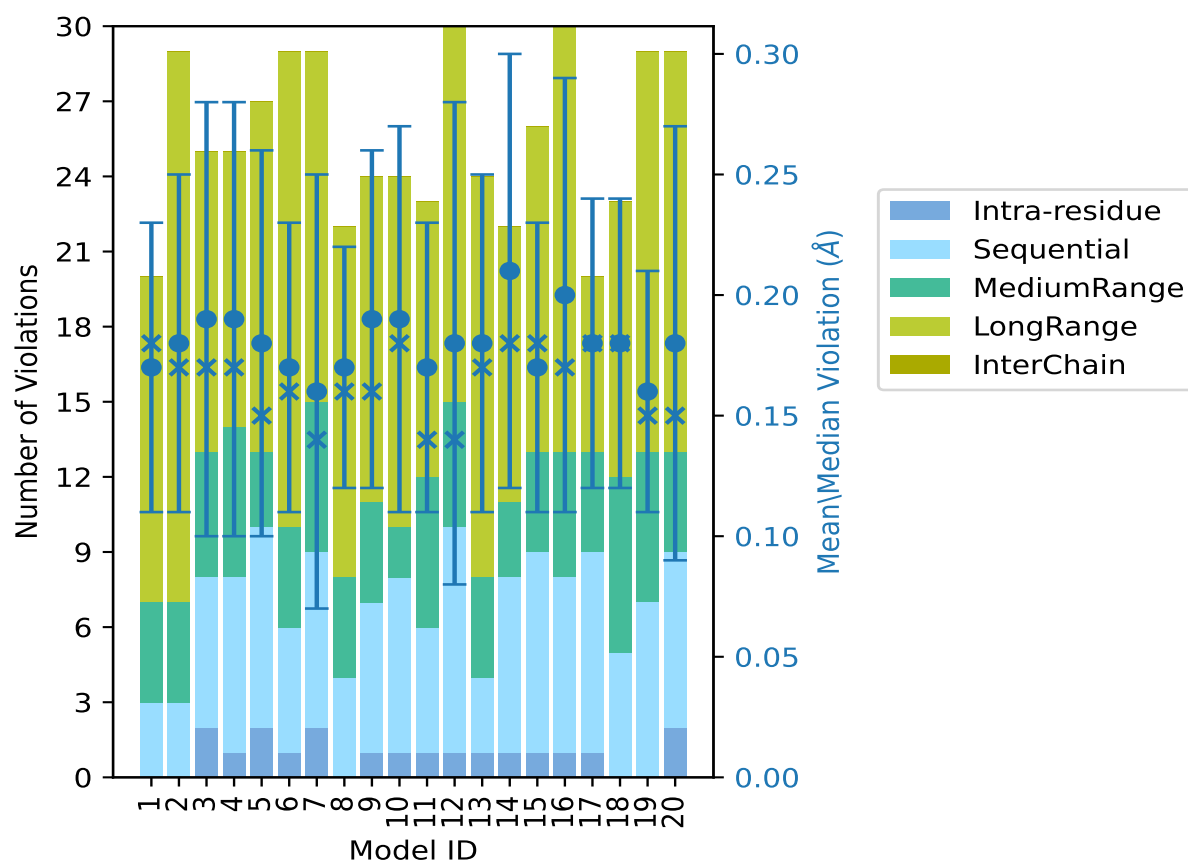
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| Model ID | Number of violations |                 |                 |                 |                 |       | Mean (Å) | Max (Å) | SD <sup>6</sup> (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
|          | IR <sup>1</sup>      | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total |          |         |                     |            |
| 11       | 1                    | 5               | 6               | 11              | 0               | 23    | 0.17     | 0.33    | 0.06                | 0.14       |
| 12       | 1                    | 9               | 5               | 15              | 0               | 30    | 0.18     | 0.45    | 0.1                 | 0.14       |
| 13       | 1                    | 3               | 4               | 16              | 0               | 24    | 0.18     | 0.34    | 0.07                | 0.17       |
| 14       | 1                    | 7               | 3               | 11              | 0               | 22    | 0.21     | 0.44    | 0.09                | 0.18       |
| 15       | 1                    | 8               | 4               | 13              | 0               | 26    | 0.17     | 0.34    | 0.06                | 0.18       |
| 16       | 1                    | 7               | 5               | 17              | 0               | 30    | 0.2      | 0.44    | 0.09                | 0.17       |
| 17       | 1                    | 8               | 4               | 7               | 0               | 20    | 0.18     | 0.39    | 0.06                | 0.18       |
| 18       | 0                    | 5               | 7               | 11              | 0               | 23    | 0.18     | 0.29    | 0.06                | 0.18       |
| 19       | 0                    | 7               | 6               | 16              | 0               | 29    | 0.16     | 0.27    | 0.05                | 0.15       |
| 20       | 2                    | 7               | 4               | 16              | 0               | 29    | 0.18     | 0.44    | 0.09                | 0.15       |

<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

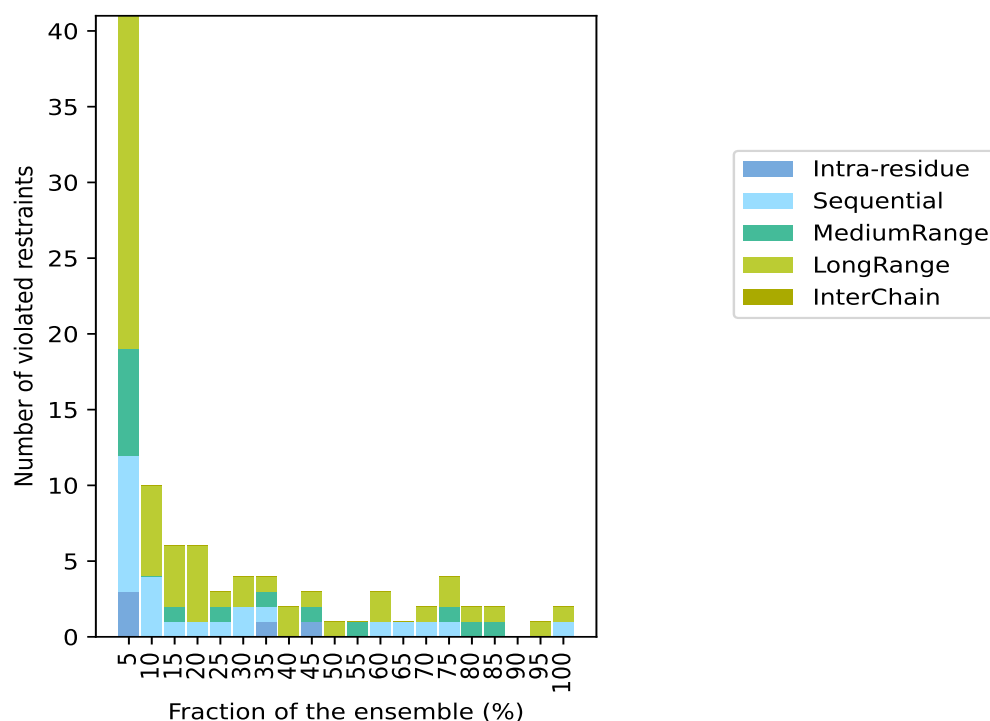
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1599(IR:289, SQ:435, MR:193, LR:682, IC:0) restraints are not violated in the ensemble.

| Number of violated restraints |                 |                 |                 |                 |       | Fraction of the ensemble |       |
|-------------------------------|-----------------|-----------------|-----------------|-----------------|-------|--------------------------|-------|
| IR <sup>1</sup>               | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total | Count <sup>6</sup>       | %     |
| 3                             | 9               | 7               | 22              | 0               | 41    | 1                        | 5.0   |
| 0                             | 4               | 0               | 6               | 0               | 10    | 2                        | 10.0  |
| 0                             | 1               | 1               | 4               | 0               | 6     | 3                        | 15.0  |
| 0                             | 1               | 0               | 5               | 0               | 6     | 4                        | 20.0  |
| 0                             | 1               | 1               | 1               | 0               | 3     | 5                        | 25.0  |
| 0                             | 2               | 0               | 2               | 0               | 4     | 6                        | 30.0  |
| 1                             | 1               | 1               | 1               | 0               | 4     | 7                        | 35.0  |
| 0                             | 0               | 0               | 2               | 0               | 2     | 8                        | 40.0  |
| 1                             | 0               | 1               | 1               | 0               | 3     | 9                        | 45.0  |
| 0                             | 0               | 0               | 1               | 0               | 1     | 10                       | 50.0  |
| 0                             | 0               | 1               | 0               | 0               | 1     | 11                       | 55.0  |
| 0                             | 1               | 0               | 2               | 0               | 3     | 12                       | 60.0  |
| 0                             | 1               | 0               | 0               | 0               | 1     | 13                       | 65.0  |
| 0                             | 1               | 0               | 1               | 0               | 2     | 14                       | 70.0  |
| 0                             | 1               | 1               | 2               | 0               | 4     | 15                       | 75.0  |
| 0                             | 0               | 1               | 1               | 0               | 2     | 16                       | 80.0  |
| 0                             | 0               | 1               | 1               | 0               | 2     | 17                       | 85.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 18                       | 90.0  |
| 0                             | 0               | 0               | 1               | 0               | 1     | 19                       | 95.0  |
| 0                             | 1               | 0               | 1               | 0               | 2     | 20                       | 100.0 |

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

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

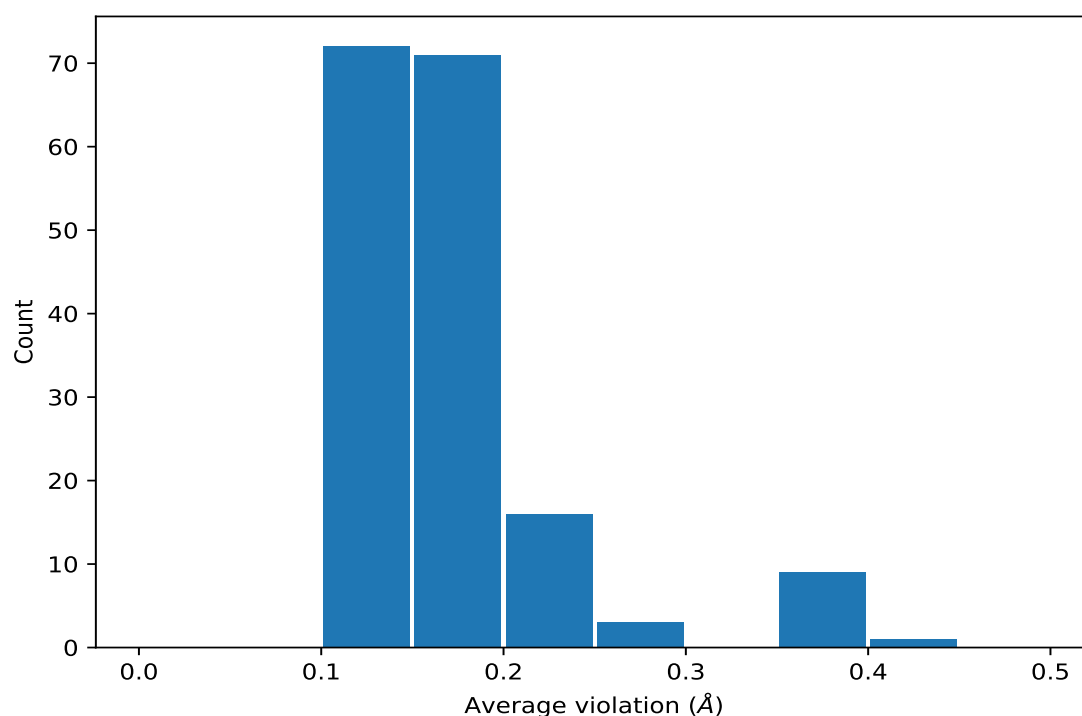
### 9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

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

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



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

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

| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (2,633)  | 1:197:A:LEU:HB3  | 1:210:A:VAL:HG21 | 20                  | 0.19     | 0.04                | 0.18       |
| (2,633)  | 1:197:A:LEU:HB3  | 1:210:A:VAL:HG22 | 20                  | 0.19     | 0.04                | 0.18       |
| (2,633)  | 1:197:A:LEU:HB3  | 1:210:A:VAL:HG23 | 20                  | 0.19     | 0.04                | 0.18       |
| (2,1435) | 1:199:A:VAL:HG11 | 1:200:A:PRO:HG2  | 20                  | 0.13     | 0.02                | 0.13       |
| (2,1435) | 1:199:A:VAL:HG12 | 1:200:A:PRO:HG2  | 20                  | 0.13     | 0.02                | 0.13       |
| (2,1435) | 1:199:A:VAL:HG13 | 1:200:A:PRO:HG2  | 20                  | 0.13     | 0.02                | 0.13       |
| (2,1435) | 1:199:A:VAL:HG21 | 1:200:A:PRO:HG2  | 20                  | 0.13     | 0.02                | 0.13       |
| (2,1435) | 1:199:A:VAL:HG22 | 1:200:A:PRO:HG2  | 20                  | 0.13     | 0.02                | 0.13       |
| (2,1435) | 1:199:A:VAL:HG23 | 1:200:A:PRO:HG2  | 20                  | 0.13     | 0.02                | 0.13       |
| (2,202)  | 1:197:A:LEU:HA   | 1:210:A:VAL:HG11 | 19                  | 0.17     | 0.05                | 0.18       |
| (2,202)  | 1:197:A:LEU:HA   | 1:210:A:VAL:HG12 | 19                  | 0.17     | 0.05                | 0.18       |
| (2,202)  | 1:197:A:LEU:HA   | 1:210:A:VAL:HG13 | 19                  | 0.17     | 0.05                | 0.18       |
| (2,65)   | 1:243:A:PRO:HG3  | 1:247:A:GLY:HA2  | 17                  | 0.23     | 0.06                | 0.23       |
| (2,91)   | 1:170:A:THR:HB   | 1:219:A:VAL:HG21 | 17                  | 0.19     | 0.04                | 0.18       |
| (2,91)   | 1:170:A:THR:HB   | 1:219:A:VAL:HG22 | 17                  | 0.19     | 0.04                | 0.18       |
| (2,91)   | 1:170:A:THR:HB   | 1:219:A:VAL:HG23 | 17                  | 0.19     | 0.04                | 0.18       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (2,247)  | 1:199:A:VAL:HA   | 1:203:A:ILE:HD11 | 16                  | 0.16     | 0.03                | 0.16       |
| (2,247)  | 1:199:A:VAL:HA   | 1:203:A:ILE:HD12 | 16                  | 0.16     | 0.03                | 0.16       |
| (2,247)  | 1:199:A:VAL:HA   | 1:203:A:ILE:HD13 | 16                  | 0.16     | 0.03                | 0.16       |
| (2,553)  | 1:193:A:LEU:HB3  | 1:249:A:LEU:HD21 | 16                  | 0.16     | 0.04                | 0.14       |
| (2,553)  | 1:193:A:LEU:HB3  | 1:249:A:LEU:HD22 | 16                  | 0.16     | 0.04                | 0.14       |
| (2,553)  | 1:193:A:LEU:HB3  | 1:249:A:LEU:HD23 | 16                  | 0.16     | 0.04                | 0.14       |
| (2,694)  | 1:197:A:LEU:HD21 | 1:221:A:VAL:HB   | 15                  | 0.26     | 0.04                | 0.26       |
| (2,694)  | 1:197:A:LEU:HD22 | 1:221:A:VAL:HB   | 15                  | 0.26     | 0.04                | 0.26       |
| (2,694)  | 1:197:A:LEU:HD23 | 1:221:A:VAL:HB   | 15                  | 0.26     | 0.04                | 0.26       |
| (2,1681) | 1:173:A:PHE:HD2  | 1:235:A:LEU:HD11 | 15                  | 0.21     | 0.1                 | 0.19       |
| (2,1681) | 1:173:A:PHE:HD2  | 1:235:A:LEU:HD12 | 15                  | 0.21     | 0.1                 | 0.19       |
| (2,1681) | 1:173:A:PHE:HD2  | 1:235:A:LEU:HD13 | 15                  | 0.21     | 0.1                 | 0.19       |
| (2,1311) | 1:233:A:LEU:HD11 | 1:235:A:LEU:HD11 | 15                  | 0.18     | 0.03                | 0.17       |
| (2,1311) | 1:233:A:LEU:HD11 | 1:235:A:LEU:HD12 | 15                  | 0.18     | 0.03                | 0.17       |
| (2,1311) | 1:233:A:LEU:HD11 | 1:235:A:LEU:HD13 | 15                  | 0.18     | 0.03                | 0.17       |
| (2,1311) | 1:233:A:LEU:HD12 | 1:235:A:LEU:HD11 | 15                  | 0.18     | 0.03                | 0.17       |
| (2,1311) | 1:233:A:LEU:HD12 | 1:235:A:LEU:HD12 | 15                  | 0.18     | 0.03                | 0.17       |
| (2,1311) | 1:233:A:LEU:HD12 | 1:235:A:LEU:HD13 | 15                  | 0.18     | 0.03                | 0.17       |
| (2,1311) | 1:233:A:LEU:HD13 | 1:235:A:LEU:HD11 | 15                  | 0.18     | 0.03                | 0.17       |
| (2,1311) | 1:233:A:LEU:HD13 | 1:235:A:LEU:HD12 | 15                  | 0.18     | 0.03                | 0.17       |
| (2,1311) | 1:233:A:LEU:HD13 | 1:235:A:LEU:HD13 | 15                  | 0.18     | 0.03                | 0.17       |
| (2,395)  | 1:194:A:TYR:HD2  | 1:195:A:ALA:HB1  | 15                  | 0.15     | 0.03                | 0.15       |
| (2,395)  | 1:194:A:TYR:HD2  | 1:195:A:ALA:HB2  | 15                  | 0.15     | 0.03                | 0.15       |
| (2,395)  | 1:194:A:TYR:HD2  | 1:195:A:ALA:HB3  | 15                  | 0.15     | 0.03                | 0.15       |
| (2,726)  | 1:174:A:TYR:HB3  | 1:251:A:LEU:HD11 | 14                  | 0.2      | 0.07                | 0.2        |
| (2,726)  | 1:174:A:TYR:HB3  | 1:251:A:LEU:HD12 | 14                  | 0.2      | 0.07                | 0.2        |
| (2,726)  | 1:174:A:TYR:HB3  | 1:251:A:LEU:HD13 | 14                  | 0.2      | 0.07                | 0.2        |
| (2,1651) | 1:236:A:LYS:HD2  | 1:237:A:GLY:H    | 14                  | 0.19     | 0.07                | 0.17       |
| (2,1651) | 1:236:A:LYS:HD3  | 1:237:A:GLY:H    | 14                  | 0.19     | 0.07                | 0.17       |
| (2,1213) | 1:231:A:ARG:HD3  | 1:232:A:LYS:H    | 13                  | 0.17     | 0.04                | 0.17       |
| (1,21)   | 1:247:A:GLY:H    | 1:240:A:PHE:O    | 13                  | 0.15     | 0.03                | 0.16       |
| (2,1525) | 1:209:A:LYS:HE2  | 1:222:A:ALA:HB1  | 12                  | 0.18     | 0.06                | 0.16       |
| (2,1525) | 1:209:A:LYS:HE2  | 1:222:A:ALA:HB2  | 12                  | 0.18     | 0.06                | 0.16       |
| (2,1525) | 1:209:A:LYS:HE2  | 1:222:A:ALA:HB3  | 12                  | 0.18     | 0.06                | 0.16       |
| (2,1525) | 1:209:A:LYS:HE3  | 1:222:A:ALA:HB1  | 12                  | 0.18     | 0.06                | 0.16       |
| (2,1525) | 1:209:A:LYS:HE3  | 1:222:A:ALA:HB2  | 12                  | 0.18     | 0.06                | 0.16       |
| (2,1525) | 1:209:A:LYS:HE3  | 1:222:A:ALA:HB3  | 12                  | 0.18     | 0.06                | 0.16       |
| (2,390)  | 1:196:A:THR:HG21 | 1:252:A:GLU:HA   | 12                  | 0.17     | 0.03                | 0.18       |
| (2,390)  | 1:196:A:THR:HG22 | 1:252:A:GLU:HA   | 12                  | 0.17     | 0.03                | 0.18       |
| (2,390)  | 1:196:A:THR:HG23 | 1:252:A:GLU:HA   | 12                  | 0.17     | 0.03                | 0.18       |
| (2,739)  | 1:225:A:PRO:HB3  | 1:226:A:ARG:HG2  | 12                  | 0.14     | 0.03                | 0.13       |
| (2,1470) | 1:202:A:PRO:HB3  | 1:205:A:VAL:HG11 | 11                  | 0.18     | 0.02                | 0.18       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (2,1470) | 1:202:A:PRO:HB3  | 1:205:A:VAL:HG12 | 11                  | 0.18     | 0.02                | 0.18       |
| (2,1470) | 1:202:A:PRO:HB3  | 1:205:A:VAL:HG13 | 11                  | 0.18     | 0.02                | 0.18       |
| (2,1470) | 1:202:A:PRO:HB3  | 1:205:A:VAL:HG21 | 11                  | 0.18     | 0.02                | 0.18       |
| (2,1470) | 1:202:A:PRO:HB3  | 1:205:A:VAL:HG22 | 11                  | 0.18     | 0.02                | 0.18       |
| (2,1470) | 1:202:A:PRO:HB3  | 1:205:A:VAL:HG23 | 11                  | 0.18     | 0.02                | 0.18       |
| (2,778)  | 1:189:A:GLY:HA3  | 1:242:A:GLY:HA3  | 10                  | 0.17     | 0.04                | 0.17       |
| (2,1626) | 1:232:A:LYS:HB3  | 1:232:A:LYS:HE2  | 9                   | 0.36     | 0.08                | 0.34       |
| (2,1626) | 1:232:A:LYS:HB3  | 1:232:A:LYS:HE3  | 9                   | 0.36     | 0.08                | 0.34       |
| (2,1663) | 1:241:A:PRO:HB2  | 1:245:A:GLY:H    | 9                   | 0.16     | 0.05                | 0.14       |
| (2,1663) | 1:241:A:PRO:HB3  | 1:245:A:GLY:H    | 9                   | 0.16     | 0.05                | 0.14       |
| (2,732)  | 1:197:A:LEU:HD21 | 1:251:A:LEU:HD11 | 9                   | 0.14     | 0.03                | 0.13       |
| (2,732)  | 1:197:A:LEU:HD21 | 1:251:A:LEU:HD12 | 9                   | 0.14     | 0.03                | 0.13       |
| (2,732)  | 1:197:A:LEU:HD21 | 1:251:A:LEU:HD13 | 9                   | 0.14     | 0.03                | 0.13       |
| (2,732)  | 1:197:A:LEU:HD22 | 1:251:A:LEU:HD11 | 9                   | 0.14     | 0.03                | 0.13       |
| (2,732)  | 1:197:A:LEU:HD22 | 1:251:A:LEU:HD12 | 9                   | 0.14     | 0.03                | 0.13       |
| (2,732)  | 1:197:A:LEU:HD22 | 1:251:A:LEU:HD13 | 9                   | 0.14     | 0.03                | 0.13       |
| (2,732)  | 1:197:A:LEU:HD23 | 1:251:A:LEU:HD11 | 9                   | 0.14     | 0.03                | 0.13       |
| (2,732)  | 1:197:A:LEU:HD23 | 1:251:A:LEU:HD12 | 9                   | 0.14     | 0.03                | 0.13       |
| (2,732)  | 1:197:A:LEU:HD23 | 1:251:A:LEU:HD13 | 9                   | 0.14     | 0.03                | 0.13       |
| (2,1633) | 1:232:A:LYS:HG2  | 1:253:A:VAL:H    | 8                   | 0.19     | 0.06                | 0.18       |
| (2,1633) | 1:232:A:LYS:HG3  | 1:253:A:VAL:H    | 8                   | 0.19     | 0.06                | 0.18       |
| (2,1006) | 1:230:A:GLY:H    | 1:255:A:ILE:HG13 | 8                   | 0.13     | 0.03                | 0.12       |
| (2,1106) | 1:205:A:VAL:H    | 1:205:A:VAL:HB   | 7                   | 0.44     | 0.01                | 0.44       |
| (2,137)  | 1:202:A:PRO:HA   | 1:205:A:VAL:HB   | 7                   | 0.38     | 0.03                | 0.37       |
| (2,951)  | 1:205:A:VAL:HB   | 1:206:A:VAL:H    | 7                   | 0.24     | 0.04                | 0.24       |
| (2,1639) | 1:232:A:LYS:HE2  | 1:252:A:GLU:HA   | 7                   | 0.13     | 0.04                | 0.12       |
| (2,1639) | 1:232:A:LYS:HE3  | 1:252:A:GLU:HA   | 7                   | 0.13     | 0.04                | 0.12       |
| (2,1578) | 1:219:A:VAL:HG21 | 1:238:A:LYS:HD2  | 6                   | 0.16     | 0.07                | 0.14       |
| (2,1578) | 1:219:A:VAL:HG21 | 1:238:A:LYS:HD3  | 6                   | 0.16     | 0.07                | 0.14       |
| (2,1578) | 1:219:A:VAL:HG22 | 1:238:A:LYS:HD2  | 6                   | 0.16     | 0.07                | 0.14       |
| (2,1578) | 1:219:A:VAL:HG22 | 1:238:A:LYS:HD3  | 6                   | 0.16     | 0.07                | 0.14       |
| (2,1578) | 1:219:A:VAL:HG23 | 1:238:A:LYS:HD2  | 6                   | 0.16     | 0.07                | 0.14       |
| (2,1578) | 1:219:A:VAL:HG23 | 1:238:A:LYS:HD3  | 6                   | 0.16     | 0.07                | 0.14       |
| (2,937)  | 1:250:A:TYR:HD2  | 1:251:A:LEU:H    | 6                   | 0.15     | 0.03                | 0.16       |
| (2,1653) | 1:236:A:LYS:HD2  | 1:246:A:ARG:HG2  | 6                   | 0.14     | 0.03                | 0.16       |
| (2,1653) | 1:236:A:LYS:HD3  | 1:246:A:ARG:HG2  | 6                   | 0.14     | 0.03                | 0.16       |
| (2,151)  | 1:193:A:LEU:HD21 | 1:194:A:TYR:HB2  | 6                   | 0.13     | 0.02                | 0.12       |
| (2,151)  | 1:193:A:LEU:HD22 | 1:194:A:TYR:HB2  | 6                   | 0.13     | 0.02                | 0.12       |
| (2,151)  | 1:193:A:LEU:HD23 | 1:194:A:TYR:HB2  | 6                   | 0.13     | 0.02                | 0.12       |
| (2,1589) | 1:221:A:VAL:HG11 | 1:222:A:ALA:H    | 5                   | 0.38     | 0.01                | 0.39       |
| (2,1589) | 1:221:A:VAL:HG12 | 1:222:A:ALA:H    | 5                   | 0.38     | 0.01                | 0.39       |
| (2,1589) | 1:221:A:VAL:HG13 | 1:222:A:ALA:H    | 5                   | 0.38     | 0.01                | 0.39       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (2,1589) | 1:221:A:VAL:HG21 | 1:222:A:ALA:H    | 5                   | 0.38     | 0.01                | 0.39       |
| (2,1589) | 1:221:A:VAL:HG22 | 1:222:A:ALA:H    | 5                   | 0.38     | 0.01                | 0.39       |
| (2,1589) | 1:221:A:VAL:HG23 | 1:222:A:ALA:H    | 5                   | 0.38     | 0.01                | 0.39       |
| (2,487)  | 1:173:A:PHE:H    | 1:175:A:THR:HG21 | 5                   | 0.19     | 0.07                | 0.19       |
| (2,487)  | 1:173:A:PHE:H    | 1:175:A:THR:HG22 | 5                   | 0.19     | 0.07                | 0.19       |
| (2,487)  | 1:173:A:PHE:H    | 1:175:A:THR:HG23 | 5                   | 0.19     | 0.07                | 0.19       |
| (2,1315) | 1:221:A:VAL:HG11 | 1:233:A:LEU:HD11 | 5                   | 0.15     | 0.02                | 0.16       |
| (2,1315) | 1:221:A:VAL:HG11 | 1:233:A:LEU:HD12 | 5                   | 0.15     | 0.02                | 0.16       |
| (2,1315) | 1:221:A:VAL:HG11 | 1:233:A:LEU:HD13 | 5                   | 0.15     | 0.02                | 0.16       |
| (2,1315) | 1:221:A:VAL:HG12 | 1:233:A:LEU:HD11 | 5                   | 0.15     | 0.02                | 0.16       |
| (2,1315) | 1:221:A:VAL:HG12 | 1:233:A:LEU:HD12 | 5                   | 0.15     | 0.02                | 0.16       |
| (2,1315) | 1:221:A:VAL:HG12 | 1:233:A:LEU:HD13 | 5                   | 0.15     | 0.02                | 0.16       |
| (2,1315) | 1:221:A:VAL:HG13 | 1:233:A:LEU:HD11 | 5                   | 0.15     | 0.02                | 0.16       |
| (2,1315) | 1:221:A:VAL:HG13 | 1:233:A:LEU:HD12 | 5                   | 0.15     | 0.02                | 0.16       |
| (2,1315) | 1:221:A:VAL:HG13 | 1:233:A:LEU:HD13 | 5                   | 0.15     | 0.02                | 0.16       |
| (2,292)  | 1:191:A:GLN:HB3  | 1:243:A:PRO:HG3  | 4                   | 0.16     | 0.02                | 0.17       |
| (2,1684) | 1:172:A:LEU:HG   | 1:219:A:VAL:HG11 | 4                   | 0.14     | 0.04                | 0.12       |
| (2,1684) | 1:172:A:LEU:HG   | 1:219:A:VAL:HG12 | 4                   | 0.14     | 0.04                | 0.12       |
| (2,1684) | 1:172:A:LEU:HG   | 1:219:A:VAL:HG13 | 4                   | 0.14     | 0.04                | 0.12       |
| (2,1684) | 1:172:A:LEU:HG   | 1:219:A:VAL:HG21 | 4                   | 0.14     | 0.04                | 0.12       |
| (2,1684) | 1:172:A:LEU:HG   | 1:219:A:VAL:HG22 | 4                   | 0.14     | 0.04                | 0.12       |
| (2,1684) | 1:172:A:LEU:HG   | 1:219:A:VAL:HG23 | 4                   | 0.14     | 0.04                | 0.12       |
| (2,1284) | 1:195:A:ALA:H    | 1:250:A:TYR:HD1  | 4                   | 0.14     | 0.03                | 0.14       |
| (2,332)  | 1:231:A:ARG:HD3  | 1:253:A:VAL:HG11 | 4                   | 0.12     | 0.02                | 0.11       |
| (2,332)  | 1:231:A:ARG:HD3  | 1:253:A:VAL:HG12 | 4                   | 0.12     | 0.02                | 0.11       |
| (2,332)  | 1:231:A:ARG:HD3  | 1:253:A:VAL:HG13 | 4                   | 0.12     | 0.02                | 0.11       |
| (2,924)  | 1:235:A:LEU:HD21 | 1:236:A:LYS:H    | 4                   | 0.12     | 0.01                | 0.12       |
| (2,924)  | 1:235:A:LEU:HD22 | 1:236:A:LYS:H    | 4                   | 0.12     | 0.01                | 0.12       |
| (2,924)  | 1:235:A:LEU:HD23 | 1:236:A:LYS:H    | 4                   | 0.12     | 0.01                | 0.12       |
| (2,773)  | 1:228:A:GLN:HG3  | 1:255:A:ILE:HG21 | 4                   | 0.11     | 0.0                 | 0.11       |
| (2,773)  | 1:228:A:GLN:HG3  | 1:255:A:ILE:HG22 | 4                   | 0.11     | 0.0                 | 0.11       |
| (2,773)  | 1:228:A:GLN:HG3  | 1:255:A:ILE:HG23 | 4                   | 0.11     | 0.0                 | 0.11       |
| (2,474)  | 1:180:A:GLY:H    | 1:231:A:ARG:HD2  | 3                   | 0.24     | 0.16                | 0.14       |
| (2,1607) | 1:223:A:VAL:HG11 | 1:231:A:ARG:HD2  | 3                   | 0.19     | 0.01                | 0.18       |
| (2,1607) | 1:223:A:VAL:HG12 | 1:231:A:ARG:HD2  | 3                   | 0.19     | 0.01                | 0.18       |
| (2,1607) | 1:223:A:VAL:HG13 | 1:231:A:ARG:HD2  | 3                   | 0.19     | 0.01                | 0.18       |
| (2,1607) | 1:223:A:VAL:HG21 | 1:231:A:ARG:HD2  | 3                   | 0.19     | 0.01                | 0.18       |
| (2,1607) | 1:223:A:VAL:HG22 | 1:231:A:ARG:HD2  | 3                   | 0.19     | 0.01                | 0.18       |
| (2,1607) | 1:223:A:VAL:HG23 | 1:231:A:ARG:HD2  | 3                   | 0.19     | 0.01                | 0.18       |
| (2,34)   | 1:194:A:TYR:HD2  | 1:249:A:LEU:HD11 | 3                   | 0.13     | 0.02                | 0.14       |
| (2,34)   | 1:194:A:TYR:HD2  | 1:249:A:LEU:HD12 | 3                   | 0.13     | 0.02                | 0.14       |
| (2,34)   | 1:194:A:TYR:HD2  | 1:249:A:LEU:HD13 | 3                   | 0.13     | 0.02                | 0.14       |

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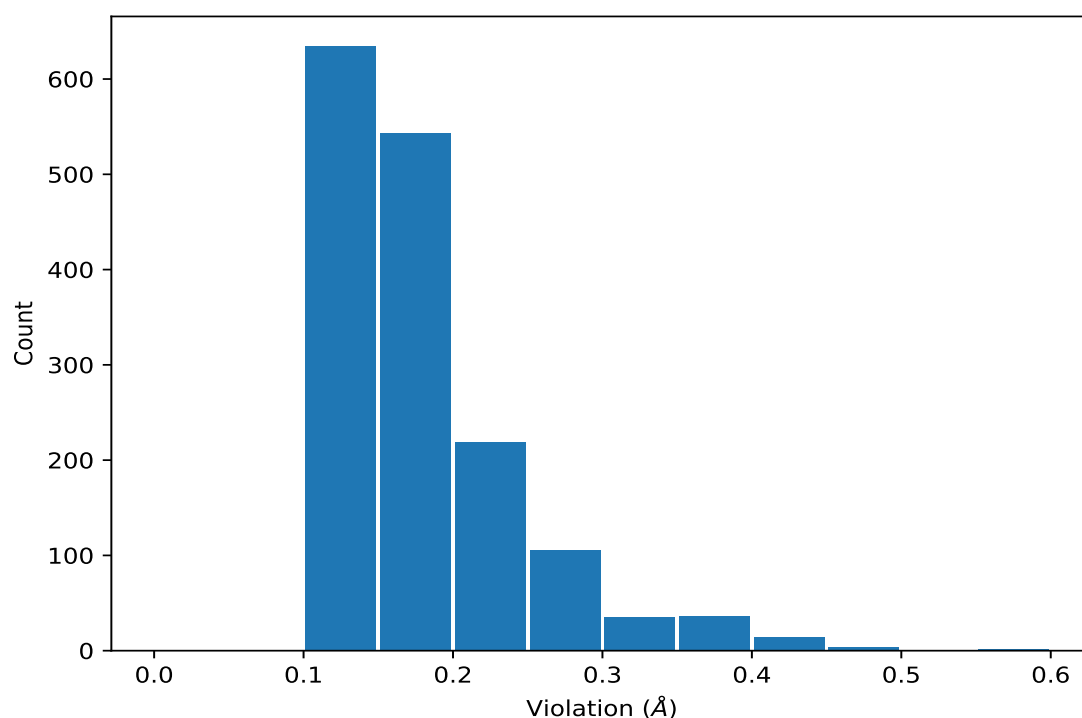
| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (2,828)  | 1:228:A:GLN:H    | 1:231:A:ARG:HB2  | 3                   | 0.13     | 0.03                | 0.11       |
| (2,1050) | 1:231:A:ARG:H    | 1:253:A:VAL:HG11 | 3                   | 0.12     | 0.02                | 0.11       |
| (2,1050) | 1:231:A:ARG:H    | 1:253:A:VAL:HG12 | 3                   | 0.12     | 0.02                | 0.11       |
| (2,1050) | 1:231:A:ARG:H    | 1:253:A:VAL:HG13 | 3                   | 0.12     | 0.02                | 0.11       |
| (2,1298) | 1:223:A:VAL:HG21 | 1:224:A:PRO:HG2  | 3                   | 0.11     | 0.02                | 0.1        |
| (2,1298) | 1:223:A:VAL:HG22 | 1:224:A:PRO:HG2  | 3                   | 0.11     | 0.02                | 0.1        |
| (2,1298) | 1:223:A:VAL:HG23 | 1:224:A:PRO:HG2  | 3                   | 0.11     | 0.02                | 0.1        |
| (2,67)   | 1:179:A:ALA:HB1  | 1:226:A:ARG:HA   | 2                   | 0.2      | 0.02                | 0.2        |
| (2,67)   | 1:179:A:ALA:HB2  | 1:226:A:ARG:HA   | 2                   | 0.2      | 0.02                | 0.2        |
| (2,67)   | 1:179:A:ALA:HB3  | 1:226:A:ARG:HA   | 2                   | 0.2      | 0.02                | 0.2        |
| (2,1207) | 1:171:A:ASP:H    | 1:172:A:LEU:H    | 2                   | 0.2      | 0.0                 | 0.2        |
| (2,30)   | 1:174:A:TYR:HE1  | 1:175:A:THR:HG21 | 2                   | 0.2      | 0.01                | 0.2        |
| (2,30)   | 1:174:A:TYR:HE1  | 1:175:A:THR:HG22 | 2                   | 0.2      | 0.01                | 0.2        |
| (2,30)   | 1:174:A:TYR:HE1  | 1:175:A:THR:HG23 | 2                   | 0.2      | 0.01                | 0.2        |
| (2,488)  | 1:170:A:THR:HG21 | 1:171:A:ASP:HA   | 2                   | 0.18     | 0.05                | 0.18       |
| (2,488)  | 1:170:A:THR:HG22 | 1:171:A:ASP:HA   | 2                   | 0.18     | 0.05                | 0.18       |
| (2,488)  | 1:170:A:THR:HG23 | 1:171:A:ASP:HA   | 2                   | 0.18     | 0.05                | 0.18       |
| (2,1524) | 1:209:A:LYS:HE2  | 1:222:A:ALA:HA   | 2                   | 0.18     | 0.01                | 0.18       |
| (2,1524) | 1:209:A:LYS:HE3  | 1:222:A:ALA:HA   | 2                   | 0.18     | 0.01                | 0.18       |
| (2,564)  | 1:178:A:ALA:HB1  | 1:233:A:LEU:HB3  | 2                   | 0.16     | 0.04                | 0.16       |
| (2,564)  | 1:178:A:ALA:HB2  | 1:233:A:LEU:HB3  | 2                   | 0.16     | 0.04                | 0.16       |
| (2,564)  | 1:178:A:ALA:HB3  | 1:233:A:LEU:HB3  | 2                   | 0.16     | 0.04                | 0.16       |
| (2,396)  | 1:225:A:PRO:HG2  | 1:226:A:ARG:HG3  | 2                   | 0.14     | 0.01                | 0.14       |
| (2,687)  | 1:197:A:LEU:HD21 | 1:212:A:ALA:H    | 2                   | 0.14     | 0.01                | 0.14       |
| (2,687)  | 1:197:A:LEU:HD22 | 1:212:A:ALA:H    | 2                   | 0.14     | 0.01                | 0.14       |
| (2,687)  | 1:197:A:LEU:HD23 | 1:212:A:ALA:H    | 2                   | 0.14     | 0.01                | 0.14       |
| (2,1262) | 1:205:A:VAL:HG21 | 1:226:A:ARG:H    | 2                   | 0.14     | 0.04                | 0.14       |
| (2,1262) | 1:205:A:VAL:HG22 | 1:226:A:ARG:H    | 2                   | 0.14     | 0.04                | 0.14       |
| (2,1262) | 1:205:A:VAL:HG23 | 1:226:A:ARG:H    | 2                   | 0.14     | 0.04                | 0.14       |
| (2,382)  | 1:198:A:ASP:HA   | 1:254:A:ARG:HB3  | 2                   | 0.12     | 0.01                | 0.12       |

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

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

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

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



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

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

| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (2,1626) | 1:232:A:LYS:HB3 | 1:232:A:LYS:HE2  | 7        | 0.59          |
| (2,1626) | 1:232:A:LYS:HB3 | 1:232:A:LYS:HE3  | 7        | 0.59          |
| (2,1106) | 1:205:A:VAL:H   | 1:205:A:VAL:HB   | 3        | 0.46          |
| (2,474)  | 1:180:A:GLY:H   | 1:231:A:ARG:HD2  | 2        | 0.46          |
| (2,1106) | 1:205:A:VAL:H   | 1:205:A:VAL:HB   | 10       | 0.45          |
| (2,1106) | 1:205:A:VAL:H   | 1:205:A:VAL:HB   | 12       | 0.45          |
| (2,1106) | 1:205:A:VAL:H   | 1:205:A:VAL:HB   | 5        | 0.44          |
| (2,1106) | 1:205:A:VAL:H   | 1:205:A:VAL:HB   | 14       | 0.44          |
| (2,1106) | 1:205:A:VAL:H   | 1:205:A:VAL:HB   | 20       | 0.44          |
| (2,137)  | 1:202:A:PRO:HA  | 1:205:A:VAL:HB   | 16       | 0.44          |
| (2,1106) | 1:205:A:VAL:H   | 1:205:A:VAL:HB   | 16       | 0.43          |
| (2,1681) | 1:173:A:PHE:HD2 | 1:235:A:LEU:HD11 | 4        | 0.42          |
| (2,1681) | 1:173:A:PHE:HD2 | 1:235:A:LEU:HD12 | 4        | 0.42          |
| (2,1681) | 1:173:A:PHE:HD2 | 1:235:A:LEU:HD13 | 4        | 0.42          |
| (2,1681) | 1:173:A:PHE:HD2 | 1:235:A:LEU:HD11 | 12       | 0.42          |
| (2,1681) | 1:173:A:PHE:HD2 | 1:235:A:LEU:HD12 | 12       | 0.42          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,1681) | 1:173:A:PHE:HD2  | 1:235:A:LEU:HD13 | 12       | 0.42          |
| (2,1626) | 1:232:A:LYS:HB3  | 1:232:A:LYS:HE2  | 4        | 0.4           |
| (2,1626) | 1:232:A:LYS:HB3  | 1:232:A:LYS:HE3  | 4        | 0.4           |
| (2,137)  | 1:202:A:PRO:HA   | 1:205:A:VAL:HB   | 12       | 0.4           |
| (2,1589) | 1:221:A:VAL:HG11 | 1:222:A:ALA:H    | 12       | 0.39          |
| (2,1589) | 1:221:A:VAL:HG12 | 1:222:A:ALA:H    | 12       | 0.39          |
| (2,1589) | 1:221:A:VAL:HG13 | 1:222:A:ALA:H    | 12       | 0.39          |
| (2,1589) | 1:221:A:VAL:HG21 | 1:222:A:ALA:H    | 12       | 0.39          |
| (2,1589) | 1:221:A:VAL:HG22 | 1:222:A:ALA:H    | 12       | 0.39          |
| (2,1589) | 1:221:A:VAL:HG23 | 1:222:A:ALA:H    | 12       | 0.39          |
| (2,1589) | 1:221:A:VAL:HG11 | 1:222:A:ALA:H    | 16       | 0.39          |
| (2,1589) | 1:221:A:VAL:HG12 | 1:222:A:ALA:H    | 16       | 0.39          |
| (2,1589) | 1:221:A:VAL:HG13 | 1:222:A:ALA:H    | 16       | 0.39          |
| (2,1589) | 1:221:A:VAL:HG21 | 1:222:A:ALA:H    | 16       | 0.39          |
| (2,1589) | 1:221:A:VAL:HG22 | 1:222:A:ALA:H    | 16       | 0.39          |
| (2,1589) | 1:221:A:VAL:HG23 | 1:222:A:ALA:H    | 16       | 0.39          |
| (2,1589) | 1:221:A:VAL:HG11 | 1:222:A:ALA:H    | 17       | 0.39          |
| (2,1589) | 1:221:A:VAL:HG12 | 1:222:A:ALA:H    | 17       | 0.39          |
| (2,1589) | 1:221:A:VAL:HG13 | 1:222:A:ALA:H    | 17       | 0.39          |
| (2,1589) | 1:221:A:VAL:HG21 | 1:222:A:ALA:H    | 17       | 0.39          |
| (2,1589) | 1:221:A:VAL:HG22 | 1:222:A:ALA:H    | 17       | 0.39          |
| (2,1589) | 1:221:A:VAL:HG23 | 1:222:A:ALA:H    | 17       | 0.39          |
| (2,137)  | 1:202:A:PRO:HA   | 1:205:A:VAL:HB   | 3        | 0.39          |
| (2,1589) | 1:221:A:VAL:HG11 | 1:222:A:ALA:H    | 14       | 0.38          |
| (2,1589) | 1:221:A:VAL:HG12 | 1:222:A:ALA:H    | 14       | 0.38          |
| (2,1589) | 1:221:A:VAL:HG13 | 1:222:A:ALA:H    | 14       | 0.38          |
| (2,1589) | 1:221:A:VAL:HG21 | 1:222:A:ALA:H    | 14       | 0.38          |
| (2,1589) | 1:221:A:VAL:HG22 | 1:222:A:ALA:H    | 14       | 0.38          |
| (2,1589) | 1:221:A:VAL:HG23 | 1:222:A:ALA:H    | 14       | 0.38          |
| (2,137)  | 1:202:A:PRO:HA   | 1:205:A:VAL:HB   | 5        | 0.37          |
| (2,137)  | 1:202:A:PRO:HA   | 1:205:A:VAL:HB   | 10       | 0.37          |
| (2,137)  | 1:202:A:PRO:HA   | 1:205:A:VAL:HB   | 20       | 0.37          |
| (2,1589) | 1:221:A:VAL:HG11 | 1:222:A:ALA:H    | 4        | 0.36          |
| (2,1589) | 1:221:A:VAL:HG12 | 1:222:A:ALA:H    | 4        | 0.36          |
| (2,1589) | 1:221:A:VAL:HG13 | 1:222:A:ALA:H    | 4        | 0.36          |
| (2,1589) | 1:221:A:VAL:HG21 | 1:222:A:ALA:H    | 4        | 0.36          |
| (2,1589) | 1:221:A:VAL:HG22 | 1:222:A:ALA:H    | 4        | 0.36          |
| (2,1589) | 1:221:A:VAL:HG23 | 1:222:A:ALA:H    | 4        | 0.36          |
| (2,137)  | 1:202:A:PRO:HA   | 1:205:A:VAL:HB   | 14       | 0.35          |
| (2,65)   | 1:243:A:PRO:HG3  | 1:247:A:GLY:HA2  | 1        | 0.35          |
| (2,1651) | 1:236:A:LYS:HD2  | 1:237:A:GLY:H    | 16       | 0.34          |
| (2,1651) | 1:236:A:LYS:HD3  | 1:237:A:GLY:H    | 16       | 0.34          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,1626) | 1:232:A:LYS:HB3  | 1:232:A:LYS:HE2  | 3        | 0.34          |
| (2,1626) | 1:232:A:LYS:HB3  | 1:232:A:LYS:HE3  | 3        | 0.34          |
| (2,1626) | 1:232:A:LYS:HB3  | 1:232:A:LYS:HE2  | 13       | 0.34          |
| (2,1626) | 1:232:A:LYS:HB3  | 1:232:A:LYS:HE3  | 13       | 0.34          |
| (2,1626) | 1:232:A:LYS:HB3  | 1:232:A:LYS:HE2  | 15       | 0.34          |
| (2,1626) | 1:232:A:LYS:HB3  | 1:232:A:LYS:HE3  | 15       | 0.34          |
| (2,694)  | 1:197:A:LEU:HD21 | 1:221:A:VAL:HB   | 9        | 0.34          |
| (2,694)  | 1:197:A:LEU:HD22 | 1:221:A:VAL:HB   | 9        | 0.34          |
| (2,694)  | 1:197:A:LEU:HD23 | 1:221:A:VAL:HB   | 9        | 0.34          |
| (2,65)   | 1:243:A:PRO:HG3  | 1:247:A:GLY:HA2  | 6        | 0.34          |
| (2,1626) | 1:232:A:LYS:HB3  | 1:232:A:LYS:HE2  | 11       | 0.33          |
| (2,1626) | 1:232:A:LYS:HB3  | 1:232:A:LYS:HE3  | 11       | 0.33          |
| (2,1681) | 1:173:A:PHE:HD2  | 1:235:A:LEU:HD11 | 14       | 0.32          |
| (2,1681) | 1:173:A:PHE:HD2  | 1:235:A:LEU:HD12 | 14       | 0.32          |
| (2,1681) | 1:173:A:PHE:HD2  | 1:235:A:LEU:HD13 | 14       | 0.32          |
| (2,1626) | 1:232:A:LYS:HB3  | 1:232:A:LYS:HE2  | 9        | 0.32          |
| (2,1626) | 1:232:A:LYS:HB3  | 1:232:A:LYS:HE3  | 9        | 0.32          |
| (2,1626) | 1:232:A:LYS:HB3  | 1:232:A:LYS:HE2  | 20       | 0.32          |
| (2,1626) | 1:232:A:LYS:HB3  | 1:232:A:LYS:HE3  | 20       | 0.32          |
| (2,726)  | 1:174:A:TYR:HB3  | 1:251:A:LEU:HD11 | 9        | 0.32          |
| (2,726)  | 1:174:A:TYR:HB3  | 1:251:A:LEU:HD12 | 9        | 0.32          |
| (2,726)  | 1:174:A:TYR:HB3  | 1:251:A:LEU:HD13 | 9        | 0.32          |
| (2,1578) | 1:219:A:VAL:HG21 | 1:238:A:LYS:HD2  | 20       | 0.31          |
| (2,1578) | 1:219:A:VAL:HG21 | 1:238:A:LYS:HD3  | 20       | 0.31          |
| (2,1578) | 1:219:A:VAL:HG22 | 1:238:A:LYS:HD2  | 20       | 0.31          |
| (2,1578) | 1:219:A:VAL:HG22 | 1:238:A:LYS:HD3  | 20       | 0.31          |
| (2,1578) | 1:219:A:VAL:HG23 | 1:238:A:LYS:HD2  | 20       | 0.31          |
| (2,1578) | 1:219:A:VAL:HG23 | 1:238:A:LYS:HD3  | 20       | 0.31          |
| (2,951)  | 1:205:A:VAL:HB   | 1:206:A:VAL:H    | 14       | 0.31          |
| (2,694)  | 1:197:A:LEU:HD21 | 1:221:A:VAL:HB   | 13       | 0.3           |
| (2,694)  | 1:197:A:LEU:HD22 | 1:221:A:VAL:HB   | 13       | 0.3           |
| (2,694)  | 1:197:A:LEU:HD23 | 1:221:A:VAL:HB   | 13       | 0.3           |
| (2,65)   | 1:243:A:PRO:HG3  | 1:247:A:GLY:HA2  | 2        | 0.3           |
| (2,1651) | 1:236:A:LYS:HD2  | 1:237:A:GLY:H    | 17       | 0.29          |
| (2,1651) | 1:236:A:LYS:HD3  | 1:237:A:GLY:H    | 17       | 0.29          |
| (2,1651) | 1:236:A:LYS:HD2  | 1:237:A:GLY:H    | 18       | 0.29          |
| (2,1651) | 1:236:A:LYS:HD3  | 1:237:A:GLY:H    | 18       | 0.29          |
| (2,1633) | 1:232:A:LYS:HG2  | 1:253:A:VAL:H    | 1        | 0.29          |
| (2,1633) | 1:232:A:LYS:HG3  | 1:253:A:VAL:H    | 1        | 0.29          |
| (2,1626) | 1:232:A:LYS:HB3  | 1:232:A:LYS:HE2  | 5        | 0.29          |
| (2,1626) | 1:232:A:LYS:HB3  | 1:232:A:LYS:HE3  | 5        | 0.29          |
| (2,1525) | 1:209:A:LYS:HE2  | 1:222:A:ALA:HB1  | 6        | 0.29          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,1525) | 1:209:A:LYS:HE2  | 1:222:A:ALA:HB2  | 6        | 0.29          |
| (2,1525) | 1:209:A:LYS:HE2  | 1:222:A:ALA:HB3  | 6        | 0.29          |
| (2,1525) | 1:209:A:LYS:HE3  | 1:222:A:ALA:HB1  | 6        | 0.29          |
| (2,1525) | 1:209:A:LYS:HE3  | 1:222:A:ALA:HB2  | 6        | 0.29          |
| (2,1525) | 1:209:A:LYS:HE3  | 1:222:A:ALA:HB3  | 6        | 0.29          |
| (2,726)  | 1:174:A:TYR:HB3  | 1:251:A:LEU:HD11 | 8        | 0.29          |
| (2,726)  | 1:174:A:TYR:HB3  | 1:251:A:LEU:HD12 | 8        | 0.29          |
| (2,726)  | 1:174:A:TYR:HB3  | 1:251:A:LEU:HD13 | 8        | 0.29          |
| (2,694)  | 1:197:A:LEU:HD21 | 1:221:A:VAL:HB   | 3        | 0.29          |
| (2,694)  | 1:197:A:LEU:HD22 | 1:221:A:VAL:HB   | 3        | 0.29          |
| (2,694)  | 1:197:A:LEU:HD23 | 1:221:A:VAL:HB   | 3        | 0.29          |
| (2,694)  | 1:197:A:LEU:HD21 | 1:221:A:VAL:HB   | 18       | 0.29          |
| (2,694)  | 1:197:A:LEU:HD22 | 1:221:A:VAL:HB   | 18       | 0.29          |
| (2,694)  | 1:197:A:LEU:HD23 | 1:221:A:VAL:HB   | 18       | 0.29          |
| (2,694)  | 1:197:A:LEU:HD21 | 1:221:A:VAL:HB   | 7        | 0.28          |
| (2,694)  | 1:197:A:LEU:HD22 | 1:221:A:VAL:HB   | 7        | 0.28          |
| (2,694)  | 1:197:A:LEU:HD23 | 1:221:A:VAL:HB   | 7        | 0.28          |
| (2,91)   | 1:170:A:THR:HB   | 1:219:A:VAL:HG21 | 2        | 0.28          |
| (2,91)   | 1:170:A:THR:HB   | 1:219:A:VAL:HG22 | 2        | 0.28          |
| (2,91)   | 1:170:A:THR:HB   | 1:219:A:VAL:HG23 | 2        | 0.28          |
| (2,1633) | 1:232:A:LYS:HG2  | 1:253:A:VAL:H    | 13       | 0.27          |
| (2,1633) | 1:232:A:LYS:HG3  | 1:253:A:VAL:H    | 13       | 0.27          |
| (2,1525) | 1:209:A:LYS:HE2  | 1:222:A:ALA:HB1  | 13       | 0.27          |
| (2,1525) | 1:209:A:LYS:HE2  | 1:222:A:ALA:HB2  | 13       | 0.27          |
| (2,1525) | 1:209:A:LYS:HE2  | 1:222:A:ALA:HB3  | 13       | 0.27          |
| (2,1525) | 1:209:A:LYS:HE3  | 1:222:A:ALA:HB1  | 13       | 0.27          |
| (2,1525) | 1:209:A:LYS:HE3  | 1:222:A:ALA:HB2  | 13       | 0.27          |
| (2,1525) | 1:209:A:LYS:HE3  | 1:222:A:ALA:HB3  | 13       | 0.27          |
| (2,951)  | 1:205:A:VAL:HB   | 1:206:A:VAL:H    | 20       | 0.27          |
| (2,694)  | 1:197:A:LEU:HD21 | 1:221:A:VAL:HB   | 6        | 0.27          |
| (2,694)  | 1:197:A:LEU:HD22 | 1:221:A:VAL:HB   | 6        | 0.27          |
| (2,694)  | 1:197:A:LEU:HD23 | 1:221:A:VAL:HB   | 6        | 0.27          |
| (2,694)  | 1:197:A:LEU:HD21 | 1:221:A:VAL:HB   | 19       | 0.27          |
| (2,694)  | 1:197:A:LEU:HD22 | 1:221:A:VAL:HB   | 19       | 0.27          |
| (2,694)  | 1:197:A:LEU:HD23 | 1:221:A:VAL:HB   | 19       | 0.27          |
| (2,633)  | 1:197:A:LEU:HB3  | 1:210:A:VAL:HG21 | 14       | 0.27          |
| (2,633)  | 1:197:A:LEU:HB3  | 1:210:A:VAL:HG22 | 14       | 0.27          |
| (2,633)  | 1:197:A:LEU:HB3  | 1:210:A:VAL:HG23 | 14       | 0.27          |
| (2,487)  | 1:173:A:PHE:H    | 1:175:A:THR:HG21 | 14       | 0.27          |
| (2,487)  | 1:173:A:PHE:H    | 1:175:A:THR:HG22 | 14       | 0.27          |
| (2,487)  | 1:173:A:PHE:H    | 1:175:A:THR:HG23 | 14       | 0.27          |
| (2,202)  | 1:197:A:LEU:HA   | 1:210:A:VAL:HG11 | 10       | 0.27          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,202)  | 1:197:A:LEU:HA   | 1:210:A:VAL:HG12 | 10       | 0.27          |
| (2,202)  | 1:197:A:LEU:HA   | 1:210:A:VAL:HG13 | 10       | 0.27          |
| (2,65)   | 1:243:A:PRO:HG3  | 1:247:A:GLY:HA2  | 3        | 0.27          |
| (2,1681) | 1:173:A:PHE:HD2  | 1:235:A:LEU:HD11 | 15       | 0.26          |
| (2,1681) | 1:173:A:PHE:HD2  | 1:235:A:LEU:HD12 | 15       | 0.26          |
| (2,1681) | 1:173:A:PHE:HD2  | 1:235:A:LEU:HD13 | 15       | 0.26          |
| (2,1311) | 1:233:A:LEU:HD11 | 1:235:A:LEU:HD11 | 18       | 0.26          |
| (2,1311) | 1:233:A:LEU:HD11 | 1:235:A:LEU:HD12 | 18       | 0.26          |
| (2,1311) | 1:233:A:LEU:HD11 | 1:235:A:LEU:HD13 | 18       | 0.26          |
| (2,1311) | 1:233:A:LEU:HD12 | 1:235:A:LEU:HD11 | 18       | 0.26          |
| (2,1311) | 1:233:A:LEU:HD12 | 1:235:A:LEU:HD12 | 18       | 0.26          |
| (2,1311) | 1:233:A:LEU:HD12 | 1:235:A:LEU:HD13 | 18       | 0.26          |
| (2,1311) | 1:233:A:LEU:HD13 | 1:235:A:LEU:HD11 | 18       | 0.26          |
| (2,1311) | 1:233:A:LEU:HD13 | 1:235:A:LEU:HD12 | 18       | 0.26          |
| (2,1311) | 1:233:A:LEU:HD13 | 1:235:A:LEU:HD13 | 18       | 0.26          |
| (2,726)  | 1:174:A:TYR:HB3  | 1:251:A:LEU:HD11 | 18       | 0.26          |
| (2,726)  | 1:174:A:TYR:HB3  | 1:251:A:LEU:HD12 | 18       | 0.26          |
| (2,726)  | 1:174:A:TYR:HB3  | 1:251:A:LEU:HD13 | 18       | 0.26          |
| (2,694)  | 1:197:A:LEU:HD21 | 1:221:A:VAL:HB   | 8        | 0.26          |
| (2,694)  | 1:197:A:LEU:HD22 | 1:221:A:VAL:HB   | 8        | 0.26          |
| (2,694)  | 1:197:A:LEU:HD23 | 1:221:A:VAL:HB   | 8        | 0.26          |
| (2,694)  | 1:197:A:LEU:HD21 | 1:221:A:VAL:HB   | 10       | 0.26          |
| (2,694)  | 1:197:A:LEU:HD22 | 1:221:A:VAL:HB   | 10       | 0.26          |
| (2,694)  | 1:197:A:LEU:HD23 | 1:221:A:VAL:HB   | 10       | 0.26          |
| (2,694)  | 1:197:A:LEU:HD21 | 1:221:A:VAL:HB   | 11       | 0.26          |
| (2,694)  | 1:197:A:LEU:HD22 | 1:221:A:VAL:HB   | 11       | 0.26          |
| (2,694)  | 1:197:A:LEU:HD23 | 1:221:A:VAL:HB   | 11       | 0.26          |
| (2,694)  | 1:197:A:LEU:HD21 | 1:221:A:VAL:HB   | 15       | 0.26          |
| (2,694)  | 1:197:A:LEU:HD22 | 1:221:A:VAL:HB   | 15       | 0.26          |
| (2,694)  | 1:197:A:LEU:HD23 | 1:221:A:VAL:HB   | 15       | 0.26          |
| (2,487)  | 1:173:A:PHE:H    | 1:175:A:THR:HG21 | 11       | 0.26          |
| (2,487)  | 1:173:A:PHE:H    | 1:175:A:THR:HG22 | 11       | 0.26          |
| (2,487)  | 1:173:A:PHE:H    | 1:175:A:THR:HG23 | 11       | 0.26          |
| (2,65)   | 1:243:A:PRO:HG3  | 1:247:A:GLY:HA2  | 4        | 0.26          |
| (2,65)   | 1:243:A:PRO:HG3  | 1:247:A:GLY:HA2  | 11       | 0.26          |
| (2,1663) | 1:241:A:PRO:HB2  | 1:245:A:GLY:H    | 9        | 0.25          |
| (2,1663) | 1:241:A:PRO:HB3  | 1:245:A:GLY:H    | 9        | 0.25          |
| (2,951)  | 1:205:A:VAL:HB   | 1:206:A:VAL:H    | 5        | 0.25          |
| (2,633)  | 1:197:A:LEU:HB3  | 1:210:A:VAL:HG21 | 13       | 0.25          |
| (2,633)  | 1:197:A:LEU:HB3  | 1:210:A:VAL:HG22 | 13       | 0.25          |
| (2,633)  | 1:197:A:LEU:HB3  | 1:210:A:VAL:HG23 | 13       | 0.25          |
| (2,417)  | 1:169:A:GLN:HA   | 1:170:A:THR:HG21 | 4        | 0.25          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,417)  | 1:169:A:GLN:HA   | 1:170:A:THR:HG22 | 4        | 0.25          |
| (2,417)  | 1:169:A:GLN:HA   | 1:170:A:THR:HG23 | 4        | 0.25          |
| (2,247)  | 1:199:A:VAL:HA   | 1:203:A:ILE:HD11 | 7        | 0.25          |
| (2,247)  | 1:199:A:VAL:HA   | 1:203:A:ILE:HD12 | 7        | 0.25          |
| (2,247)  | 1:199:A:VAL:HA   | 1:203:A:ILE:HD13 | 7        | 0.25          |
| (2,202)  | 1:197:A:LEU:HA   | 1:210:A:VAL:HG11 | 2        | 0.25          |
| (2,202)  | 1:197:A:LEU:HA   | 1:210:A:VAL:HG12 | 2        | 0.25          |
| (2,202)  | 1:197:A:LEU:HA   | 1:210:A:VAL:HG13 | 2        | 0.25          |
| (2,91)   | 1:170:A:THR:HB   | 1:219:A:VAL:HG21 | 18       | 0.25          |
| (2,91)   | 1:170:A:THR:HB   | 1:219:A:VAL:HG22 | 18       | 0.25          |
| (2,91)   | 1:170:A:THR:HB   | 1:219:A:VAL:HG23 | 18       | 0.25          |
| (2,65)   | 1:243:A:PRO:HG3  | 1:247:A:GLY:HA2  | 16       | 0.25          |
| (2,65)   | 1:243:A:PRO:HG3  | 1:247:A:GLY:HA2  | 20       | 0.25          |
| (2,951)  | 1:205:A:VAL:HB   | 1:206:A:VAL:H    | 3        | 0.24          |
| (2,778)  | 1:189:A:GLY:HA3  | 1:242:A:GLY:HA3  | 4        | 0.24          |
| (2,726)  | 1:174:A:TYR:HB3  | 1:251:A:LEU:HD11 | 13       | 0.24          |
| (2,726)  | 1:174:A:TYR:HB3  | 1:251:A:LEU:HD12 | 13       | 0.24          |
| (2,726)  | 1:174:A:TYR:HB3  | 1:251:A:LEU:HD13 | 13       | 0.24          |
| (2,633)  | 1:197:A:LEU:HB3  | 1:210:A:VAL:HG21 | 2        | 0.24          |
| (2,633)  | 1:197:A:LEU:HB3  | 1:210:A:VAL:HG22 | 2        | 0.24          |
| (2,633)  | 1:197:A:LEU:HB3  | 1:210:A:VAL:HG23 | 2        | 0.24          |
| (2,488)  | 1:170:A:THR:HG21 | 1:171:A:ASP:HA   | 19       | 0.24          |
| (2,488)  | 1:170:A:THR:HG22 | 1:171:A:ASP:HA   | 19       | 0.24          |
| (2,488)  | 1:170:A:THR:HG23 | 1:171:A:ASP:HA   | 19       | 0.24          |
| (2,1651) | 1:236:A:LYS:HD2  | 1:237:A:GLY:H    | 8        | 0.23          |
| (2,1651) | 1:236:A:LYS:HD3  | 1:237:A:GLY:H    | 8        | 0.23          |
| (2,1311) | 1:233:A:LEU:HD11 | 1:235:A:LEU:HD11 | 6        | 0.23          |
| (2,1311) | 1:233:A:LEU:HD11 | 1:235:A:LEU:HD12 | 6        | 0.23          |
| (2,1311) | 1:233:A:LEU:HD11 | 1:235:A:LEU:HD13 | 6        | 0.23          |
| (2,1311) | 1:233:A:LEU:HD12 | 1:235:A:LEU:HD11 | 6        | 0.23          |
| (2,1311) | 1:233:A:LEU:HD12 | 1:235:A:LEU:HD12 | 6        | 0.23          |
| (2,1311) | 1:233:A:LEU:HD12 | 1:235:A:LEU:HD13 | 6        | 0.23          |
| (2,1311) | 1:233:A:LEU:HD13 | 1:235:A:LEU:HD11 | 6        | 0.23          |
| (2,1311) | 1:233:A:LEU:HD13 | 1:235:A:LEU:HD12 | 6        | 0.23          |
| (2,1311) | 1:233:A:LEU:HD13 | 1:235:A:LEU:HD13 | 6        | 0.23          |
| (2,726)  | 1:174:A:TYR:HB3  | 1:251:A:LEU:HD11 | 2        | 0.23          |
| (2,726)  | 1:174:A:TYR:HB3  | 1:251:A:LEU:HD12 | 2        | 0.23          |
| (2,726)  | 1:174:A:TYR:HB3  | 1:251:A:LEU:HD13 | 2        | 0.23          |
| (2,202)  | 1:197:A:LEU:HA   | 1:210:A:VAL:HG11 | 6        | 0.23          |
| (2,202)  | 1:197:A:LEU:HA   | 1:210:A:VAL:HG12 | 6        | 0.23          |
| (2,202)  | 1:197:A:LEU:HA   | 1:210:A:VAL:HG13 | 6        | 0.23          |
| (2,91)   | 1:170:A:THR:HB   | 1:219:A:VAL:HG21 | 19       | 0.23          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,91)   | 1:170:A:THR:HB   | 1:219:A:VAL:HG22 | 19       | 0.23          |
| (2,91)   | 1:170:A:THR:HB   | 1:219:A:VAL:HG23 | 19       | 0.23          |
| (2,65)   | 1:243:A:PRO:HG3  | 1:247:A:GLY:HA2  | 9        | 0.23          |
| (2,65)   | 1:243:A:PRO:HG3  | 1:247:A:GLY:HA2  | 12       | 0.23          |
| (2,1681) | 1:173:A:PHE:HD2  | 1:235:A:LEU:HD11 | 6        | 0.22          |
| (2,1681) | 1:173:A:PHE:HD2  | 1:235:A:LEU:HD12 | 6        | 0.22          |
| (2,1681) | 1:173:A:PHE:HD2  | 1:235:A:LEU:HD13 | 6        | 0.22          |
| (2,1681) | 1:173:A:PHE:HD2  | 1:235:A:LEU:HD11 | 9        | 0.22          |
| (2,1681) | 1:173:A:PHE:HD2  | 1:235:A:LEU:HD12 | 9        | 0.22          |
| (2,1681) | 1:173:A:PHE:HD2  | 1:235:A:LEU:HD13 | 9        | 0.22          |
| (2,1525) | 1:209:A:LYS:HE2  | 1:222:A:ALA:HB1  | 8        | 0.22          |
| (2,1525) | 1:209:A:LYS:HE2  | 1:222:A:ALA:HB2  | 8        | 0.22          |
| (2,1525) | 1:209:A:LYS:HE2  | 1:222:A:ALA:HB3  | 8        | 0.22          |
| (2,1525) | 1:209:A:LYS:HE3  | 1:222:A:ALA:HB1  | 8        | 0.22          |
| (2,1525) | 1:209:A:LYS:HE3  | 1:222:A:ALA:HB2  | 8        | 0.22          |
| (2,1525) | 1:209:A:LYS:HE3  | 1:222:A:ALA:HB3  | 8        | 0.22          |
| (2,1213) | 1:231:A:ARG:HD3  | 1:232:A:LYS:H    | 12       | 0.22          |
| (2,1213) | 1:231:A:ARG:HD3  | 1:232:A:LYS:H    | 15       | 0.22          |
| (2,726)  | 1:174:A:TYR:HB3  | 1:251:A:LEU:HD11 | 19       | 0.22          |
| (2,726)  | 1:174:A:TYR:HB3  | 1:251:A:LEU:HD12 | 19       | 0.22          |
| (2,726)  | 1:174:A:TYR:HB3  | 1:251:A:LEU:HD13 | 19       | 0.22          |
| (2,694)  | 1:197:A:LEU:HD21 | 1:221:A:VAL:HB   | 1        | 0.22          |
| (2,694)  | 1:197:A:LEU:HD22 | 1:221:A:VAL:HB   | 1        | 0.22          |
| (2,694)  | 1:197:A:LEU:HD23 | 1:221:A:VAL:HB   | 1        | 0.22          |
| (2,694)  | 1:197:A:LEU:HD21 | 1:221:A:VAL:HB   | 2        | 0.22          |
| (2,694)  | 1:197:A:LEU:HD22 | 1:221:A:VAL:HB   | 2        | 0.22          |
| (2,694)  | 1:197:A:LEU:HD23 | 1:221:A:VAL:HB   | 2        | 0.22          |
| (2,633)  | 1:197:A:LEU:HB3  | 1:210:A:VAL:HG21 | 5        | 0.22          |
| (2,633)  | 1:197:A:LEU:HB3  | 1:210:A:VAL:HG22 | 5        | 0.22          |
| (2,633)  | 1:197:A:LEU:HB3  | 1:210:A:VAL:HG23 | 5        | 0.22          |
| (2,390)  | 1:196:A:THR:HG21 | 1:252:A:GLU:HA   | 12       | 0.22          |
| (2,390)  | 1:196:A:THR:HG22 | 1:252:A:GLU:HA   | 12       | 0.22          |
| (2,390)  | 1:196:A:THR:HG23 | 1:252:A:GLU:HA   | 12       | 0.22          |
| (2,91)   | 1:170:A:THR:HB   | 1:219:A:VAL:HG21 | 16       | 0.22          |
| (2,91)   | 1:170:A:THR:HB   | 1:219:A:VAL:HG22 | 16       | 0.22          |
| (2,91)   | 1:170:A:THR:HB   | 1:219:A:VAL:HG23 | 16       | 0.22          |
| (2,67)   | 1:179:A:ALA:HB1  | 1:226:A:ARG:HA   | 8        | 0.22          |
| (2,67)   | 1:179:A:ALA:HB2  | 1:226:A:ARG:HA   | 8        | 0.22          |
| (2,67)   | 1:179:A:ALA:HB3  | 1:226:A:ARG:HA   | 8        | 0.22          |
| (2,65)   | 1:243:A:PRO:HG3  | 1:247:A:GLY:HA2  | 15       | 0.22          |
| (2,1684) | 1:172:A:LEU:HG   | 1:219:A:VAL:HG11 | 6        | 0.21          |
| (2,1684) | 1:172:A:LEU:HG   | 1:219:A:VAL:HG12 | 6        | 0.21          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,1684) | 1:172:A:LEU:HG   | 1:219:A:VAL:HG13 | 6        | 0.21          |
| (2,1684) | 1:172:A:LEU:HG   | 1:219:A:VAL:HG21 | 6        | 0.21          |
| (2,1684) | 1:172:A:LEU:HG   | 1:219:A:VAL:HG22 | 6        | 0.21          |
| (2,1684) | 1:172:A:LEU:HG   | 1:219:A:VAL:HG23 | 6        | 0.21          |
| (2,1663) | 1:241:A:PRO:HB2  | 1:245:A:GLY:H    | 17       | 0.21          |
| (2,1663) | 1:241:A:PRO:HB3  | 1:245:A:GLY:H    | 17       | 0.21          |
| (2,1639) | 1:232:A:LYS:HE2  | 1:252:A:GLU:HA   | 6        | 0.21          |
| (2,1639) | 1:232:A:LYS:HE3  | 1:252:A:GLU:HA   | 6        | 0.21          |
| (2,1581) | 1:220:A:GLU:H    | 1:220:A:GLU:HG2  | 17       | 0.21          |
| (2,1581) | 1:220:A:GLU:H    | 1:220:A:GLU:HG3  | 17       | 0.21          |
| (2,1470) | 1:202:A:PRO:HB3  | 1:205:A:VAL:HG11 | 15       | 0.21          |
| (2,1470) | 1:202:A:PRO:HB3  | 1:205:A:VAL:HG12 | 15       | 0.21          |
| (2,1470) | 1:202:A:PRO:HB3  | 1:205:A:VAL:HG13 | 15       | 0.21          |
| (2,1470) | 1:202:A:PRO:HB3  | 1:205:A:VAL:HG21 | 15       | 0.21          |
| (2,1470) | 1:202:A:PRO:HB3  | 1:205:A:VAL:HG22 | 15       | 0.21          |
| (2,1470) | 1:202:A:PRO:HB3  | 1:205:A:VAL:HG23 | 15       | 0.21          |
| (2,1213) | 1:231:A:ARG:HD3  | 1:232:A:LYS:H    | 2        | 0.21          |
| (2,1213) | 1:231:A:ARG:HD3  | 1:232:A:LYS:H    | 17       | 0.21          |
| (2,951)  | 1:205:A:VAL:HB   | 1:206:A:VAL:H    | 16       | 0.21          |
| (2,778)  | 1:189:A:GLY:HA3  | 1:242:A:GLY:HA3  | 9        | 0.21          |
| (2,726)  | 1:174:A:TYR:HB3  | 1:251:A:LEU:HD11 | 10       | 0.21          |
| (2,726)  | 1:174:A:TYR:HB3  | 1:251:A:LEU:HD12 | 10       | 0.21          |
| (2,726)  | 1:174:A:TYR:HB3  | 1:251:A:LEU:HD13 | 10       | 0.21          |
| (2,694)  | 1:197:A:LEU:HD21 | 1:221:A:VAL:HB   | 20       | 0.21          |
| (2,694)  | 1:197:A:LEU:HD22 | 1:221:A:VAL:HB   | 20       | 0.21          |
| (2,694)  | 1:197:A:LEU:HD23 | 1:221:A:VAL:HB   | 20       | 0.21          |
| (2,633)  | 1:197:A:LEU:HB3  | 1:210:A:VAL:HG21 | 16       | 0.21          |
| (2,633)  | 1:197:A:LEU:HB3  | 1:210:A:VAL:HG22 | 16       | 0.21          |
| (2,633)  | 1:197:A:LEU:HB3  | 1:210:A:VAL:HG23 | 16       | 0.21          |
| (2,553)  | 1:193:A:LEU:HB3  | 1:249:A:LEU:HD21 | 1        | 0.21          |
| (2,553)  | 1:193:A:LEU:HB3  | 1:249:A:LEU:HD22 | 1        | 0.21          |
| (2,553)  | 1:193:A:LEU:HB3  | 1:249:A:LEU:HD23 | 1        | 0.21          |
| (2,553)  | 1:193:A:LEU:HB3  | 1:249:A:LEU:HD21 | 13       | 0.21          |
| (2,553)  | 1:193:A:LEU:HB3  | 1:249:A:LEU:HD22 | 13       | 0.21          |
| (2,553)  | 1:193:A:LEU:HB3  | 1:249:A:LEU:HD23 | 13       | 0.21          |
| (2,202)  | 1:197:A:LEU:HA   | 1:210:A:VAL:HG11 | 3        | 0.21          |
| (2,202)  | 1:197:A:LEU:HA   | 1:210:A:VAL:HG12 | 3        | 0.21          |
| (2,202)  | 1:197:A:LEU:HA   | 1:210:A:VAL:HG13 | 3        | 0.21          |
| (2,91)   | 1:170:A:THR:HB   | 1:219:A:VAL:HG21 | 8        | 0.21          |
| (2,91)   | 1:170:A:THR:HB   | 1:219:A:VAL:HG22 | 8        | 0.21          |
| (2,91)   | 1:170:A:THR:HB   | 1:219:A:VAL:HG23 | 8        | 0.21          |
| (2,91)   | 1:170:A:THR:HB   | 1:219:A:VAL:HG21 | 11       | 0.21          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,91)   | 1:170:A:THR:HB   | 1:219:A:VAL:HG22 | 11       | 0.21          |
| (2,91)   | 1:170:A:THR:HB   | 1:219:A:VAL:HG23 | 11       | 0.21          |
| (2,91)   | 1:170:A:THR:HB   | 1:219:A:VAL:HG21 | 14       | 0.21          |
| (2,91)   | 1:170:A:THR:HB   | 1:219:A:VAL:HG22 | 14       | 0.21          |
| (2,91)   | 1:170:A:THR:HB   | 1:219:A:VAL:HG23 | 14       | 0.21          |
| (2,65)   | 1:243:A:PRO:HG3  | 1:247:A:GLY:HA2  | 14       | 0.21          |
| (1,21)   | 1:247:A:GLY:H    | 1:240:A:PHE:O    | 13       | 0.21          |
| (2,1681) | 1:173:A:PHE:HD2  | 1:235:A:LEU:HD11 | 1        | 0.2           |
| (2,1681) | 1:173:A:PHE:HD2  | 1:235:A:LEU:HD12 | 1        | 0.2           |
| (2,1681) | 1:173:A:PHE:HD2  | 1:235:A:LEU:HD13 | 1        | 0.2           |
| (2,1651) | 1:236:A:LYS:HD2  | 1:237:A:GLY:H    | 19       | 0.2           |
| (2,1651) | 1:236:A:LYS:HD3  | 1:237:A:GLY:H    | 19       | 0.2           |
| (2,1633) | 1:232:A:LYS:HG2  | 1:253:A:VAL:H    | 4        | 0.2           |
| (2,1633) | 1:232:A:LYS:HG3  | 1:253:A:VAL:H    | 4        | 0.2           |
| (2,1607) | 1:223:A:VAL:HG11 | 1:231:A:ARG:HD2  | 2        | 0.2           |
| (2,1607) | 1:223:A:VAL:HG12 | 1:231:A:ARG:HD2  | 2        | 0.2           |
| (2,1607) | 1:223:A:VAL:HG13 | 1:231:A:ARG:HD2  | 2        | 0.2           |
| (2,1607) | 1:223:A:VAL:HG21 | 1:231:A:ARG:HD2  | 2        | 0.2           |
| (2,1607) | 1:223:A:VAL:HG22 | 1:231:A:ARG:HD2  | 2        | 0.2           |
| (2,1607) | 1:223:A:VAL:HG23 | 1:231:A:ARG:HD2  | 2        | 0.2           |
| (2,1525) | 1:209:A:LYS:HE2  | 1:222:A:ALA:HB1  | 3        | 0.2           |
| (2,1525) | 1:209:A:LYS:HE2  | 1:222:A:ALA:HB2  | 3        | 0.2           |
| (2,1525) | 1:209:A:LYS:HE2  | 1:222:A:ALA:HB3  | 3        | 0.2           |
| (2,1525) | 1:209:A:LYS:HE3  | 1:222:A:ALA:HB1  | 3        | 0.2           |
| (2,1525) | 1:209:A:LYS:HE3  | 1:222:A:ALA:HB2  | 3        | 0.2           |
| (2,1525) | 1:209:A:LYS:HE3  | 1:222:A:ALA:HB3  | 3        | 0.2           |
| (2,1470) | 1:202:A:PRO:HB3  | 1:205:A:VAL:HG11 | 13       | 0.2           |
| (2,1470) | 1:202:A:PRO:HB3  | 1:205:A:VAL:HG12 | 13       | 0.2           |
| (2,1470) | 1:202:A:PRO:HB3  | 1:205:A:VAL:HG13 | 13       | 0.2           |
| (2,1470) | 1:202:A:PRO:HB3  | 1:205:A:VAL:HG21 | 13       | 0.2           |
| (2,1470) | 1:202:A:PRO:HB3  | 1:205:A:VAL:HG22 | 13       | 0.2           |
| (2,1470) | 1:202:A:PRO:HB3  | 1:205:A:VAL:HG23 | 13       | 0.2           |
| (2,1470) | 1:202:A:PRO:HB3  | 1:205:A:VAL:HG11 | 19       | 0.2           |
| (2,1470) | 1:202:A:PRO:HB3  | 1:205:A:VAL:HG12 | 19       | 0.2           |
| (2,1470) | 1:202:A:PRO:HB3  | 1:205:A:VAL:HG13 | 19       | 0.2           |
| (2,1470) | 1:202:A:PRO:HB3  | 1:205:A:VAL:HG21 | 19       | 0.2           |
| (2,1470) | 1:202:A:PRO:HB3  | 1:205:A:VAL:HG22 | 19       | 0.2           |
| (2,1470) | 1:202:A:PRO:HB3  | 1:205:A:VAL:HG23 | 19       | 0.2           |
| (2,1311) | 1:233:A:LEU:HD11 | 1:235:A:LEU:HD11 | 10       | 0.2           |
| (2,1311) | 1:233:A:LEU:HD11 | 1:235:A:LEU:HD12 | 10       | 0.2           |
| (2,1311) | 1:233:A:LEU:HD11 | 1:235:A:LEU:HD13 | 10       | 0.2           |
| (2,1311) | 1:233:A:LEU:HD12 | 1:235:A:LEU:HD11 | 10       | 0.2           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,1311) | 1:233:A:LEU:HD12 | 1:235:A:LEU:HD12 | 10       | 0.2           |
| (2,1311) | 1:233:A:LEU:HD12 | 1:235:A:LEU:HD13 | 10       | 0.2           |
| (2,1311) | 1:233:A:LEU:HD13 | 1:235:A:LEU:HD11 | 10       | 0.2           |
| (2,1311) | 1:233:A:LEU:HD13 | 1:235:A:LEU:HD12 | 10       | 0.2           |
| (2,1311) | 1:233:A:LEU:HD13 | 1:235:A:LEU:HD13 | 10       | 0.2           |
| (2,1311) | 1:233:A:LEU:HD11 | 1:235:A:LEU:HD11 | 15       | 0.2           |
| (2,1311) | 1:233:A:LEU:HD11 | 1:235:A:LEU:HD12 | 15       | 0.2           |
| (2,1311) | 1:233:A:LEU:HD11 | 1:235:A:LEU:HD13 | 15       | 0.2           |
| (2,1311) | 1:233:A:LEU:HD12 | 1:235:A:LEU:HD11 | 15       | 0.2           |
| (2,1311) | 1:233:A:LEU:HD12 | 1:235:A:LEU:HD12 | 15       | 0.2           |
| (2,1311) | 1:233:A:LEU:HD12 | 1:235:A:LEU:HD13 | 15       | 0.2           |
| (2,1311) | 1:233:A:LEU:HD13 | 1:235:A:LEU:HD11 | 15       | 0.2           |
| (2,1311) | 1:233:A:LEU:HD13 | 1:235:A:LEU:HD12 | 15       | 0.2           |
| (2,1311) | 1:233:A:LEU:HD13 | 1:235:A:LEU:HD13 | 15       | 0.2           |
| (2,1213) | 1:231:A:ARG:HD3  | 1:232:A:LYS:H    | 20       | 0.2           |
| (2,1207) | 1:171:A:ASP:H    | 1:172:A:LEU:H    | 15       | 0.2           |
| (2,1207) | 1:171:A:ASP:H    | 1:172:A:LEU:H    | 18       | 0.2           |
| (2,951)  | 1:205:A:VAL:HB   | 1:206:A:VAL:H    | 10       | 0.2           |
| (2,951)  | 1:205:A:VAL:HB   | 1:206:A:VAL:H    | 12       | 0.2           |
| (2,739)  | 1:225:A:PRO:HB3  | 1:226:A:ARG:HG2  | 4        | 0.2           |
| (2,732)  | 1:197:A:LEU:HD21 | 1:251:A:LEU:HD11 | 11       | 0.2           |
| (2,732)  | 1:197:A:LEU:HD21 | 1:251:A:LEU:HD12 | 11       | 0.2           |
| (2,732)  | 1:197:A:LEU:HD21 | 1:251:A:LEU:HD13 | 11       | 0.2           |
| (2,732)  | 1:197:A:LEU:HD22 | 1:251:A:LEU:HD11 | 11       | 0.2           |
| (2,732)  | 1:197:A:LEU:HD22 | 1:251:A:LEU:HD12 | 11       | 0.2           |
| (2,732)  | 1:197:A:LEU:HD22 | 1:251:A:LEU:HD13 | 11       | 0.2           |
| (2,732)  | 1:197:A:LEU:HD23 | 1:251:A:LEU:HD11 | 11       | 0.2           |
| (2,732)  | 1:197:A:LEU:HD23 | 1:251:A:LEU:HD12 | 11       | 0.2           |
| (2,732)  | 1:197:A:LEU:HD23 | 1:251:A:LEU:HD13 | 11       | 0.2           |
| (2,726)  | 1:174:A:TYR:HB3  | 1:251:A:LEU:HD11 | 1        | 0.2           |
| (2,726)  | 1:174:A:TYR:HB3  | 1:251:A:LEU:HD12 | 1        | 0.2           |
| (2,726)  | 1:174:A:TYR:HB3  | 1:251:A:LEU:HD13 | 1        | 0.2           |
| (2,633)  | 1:197:A:LEU:HB3  | 1:210:A:VAL:HG21 | 11       | 0.2           |
| (2,633)  | 1:197:A:LEU:HB3  | 1:210:A:VAL:HG22 | 11       | 0.2           |
| (2,633)  | 1:197:A:LEU:HB3  | 1:210:A:VAL:HG23 | 11       | 0.2           |
| (2,553)  | 1:193:A:LEU:HB3  | 1:249:A:LEU:HD21 | 5        | 0.2           |
| (2,553)  | 1:193:A:LEU:HB3  | 1:249:A:LEU:HD22 | 5        | 0.2           |
| (2,553)  | 1:193:A:LEU:HB3  | 1:249:A:LEU:HD23 | 5        | 0.2           |
| (2,553)  | 1:193:A:LEU:HB3  | 1:249:A:LEU:HD21 | 8        | 0.2           |
| (2,553)  | 1:193:A:LEU:HB3  | 1:249:A:LEU:HD22 | 8        | 0.2           |
| (2,553)  | 1:193:A:LEU:HB3  | 1:249:A:LEU:HD23 | 8        | 0.2           |
| (2,390)  | 1:196:A:THR:HG21 | 1:252:A:GLU:HA   | 3        | 0.2           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,390)  | 1:196:A:THR:HG22 | 1:252:A:GLU:HA   | 3        | 0.2           |
| (2,390)  | 1:196:A:THR:HG23 | 1:252:A:GLU:HA   | 3        | 0.2           |
| (2,390)  | 1:196:A:THR:HG21 | 1:252:A:GLU:HA   | 14       | 0.2           |
| (2,390)  | 1:196:A:THR:HG22 | 1:252:A:GLU:HA   | 14       | 0.2           |
| (2,390)  | 1:196:A:THR:HG23 | 1:252:A:GLU:HA   | 14       | 0.2           |
| (2,390)  | 1:196:A:THR:HG21 | 1:252:A:GLU:HA   | 15       | 0.2           |
| (2,390)  | 1:196:A:THR:HG22 | 1:252:A:GLU:HA   | 15       | 0.2           |
| (2,390)  | 1:196:A:THR:HG23 | 1:252:A:GLU:HA   | 15       | 0.2           |
| (2,202)  | 1:197:A:LEU:HA   | 1:210:A:VAL:HG11 | 9        | 0.2           |
| (2,202)  | 1:197:A:LEU:HA   | 1:210:A:VAL:HG12 | 9        | 0.2           |
| (2,202)  | 1:197:A:LEU:HA   | 1:210:A:VAL:HG13 | 9        | 0.2           |
| (2,202)  | 1:197:A:LEU:HA   | 1:210:A:VAL:HG11 | 12       | 0.2           |
| (2,202)  | 1:197:A:LEU:HA   | 1:210:A:VAL:HG12 | 12       | 0.2           |
| (2,202)  | 1:197:A:LEU:HA   | 1:210:A:VAL:HG13 | 12       | 0.2           |
| (2,202)  | 1:197:A:LEU:HA   | 1:210:A:VAL:HG11 | 18       | 0.2           |
| (2,202)  | 1:197:A:LEU:HA   | 1:210:A:VAL:HG12 | 18       | 0.2           |
| (2,202)  | 1:197:A:LEU:HA   | 1:210:A:VAL:HG13 | 18       | 0.2           |
| (2,65)   | 1:243:A:PRO:HG3  | 1:247:A:GLY:HA2  | 18       | 0.2           |
| (2,65)   | 1:243:A:PRO:HG3  | 1:247:A:GLY:HA2  | 19       | 0.2           |
| (2,30)   | 1:174:A:TYR:HE1  | 1:175:A:THR:HG21 | 9        | 0.2           |
| (2,30)   | 1:174:A:TYR:HE1  | 1:175:A:THR:HG22 | 9        | 0.2           |
| (2,30)   | 1:174:A:TYR:HE1  | 1:175:A:THR:HG23 | 9        | 0.2           |
| (2,1681) | 1:173:A:PHE:HD2  | 1:235:A:LEU:HD11 | 16       | 0.19          |
| (2,1681) | 1:173:A:PHE:HD2  | 1:235:A:LEU:HD12 | 16       | 0.19          |
| (2,1681) | 1:173:A:PHE:HD2  | 1:235:A:LEU:HD13 | 16       | 0.19          |
| (2,1663) | 1:241:A:PRO:HB2  | 1:245:A:GLY:H    | 16       | 0.19          |
| (2,1663) | 1:241:A:PRO:HB3  | 1:245:A:GLY:H    | 16       | 0.19          |
| (2,1633) | 1:232:A:LYS:HG2  | 1:253:A:VAL:H    | 9        | 0.19          |
| (2,1633) | 1:232:A:LYS:HG3  | 1:253:A:VAL:H    | 9        | 0.19          |
| (2,1524) | 1:209:A:LYS:HE2  | 1:222:A:ALA:HA   | 13       | 0.19          |
| (2,1524) | 1:209:A:LYS:HE3  | 1:222:A:ALA:HA   | 13       | 0.19          |
| (2,1470) | 1:202:A:PRO:HB3  | 1:205:A:VAL:HG11 | 6        | 0.19          |
| (2,1470) | 1:202:A:PRO:HB3  | 1:205:A:VAL:HG12 | 6        | 0.19          |
| (2,1470) | 1:202:A:PRO:HB3  | 1:205:A:VAL:HG13 | 6        | 0.19          |
| (2,1470) | 1:202:A:PRO:HB3  | 1:205:A:VAL:HG21 | 6        | 0.19          |
| (2,1470) | 1:202:A:PRO:HB3  | 1:205:A:VAL:HG22 | 6        | 0.19          |
| (2,1470) | 1:202:A:PRO:HB3  | 1:205:A:VAL:HG23 | 6        | 0.19          |
| (2,1311) | 1:233:A:LEU:HD11 | 1:235:A:LEU:HD11 | 13       | 0.19          |
| (2,1311) | 1:233:A:LEU:HD11 | 1:235:A:LEU:HD12 | 13       | 0.19          |
| (2,1311) | 1:233:A:LEU:HD11 | 1:235:A:LEU:HD13 | 13       | 0.19          |
| (2,1311) | 1:233:A:LEU:HD12 | 1:235:A:LEU:HD11 | 13       | 0.19          |
| (2,1311) | 1:233:A:LEU:HD12 | 1:235:A:LEU:HD12 | 13       | 0.19          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,1311) | 1:233:A:LEU:HD12 | 1:235:A:LEU:HD13 | 13       | 0.19          |
| (2,1311) | 1:233:A:LEU:HD13 | 1:235:A:LEU:HD11 | 13       | 0.19          |
| (2,1311) | 1:233:A:LEU:HD13 | 1:235:A:LEU:HD12 | 13       | 0.19          |
| (2,1311) | 1:233:A:LEU:HD13 | 1:235:A:LEU:HD13 | 13       | 0.19          |
| (2,739)  | 1:225:A:PRO:HB3  | 1:226:A:ARG:HG2  | 17       | 0.19          |
| (2,633)  | 1:197:A:LEU:HB3  | 1:210:A:VAL:HG21 | 1        | 0.19          |
| (2,633)  | 1:197:A:LEU:HB3  | 1:210:A:VAL:HG22 | 1        | 0.19          |
| (2,633)  | 1:197:A:LEU:HB3  | 1:210:A:VAL:HG23 | 1        | 0.19          |
| (2,633)  | 1:197:A:LEU:HB3  | 1:210:A:VAL:HG21 | 8        | 0.19          |
| (2,633)  | 1:197:A:LEU:HB3  | 1:210:A:VAL:HG22 | 8        | 0.19          |
| (2,633)  | 1:197:A:LEU:HB3  | 1:210:A:VAL:HG23 | 8        | 0.19          |
| (2,633)  | 1:197:A:LEU:HB3  | 1:210:A:VAL:HG21 | 12       | 0.19          |
| (2,633)  | 1:197:A:LEU:HB3  | 1:210:A:VAL:HG22 | 12       | 0.19          |
| (2,633)  | 1:197:A:LEU:HB3  | 1:210:A:VAL:HG23 | 12       | 0.19          |
| (2,633)  | 1:197:A:LEU:HB3  | 1:210:A:VAL:HG21 | 17       | 0.19          |
| (2,633)  | 1:197:A:LEU:HB3  | 1:210:A:VAL:HG22 | 17       | 0.19          |
| (2,633)  | 1:197:A:LEU:HB3  | 1:210:A:VAL:HG23 | 17       | 0.19          |
| (2,564)  | 1:178:A:ALA:HB1  | 1:233:A:LEU:HB3  | 18       | 0.19          |
| (2,564)  | 1:178:A:ALA:HB2  | 1:233:A:LEU:HB3  | 18       | 0.19          |
| (2,564)  | 1:178:A:ALA:HB3  | 1:233:A:LEU:HB3  | 18       | 0.19          |
| (2,553)  | 1:193:A:LEU:HB3  | 1:249:A:LEU:HD21 | 6        | 0.19          |
| (2,553)  | 1:193:A:LEU:HB3  | 1:249:A:LEU:HD22 | 6        | 0.19          |
| (2,553)  | 1:193:A:LEU:HB3  | 1:249:A:LEU:HD23 | 6        | 0.19          |
| (2,553)  | 1:193:A:LEU:HB3  | 1:249:A:LEU:HD21 | 14       | 0.19          |
| (2,553)  | 1:193:A:LEU:HB3  | 1:249:A:LEU:HD22 | 14       | 0.19          |
| (2,553)  | 1:193:A:LEU:HB3  | 1:249:A:LEU:HD23 | 14       | 0.19          |
| (2,487)  | 1:173:A:PHE:H    | 1:175:A:THR:HG21 | 6        | 0.19          |
| (2,487)  | 1:173:A:PHE:H    | 1:175:A:THR:HG22 | 6        | 0.19          |
| (2,487)  | 1:173:A:PHE:H    | 1:175:A:THR:HG23 | 6        | 0.19          |
| (2,395)  | 1:194:A:TYR:HD2  | 1:195:A:ALA:HB1  | 20       | 0.19          |
| (2,395)  | 1:194:A:TYR:HD2  | 1:195:A:ALA:HB2  | 20       | 0.19          |
| (2,395)  | 1:194:A:TYR:HD2  | 1:195:A:ALA:HB3  | 20       | 0.19          |
| (2,390)  | 1:196:A:THR:HG21 | 1:252:A:GLU:HA   | 13       | 0.19          |
| (2,390)  | 1:196:A:THR:HG22 | 1:252:A:GLU:HA   | 13       | 0.19          |
| (2,390)  | 1:196:A:THR:HG23 | 1:252:A:GLU:HA   | 13       | 0.19          |
| (2,292)  | 1:191:A:GLN:HB3  | 1:243:A:PRO:HG3  | 4        | 0.19          |
| (2,247)  | 1:199:A:VAL:HA   | 1:203:A:ILE:HD11 | 17       | 0.19          |
| (2,247)  | 1:199:A:VAL:HA   | 1:203:A:ILE:HD12 | 17       | 0.19          |
| (2,247)  | 1:199:A:VAL:HA   | 1:203:A:ILE:HD13 | 17       | 0.19          |
| (2,202)  | 1:197:A:LEU:HA   | 1:210:A:VAL:HG11 | 15       | 0.19          |
| (2,202)  | 1:197:A:LEU:HA   | 1:210:A:VAL:HG12 | 15       | 0.19          |
| (2,202)  | 1:197:A:LEU:HA   | 1:210:A:VAL:HG13 | 15       | 0.19          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,91)   | 1:170:A:THR:HB   | 1:219:A:VAL:HG21 | 15       | 0.19          |
| (2,91)   | 1:170:A:THR:HB   | 1:219:A:VAL:HG22 | 15       | 0.19          |
| (2,91)   | 1:170:A:THR:HB   | 1:219:A:VAL:HG23 | 15       | 0.19          |
| (2,67)   | 1:179:A:ALA:HB1  | 1:226:A:ARG:HA   | 2        | 0.19          |
| (2,67)   | 1:179:A:ALA:HB2  | 1:226:A:ARG:HA   | 2        | 0.19          |
| (2,67)   | 1:179:A:ALA:HB3  | 1:226:A:ARG:HA   | 2        | 0.19          |
| (2,65)   | 1:243:A:PRO:HG3  | 1:247:A:GLY:HA2  | 5        | 0.19          |
| (2,30)   | 1:174:A:TYR:HE1  | 1:175:A:THR:HG21 | 17       | 0.19          |
| (2,30)   | 1:174:A:TYR:HE1  | 1:175:A:THR:HG22 | 17       | 0.19          |
| (2,30)   | 1:174:A:TYR:HE1  | 1:175:A:THR:HG23 | 17       | 0.19          |
| (2,1651) | 1:236:A:LYS:HD2  | 1:237:A:GLY:H    | 1        | 0.18          |
| (2,1651) | 1:236:A:LYS:HD3  | 1:237:A:GLY:H    | 1        | 0.18          |
| (2,1607) | 1:223:A:VAL:HG11 | 1:231:A:ARG:HD2  | 18       | 0.18          |
| (2,1607) | 1:223:A:VAL:HG12 | 1:231:A:ARG:HD2  | 18       | 0.18          |
| (2,1607) | 1:223:A:VAL:HG13 | 1:231:A:ARG:HD2  | 18       | 0.18          |
| (2,1607) | 1:223:A:VAL:HG21 | 1:231:A:ARG:HD2  | 18       | 0.18          |
| (2,1607) | 1:223:A:VAL:HG22 | 1:231:A:ARG:HD2  | 18       | 0.18          |
| (2,1607) | 1:223:A:VAL:HG23 | 1:231:A:ARG:HD2  | 18       | 0.18          |
| (2,1607) | 1:223:A:VAL:HG11 | 1:231:A:ARG:HD2  | 19       | 0.18          |
| (2,1607) | 1:223:A:VAL:HG12 | 1:231:A:ARG:HD2  | 19       | 0.18          |
| (2,1607) | 1:223:A:VAL:HG13 | 1:231:A:ARG:HD2  | 19       | 0.18          |
| (2,1607) | 1:223:A:VAL:HG21 | 1:231:A:ARG:HD2  | 19       | 0.18          |
| (2,1607) | 1:223:A:VAL:HG22 | 1:231:A:ARG:HD2  | 19       | 0.18          |
| (2,1607) | 1:223:A:VAL:HG23 | 1:231:A:ARG:HD2  | 19       | 0.18          |
| (2,1470) | 1:202:A:PRO:HB3  | 1:205:A:VAL:HG11 | 11       | 0.18          |
| (2,1470) | 1:202:A:PRO:HB3  | 1:205:A:VAL:HG12 | 11       | 0.18          |
| (2,1470) | 1:202:A:PRO:HB3  | 1:205:A:VAL:HG13 | 11       | 0.18          |
| (2,1470) | 1:202:A:PRO:HB3  | 1:205:A:VAL:HG21 | 11       | 0.18          |
| (2,1470) | 1:202:A:PRO:HB3  | 1:205:A:VAL:HG22 | 11       | 0.18          |
| (2,1470) | 1:202:A:PRO:HB3  | 1:205:A:VAL:HG23 | 11       | 0.18          |
| (2,1470) | 1:202:A:PRO:HB3  | 1:205:A:VAL:HG11 | 17       | 0.18          |
| (2,1470) | 1:202:A:PRO:HB3  | 1:205:A:VAL:HG12 | 17       | 0.18          |
| (2,1470) | 1:202:A:PRO:HB3  | 1:205:A:VAL:HG13 | 17       | 0.18          |
| (2,1470) | 1:202:A:PRO:HB3  | 1:205:A:VAL:HG21 | 17       | 0.18          |
| (2,1470) | 1:202:A:PRO:HB3  | 1:205:A:VAL:HG22 | 17       | 0.18          |
| (2,1470) | 1:202:A:PRO:HB3  | 1:205:A:VAL:HG23 | 17       | 0.18          |
| (2,1470) | 1:202:A:PRO:HB3  | 1:205:A:VAL:HG11 | 18       | 0.18          |
| (2,1470) | 1:202:A:PRO:HB3  | 1:205:A:VAL:HG12 | 18       | 0.18          |
| (2,1470) | 1:202:A:PRO:HB3  | 1:205:A:VAL:HG13 | 18       | 0.18          |
| (2,1470) | 1:202:A:PRO:HB3  | 1:205:A:VAL:HG21 | 18       | 0.18          |
| (2,1470) | 1:202:A:PRO:HB3  | 1:205:A:VAL:HG22 | 18       | 0.18          |
| (2,1470) | 1:202:A:PRO:HB3  | 1:205:A:VAL:HG23 | 18       | 0.18          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,1435) | 1:199:A:VAL:HG11 | 1:200:A:PRO:HG2  | 10       | 0.18          |
| (2,1435) | 1:199:A:VAL:HG12 | 1:200:A:PRO:HG2  | 10       | 0.18          |
| (2,1435) | 1:199:A:VAL:HG13 | 1:200:A:PRO:HG2  | 10       | 0.18          |
| (2,1435) | 1:199:A:VAL:HG21 | 1:200:A:PRO:HG2  | 10       | 0.18          |
| (2,1435) | 1:199:A:VAL:HG22 | 1:200:A:PRO:HG2  | 10       | 0.18          |
| (2,1435) | 1:199:A:VAL:HG23 | 1:200:A:PRO:HG2  | 10       | 0.18          |
| (2,1315) | 1:221:A:VAL:HG11 | 1:233:A:LEU:HD11 | 4        | 0.18          |
| (2,1315) | 1:221:A:VAL:HG11 | 1:233:A:LEU:HD12 | 4        | 0.18          |
| (2,1315) | 1:221:A:VAL:HG11 | 1:233:A:LEU:HD13 | 4        | 0.18          |
| (2,1315) | 1:221:A:VAL:HG12 | 1:233:A:LEU:HD11 | 4        | 0.18          |
| (2,1315) | 1:221:A:VAL:HG12 | 1:233:A:LEU:HD12 | 4        | 0.18          |
| (2,1315) | 1:221:A:VAL:HG12 | 1:233:A:LEU:HD13 | 4        | 0.18          |
| (2,1315) | 1:221:A:VAL:HG13 | 1:233:A:LEU:HD11 | 4        | 0.18          |
| (2,1315) | 1:221:A:VAL:HG13 | 1:233:A:LEU:HD12 | 4        | 0.18          |
| (2,1315) | 1:221:A:VAL:HG13 | 1:233:A:LEU:HD13 | 4        | 0.18          |
| (2,1311) | 1:233:A:LEU:HD11 | 1:235:A:LEU:HD11 | 3        | 0.18          |
| (2,1311) | 1:233:A:LEU:HD11 | 1:235:A:LEU:HD12 | 3        | 0.18          |
| (2,1311) | 1:233:A:LEU:HD11 | 1:235:A:LEU:HD13 | 3        | 0.18          |
| (2,1311) | 1:233:A:LEU:HD12 | 1:235:A:LEU:HD11 | 3        | 0.18          |
| (2,1311) | 1:233:A:LEU:HD12 | 1:235:A:LEU:HD12 | 3        | 0.18          |
| (2,1311) | 1:233:A:LEU:HD12 | 1:235:A:LEU:HD13 | 3        | 0.18          |
| (2,1311) | 1:233:A:LEU:HD13 | 1:235:A:LEU:HD11 | 3        | 0.18          |
| (2,1311) | 1:233:A:LEU:HD13 | 1:235:A:LEU:HD12 | 3        | 0.18          |
| (2,1311) | 1:233:A:LEU:HD13 | 1:235:A:LEU:HD13 | 3        | 0.18          |
| (2,1311) | 1:233:A:LEU:HD11 | 1:235:A:LEU:HD11 | 4        | 0.18          |
| (2,1311) | 1:233:A:LEU:HD11 | 1:235:A:LEU:HD12 | 4        | 0.18          |
| (2,1311) | 1:233:A:LEU:HD11 | 1:235:A:LEU:HD13 | 4        | 0.18          |
| (2,1311) | 1:233:A:LEU:HD12 | 1:235:A:LEU:HD11 | 4        | 0.18          |
| (2,1311) | 1:233:A:LEU:HD12 | 1:235:A:LEU:HD12 | 4        | 0.18          |
| (2,1311) | 1:233:A:LEU:HD12 | 1:235:A:LEU:HD13 | 4        | 0.18          |
| (2,1311) | 1:233:A:LEU:HD13 | 1:235:A:LEU:HD11 | 4        | 0.18          |
| (2,1311) | 1:233:A:LEU:HD13 | 1:235:A:LEU:HD12 | 4        | 0.18          |
| (2,1311) | 1:233:A:LEU:HD13 | 1:235:A:LEU:HD13 | 4        | 0.18          |
| (2,1284) | 1:195:A:ALA:H    | 1:250:A:TYR:HD1  | 16       | 0.18          |
| (2,1213) | 1:231:A:ARG:HD3  | 1:232:A:LYS:H    | 10       | 0.18          |
| (2,1006) | 1:230:A:GLY:H    | 1:255:A:ILE:HG13 | 16       | 0.18          |
| (2,868)  | 1:170:A:THR:HG21 | 1:172:A:LEU:H    | 18       | 0.18          |
| (2,868)  | 1:170:A:THR:HG22 | 1:172:A:LEU:H    | 18       | 0.18          |
| (2,868)  | 1:170:A:THR:HG23 | 1:172:A:LEU:H    | 18       | 0.18          |
| (2,778)  | 1:189:A:GLY:HA3  | 1:242:A:GLY:HA3  | 7        | 0.18          |
| (2,778)  | 1:189:A:GLY:HA3  | 1:242:A:GLY:HA3  | 15       | 0.18          |
| (2,739)  | 1:225:A:PRO:HB3  | 1:226:A:ARG:HG2  | 16       | 0.18          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (2,732) | 1:197:A:LEU:HD21 | 1:251:A:LEU:HD11 | 5        | 0.18          |
| (2,732) | 1:197:A:LEU:HD21 | 1:251:A:LEU:HD12 | 5        | 0.18          |
| (2,732) | 1:197:A:LEU:HD21 | 1:251:A:LEU:HD13 | 5        | 0.18          |
| (2,732) | 1:197:A:LEU:HD22 | 1:251:A:LEU:HD11 | 5        | 0.18          |
| (2,732) | 1:197:A:LEU:HD22 | 1:251:A:LEU:HD12 | 5        | 0.18          |
| (2,732) | 1:197:A:LEU:HD22 | 1:251:A:LEU:HD13 | 5        | 0.18          |
| (2,732) | 1:197:A:LEU:HD23 | 1:251:A:LEU:HD11 | 5        | 0.18          |
| (2,732) | 1:197:A:LEU:HD23 | 1:251:A:LEU:HD12 | 5        | 0.18          |
| (2,732) | 1:197:A:LEU:HD23 | 1:251:A:LEU:HD13 | 5        | 0.18          |
| (2,726) | 1:174:A:TYR:HB3  | 1:251:A:LEU:HD11 | 17       | 0.18          |
| (2,726) | 1:174:A:TYR:HB3  | 1:251:A:LEU:HD12 | 17       | 0.18          |
| (2,726) | 1:174:A:TYR:HB3  | 1:251:A:LEU:HD13 | 17       | 0.18          |
| (2,633) | 1:197:A:LEU:HB3  | 1:210:A:VAL:HG21 | 4        | 0.18          |
| (2,633) | 1:197:A:LEU:HB3  | 1:210:A:VAL:HG22 | 4        | 0.18          |
| (2,633) | 1:197:A:LEU:HB3  | 1:210:A:VAL:HG23 | 4        | 0.18          |
| (2,633) | 1:197:A:LEU:HB3  | 1:210:A:VAL:HG21 | 7        | 0.18          |
| (2,633) | 1:197:A:LEU:HB3  | 1:210:A:VAL:HG22 | 7        | 0.18          |
| (2,633) | 1:197:A:LEU:HB3  | 1:210:A:VAL:HG23 | 7        | 0.18          |
| (2,633) | 1:197:A:LEU:HB3  | 1:210:A:VAL:HG21 | 10       | 0.18          |
| (2,633) | 1:197:A:LEU:HB3  | 1:210:A:VAL:HG22 | 10       | 0.18          |
| (2,633) | 1:197:A:LEU:HB3  | 1:210:A:VAL:HG23 | 10       | 0.18          |
| (2,633) | 1:197:A:LEU:HB3  | 1:210:A:VAL:HG21 | 15       | 0.18          |
| (2,633) | 1:197:A:LEU:HB3  | 1:210:A:VAL:HG22 | 15       | 0.18          |
| (2,633) | 1:197:A:LEU:HB3  | 1:210:A:VAL:HG23 | 15       | 0.18          |
| (2,633) | 1:197:A:LEU:HB3  | 1:210:A:VAL:HG21 | 18       | 0.18          |
| (2,633) | 1:197:A:LEU:HB3  | 1:210:A:VAL:HG22 | 18       | 0.18          |
| (2,633) | 1:197:A:LEU:HB3  | 1:210:A:VAL:HG23 | 18       | 0.18          |
| (2,553) | 1:193:A:LEU:HB3  | 1:249:A:LEU:HD21 | 10       | 0.18          |
| (2,553) | 1:193:A:LEU:HB3  | 1:249:A:LEU:HD22 | 10       | 0.18          |
| (2,553) | 1:193:A:LEU:HB3  | 1:249:A:LEU:HD23 | 10       | 0.18          |
| (2,467) | 1:198:A:ASP:H    | 1:254:A:ARG:HB2  | 16       | 0.18          |
| (2,395) | 1:194:A:TYR:HD2  | 1:195:A:ALA:HB1  | 3        | 0.18          |
| (2,395) | 1:194:A:TYR:HD2  | 1:195:A:ALA:HB2  | 3        | 0.18          |
| (2,395) | 1:194:A:TYR:HD2  | 1:195:A:ALA:HB3  | 3        | 0.18          |
| (2,395) | 1:194:A:TYR:HD2  | 1:195:A:ALA:HB1  | 10       | 0.18          |
| (2,395) | 1:194:A:TYR:HD2  | 1:195:A:ALA:HB2  | 10       | 0.18          |
| (2,395) | 1:194:A:TYR:HD2  | 1:195:A:ALA:HB3  | 10       | 0.18          |
| (2,395) | 1:194:A:TYR:HD2  | 1:195:A:ALA:HB1  | 19       | 0.18          |
| (2,395) | 1:194:A:TYR:HD2  | 1:195:A:ALA:HB2  | 19       | 0.18          |
| (2,395) | 1:194:A:TYR:HD2  | 1:195:A:ALA:HB3  | 19       | 0.18          |
| (2,390) | 1:196:A:THR:HG21 | 1:252:A:GLU:HA   | 1        | 0.18          |
| (2,390) | 1:196:A:THR:HG22 | 1:252:A:GLU:HA   | 1        | 0.18          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,390)  | 1:196:A:THR:HG23 | 1:252:A:GLU:HA   | 1        | 0.18          |
| (2,329)  | 1:224:A:PRO:HG2  | 1:231:A:ARG:HD3  | 2        | 0.18          |
| (2,292)  | 1:191:A:GLN:HB3  | 1:243:A:PRO:HG3  | 17       | 0.18          |
| (2,247)  | 1:199:A:VAL:HA   | 1:203:A:ILE:HD11 | 1        | 0.18          |
| (2,247)  | 1:199:A:VAL:HA   | 1:203:A:ILE:HD12 | 1        | 0.18          |
| (2,247)  | 1:199:A:VAL:HA   | 1:203:A:ILE:HD13 | 1        | 0.18          |
| (2,247)  | 1:199:A:VAL:HA   | 1:203:A:ILE:HD11 | 3        | 0.18          |
| (2,247)  | 1:199:A:VAL:HA   | 1:203:A:ILE:HD12 | 3        | 0.18          |
| (2,247)  | 1:199:A:VAL:HA   | 1:203:A:ILE:HD13 | 3        | 0.18          |
| (2,247)  | 1:199:A:VAL:HA   | 1:203:A:ILE:HD11 | 12       | 0.18          |
| (2,247)  | 1:199:A:VAL:HA   | 1:203:A:ILE:HD12 | 12       | 0.18          |
| (2,247)  | 1:199:A:VAL:HA   | 1:203:A:ILE:HD13 | 12       | 0.18          |
| (2,202)  | 1:197:A:LEU:HA   | 1:210:A:VAL:HG11 | 11       | 0.18          |
| (2,202)  | 1:197:A:LEU:HA   | 1:210:A:VAL:HG12 | 11       | 0.18          |
| (2,202)  | 1:197:A:LEU:HA   | 1:210:A:VAL:HG13 | 11       | 0.18          |
| (2,202)  | 1:197:A:LEU:HA   | 1:210:A:VAL:HG11 | 19       | 0.18          |
| (2,202)  | 1:197:A:LEU:HA   | 1:210:A:VAL:HG12 | 19       | 0.18          |
| (2,202)  | 1:197:A:LEU:HA   | 1:210:A:VAL:HG13 | 19       | 0.18          |
| (2,91)   | 1:170:A:THR:HB   | 1:219:A:VAL:HG21 | 9        | 0.18          |
| (2,91)   | 1:170:A:THR:HB   | 1:219:A:VAL:HG22 | 9        | 0.18          |
| (2,91)   | 1:170:A:THR:HB   | 1:219:A:VAL:HG23 | 9        | 0.18          |
| (2,91)   | 1:170:A:THR:HB   | 1:219:A:VAL:HG21 | 17       | 0.18          |
| (2,91)   | 1:170:A:THR:HB   | 1:219:A:VAL:HG22 | 17       | 0.18          |
| (2,91)   | 1:170:A:THR:HB   | 1:219:A:VAL:HG23 | 17       | 0.18          |
| (1,21)   | 1:247:A:GLY:H    | 1:240:A:PHE:O    | 10       | 0.18          |
| (1,21)   | 1:247:A:GLY:H    | 1:240:A:PHE:O    | 14       | 0.18          |
| (1,21)   | 1:247:A:GLY:H    | 1:240:A:PHE:O    | 20       | 0.18          |
| (2,1663) | 1:241:A:PRO:HB2  | 1:245:A:GLY:H    | 4        | 0.17          |
| (2,1663) | 1:241:A:PRO:HB3  | 1:245:A:GLY:H    | 4        | 0.17          |
| (2,1653) | 1:236:A:LYS:HD2  | 1:246:A:ARG:HG2  | 2        | 0.17          |
| (2,1653) | 1:236:A:LYS:HD3  | 1:246:A:ARG:HG2  | 2        | 0.17          |
| (2,1651) | 1:236:A:LYS:HD2  | 1:237:A:GLY:H    | 10       | 0.17          |
| (2,1651) | 1:236:A:LYS:HD3  | 1:237:A:GLY:H    | 10       | 0.17          |
| (2,1651) | 1:236:A:LYS:HD2  | 1:237:A:GLY:H    | 14       | 0.17          |
| (2,1651) | 1:236:A:LYS:HD3  | 1:237:A:GLY:H    | 14       | 0.17          |
| (2,1542) | 1:211:A:ARG:HG2  | 1:219:A:VAL:H    | 8        | 0.17          |
| (2,1542) | 1:211:A:ARG:HG3  | 1:219:A:VAL:H    | 8        | 0.17          |
| (2,1536) | 1:211:A:ARG:HB2  | 1:220:A:GLU:HG2  | 2        | 0.17          |
| (2,1536) | 1:211:A:ARG:HB2  | 1:220:A:GLU:HG3  | 2        | 0.17          |
| (2,1536) | 1:211:A:ARG:HB3  | 1:220:A:GLU:HG2  | 2        | 0.17          |
| (2,1536) | 1:211:A:ARG:HB3  | 1:220:A:GLU:HG3  | 2        | 0.17          |
| (2,1525) | 1:209:A:LYS:HE2  | 1:222:A:ALA:HB1  | 2        | 0.17          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,1525) | 1:209:A:LYS:HE2  | 1:222:A:ALA:HB2  | 2        | 0.17          |
| (2,1525) | 1:209:A:LYS:HE2  | 1:222:A:ALA:HB3  | 2        | 0.17          |
| (2,1525) | 1:209:A:LYS:HE3  | 1:222:A:ALA:HB1  | 2        | 0.17          |
| (2,1525) | 1:209:A:LYS:HE3  | 1:222:A:ALA:HB2  | 2        | 0.17          |
| (2,1525) | 1:209:A:LYS:HE3  | 1:222:A:ALA:HB3  | 2        | 0.17          |
| (2,1525) | 1:209:A:LYS:HE2  | 1:222:A:ALA:HB1  | 16       | 0.17          |
| (2,1525) | 1:209:A:LYS:HE2  | 1:222:A:ALA:HB2  | 16       | 0.17          |
| (2,1525) | 1:209:A:LYS:HE2  | 1:222:A:ALA:HB3  | 16       | 0.17          |
| (2,1525) | 1:209:A:LYS:HE3  | 1:222:A:ALA:HB1  | 16       | 0.17          |
| (2,1525) | 1:209:A:LYS:HE3  | 1:222:A:ALA:HB2  | 16       | 0.17          |
| (2,1525) | 1:209:A:LYS:HE3  | 1:222:A:ALA:HB3  | 16       | 0.17          |
| (2,1524) | 1:209:A:LYS:HE2  | 1:222:A:ALA:HA   | 6        | 0.17          |
| (2,1524) | 1:209:A:LYS:HE3  | 1:222:A:ALA:HA   | 6        | 0.17          |
| (2,1470) | 1:202:A:PRO:HB3  | 1:205:A:VAL:HG11 | 9        | 0.17          |
| (2,1470) | 1:202:A:PRO:HB3  | 1:205:A:VAL:HG12 | 9        | 0.17          |
| (2,1470) | 1:202:A:PRO:HB3  | 1:205:A:VAL:HG13 | 9        | 0.17          |
| (2,1470) | 1:202:A:PRO:HB3  | 1:205:A:VAL:HG21 | 9        | 0.17          |
| (2,1470) | 1:202:A:PRO:HB3  | 1:205:A:VAL:HG22 | 9        | 0.17          |
| (2,1470) | 1:202:A:PRO:HB3  | 1:205:A:VAL:HG23 | 9        | 0.17          |
| (2,1417) | 1:196:A:THR:HB   | 1:252:A:GLU:HB2  | 20       | 0.17          |
| (2,1417) | 1:196:A:THR:HB   | 1:252:A:GLU:HB3  | 20       | 0.17          |
| (2,1315) | 1:221:A:VAL:HG11 | 1:233:A:LEU:HD11 | 16       | 0.17          |
| (2,1315) | 1:221:A:VAL:HG11 | 1:233:A:LEU:HD12 | 16       | 0.17          |
| (2,1315) | 1:221:A:VAL:HG11 | 1:233:A:LEU:HD13 | 16       | 0.17          |
| (2,1315) | 1:221:A:VAL:HG12 | 1:233:A:LEU:HD11 | 16       | 0.17          |
| (2,1315) | 1:221:A:VAL:HG12 | 1:233:A:LEU:HD12 | 16       | 0.17          |
| (2,1315) | 1:221:A:VAL:HG12 | 1:233:A:LEU:HD13 | 16       | 0.17          |
| (2,1315) | 1:221:A:VAL:HG13 | 1:233:A:LEU:HD11 | 16       | 0.17          |
| (2,1315) | 1:221:A:VAL:HG13 | 1:233:A:LEU:HD12 | 16       | 0.17          |
| (2,1315) | 1:221:A:VAL:HG13 | 1:233:A:LEU:HD13 | 16       | 0.17          |
| (2,1311) | 1:233:A:LEU:HD11 | 1:235:A:LEU:HD11 | 1        | 0.17          |
| (2,1311) | 1:233:A:LEU:HD11 | 1:235:A:LEU:HD12 | 1        | 0.17          |
| (2,1311) | 1:233:A:LEU:HD11 | 1:235:A:LEU:HD13 | 1        | 0.17          |
| (2,1311) | 1:233:A:LEU:HD12 | 1:235:A:LEU:HD11 | 1        | 0.17          |
| (2,1311) | 1:233:A:LEU:HD12 | 1:235:A:LEU:HD12 | 1        | 0.17          |
| (2,1311) | 1:233:A:LEU:HD12 | 1:235:A:LEU:HD13 | 1        | 0.17          |
| (2,1311) | 1:233:A:LEU:HD13 | 1:235:A:LEU:HD11 | 1        | 0.17          |
| (2,1311) | 1:233:A:LEU:HD13 | 1:235:A:LEU:HD12 | 1        | 0.17          |
| (2,1311) | 1:233:A:LEU:HD13 | 1:235:A:LEU:HD13 | 1        | 0.17          |
| (2,1311) | 1:233:A:LEU:HD11 | 1:235:A:LEU:HD11 | 20       | 0.17          |
| (2,1311) | 1:233:A:LEU:HD11 | 1:235:A:LEU:HD12 | 20       | 0.17          |
| (2,1311) | 1:233:A:LEU:HD11 | 1:235:A:LEU:HD13 | 20       | 0.17          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,1311) | 1:233:A:LEU:HD12 | 1:235:A:LEU:HD11 | 20       | 0.17          |
| (2,1311) | 1:233:A:LEU:HD12 | 1:235:A:LEU:HD12 | 20       | 0.17          |
| (2,1311) | 1:233:A:LEU:HD12 | 1:235:A:LEU:HD13 | 20       | 0.17          |
| (2,1311) | 1:233:A:LEU:HD13 | 1:235:A:LEU:HD11 | 20       | 0.17          |
| (2,1311) | 1:233:A:LEU:HD13 | 1:235:A:LEU:HD12 | 20       | 0.17          |
| (2,1311) | 1:233:A:LEU:HD13 | 1:235:A:LEU:HD13 | 20       | 0.17          |
| (2,1262) | 1:205:A:VAL:HG21 | 1:226:A:ARG:H    | 16       | 0.17          |
| (2,1262) | 1:205:A:VAL:HG22 | 1:226:A:ARG:H    | 16       | 0.17          |
| (2,1262) | 1:205:A:VAL:HG23 | 1:226:A:ARG:H    | 16       | 0.17          |
| (2,1213) | 1:231:A:ARG:HD3  | 1:232:A:LYS:H    | 5        | 0.17          |
| (2,1006) | 1:230:A:GLY:H    | 1:255:A:ILE:HG13 | 2        | 0.17          |
| (2,937)  | 1:250:A:TYR:HD2  | 1:251:A:LEU:H    | 3        | 0.17          |
| (2,937)  | 1:250:A:TYR:HD2  | 1:251:A:LEU:H    | 6        | 0.17          |
| (2,937)  | 1:250:A:TYR:HD2  | 1:251:A:LEU:H    | 10       | 0.17          |
| (2,828)  | 1:228:A:GLN:H    | 1:231:A:ARG:HB2  | 1        | 0.17          |
| (2,778)  | 1:189:A:GLY:HA3  | 1:242:A:GLY:HA3  | 2        | 0.17          |
| (2,778)  | 1:189:A:GLY:HA3  | 1:242:A:GLY:HA3  | 20       | 0.17          |
| (2,732)  | 1:197:A:LEU:HD21 | 1:251:A:LEU:HD11 | 10       | 0.17          |
| (2,732)  | 1:197:A:LEU:HD21 | 1:251:A:LEU:HD12 | 10       | 0.17          |
| (2,732)  | 1:197:A:LEU:HD21 | 1:251:A:LEU:HD13 | 10       | 0.17          |
| (2,732)  | 1:197:A:LEU:HD22 | 1:251:A:LEU:HD11 | 10       | 0.17          |
| (2,732)  | 1:197:A:LEU:HD22 | 1:251:A:LEU:HD12 | 10       | 0.17          |
| (2,732)  | 1:197:A:LEU:HD22 | 1:251:A:LEU:HD13 | 10       | 0.17          |
| (2,732)  | 1:197:A:LEU:HD23 | 1:251:A:LEU:HD11 | 10       | 0.17          |
| (2,732)  | 1:197:A:LEU:HD23 | 1:251:A:LEU:HD12 | 10       | 0.17          |
| (2,732)  | 1:197:A:LEU:HD23 | 1:251:A:LEU:HD13 | 10       | 0.17          |
| (2,726)  | 1:174:A:TYR:HB3  | 1:251:A:LEU:HD11 | 7        | 0.17          |
| (2,726)  | 1:174:A:TYR:HB3  | 1:251:A:LEU:HD12 | 7        | 0.17          |
| (2,726)  | 1:174:A:TYR:HB3  | 1:251:A:LEU:HD13 | 7        | 0.17          |
| (2,694)  | 1:197:A:LEU:HD21 | 1:221:A:VAL:HB   | 5        | 0.17          |
| (2,694)  | 1:197:A:LEU:HD22 | 1:221:A:VAL:HB   | 5        | 0.17          |
| (2,694)  | 1:197:A:LEU:HD23 | 1:221:A:VAL:HB   | 5        | 0.17          |
| (2,633)  | 1:197:A:LEU:HB3  | 1:210:A:VAL:HG21 | 6        | 0.17          |
| (2,633)  | 1:197:A:LEU:HB3  | 1:210:A:VAL:HG22 | 6        | 0.17          |
| (2,633)  | 1:197:A:LEU:HB3  | 1:210:A:VAL:HG23 | 6        | 0.17          |
| (2,395)  | 1:194:A:TYR:HD2  | 1:195:A:ALA:HB1  | 17       | 0.17          |
| (2,395)  | 1:194:A:TYR:HD2  | 1:195:A:ALA:HB2  | 17       | 0.17          |
| (2,395)  | 1:194:A:TYR:HD2  | 1:195:A:ALA:HB3  | 17       | 0.17          |
| (2,390)  | 1:196:A:THR:HG21 | 1:252:A:GLU:HA   | 5        | 0.17          |
| (2,390)  | 1:196:A:THR:HG22 | 1:252:A:GLU:HA   | 5        | 0.17          |
| (2,390)  | 1:196:A:THR:HG23 | 1:252:A:GLU:HA   | 5        | 0.17          |
| (2,390)  | 1:196:A:THR:HG21 | 1:252:A:GLU:HA   | 16       | 0.17          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,390)  | 1:196:A:THR:HG22 | 1:252:A:GLU:HA   | 16       | 0.17          |
| (2,390)  | 1:196:A:THR:HG23 | 1:252:A:GLU:HA   | 16       | 0.17          |
| (2,247)  | 1:199:A:VAL:HA   | 1:203:A:ILE:HD11 | 15       | 0.17          |
| (2,247)  | 1:199:A:VAL:HA   | 1:203:A:ILE:HD12 | 15       | 0.17          |
| (2,247)  | 1:199:A:VAL:HA   | 1:203:A:ILE:HD13 | 15       | 0.17          |
| (2,202)  | 1:197:A:LEU:HA   | 1:210:A:VAL:HG11 | 17       | 0.17          |
| (2,202)  | 1:197:A:LEU:HA   | 1:210:A:VAL:HG12 | 17       | 0.17          |
| (2,202)  | 1:197:A:LEU:HA   | 1:210:A:VAL:HG13 | 17       | 0.17          |
| (2,91)   | 1:170:A:THR:HB   | 1:219:A:VAL:HG21 | 3        | 0.17          |
| (2,91)   | 1:170:A:THR:HB   | 1:219:A:VAL:HG22 | 3        | 0.17          |
| (2,91)   | 1:170:A:THR:HB   | 1:219:A:VAL:HG23 | 3        | 0.17          |
| (2,91)   | 1:170:A:THR:HB   | 1:219:A:VAL:HG21 | 7        | 0.17          |
| (2,91)   | 1:170:A:THR:HB   | 1:219:A:VAL:HG22 | 7        | 0.17          |
| (2,91)   | 1:170:A:THR:HB   | 1:219:A:VAL:HG23 | 7        | 0.17          |
| (1,21)   | 1:247:A:GLY:H    | 1:240:A:PHE:O    | 7        | 0.17          |
| (1,21)   | 1:247:A:GLY:H    | 1:240:A:PHE:O    | 8        | 0.17          |
| (2,1694) | 1:174:A:TYR:HD2  | 1:197:A:LEU:HD11 | 2        | 0.16          |
| (2,1694) | 1:174:A:TYR:HD2  | 1:197:A:LEU:HD12 | 2        | 0.16          |
| (2,1694) | 1:174:A:TYR:HD2  | 1:197:A:LEU:HD13 | 2        | 0.16          |
| (2,1694) | 1:174:A:TYR:HD2  | 1:197:A:LEU:HD21 | 2        | 0.16          |
| (2,1694) | 1:174:A:TYR:HD2  | 1:197:A:LEU:HD22 | 2        | 0.16          |
| (2,1694) | 1:174:A:TYR:HD2  | 1:197:A:LEU:HD23 | 2        | 0.16          |
| (2,1653) | 1:236:A:LYS:HD2  | 1:246:A:ARG:HG2  | 6        | 0.16          |
| (2,1653) | 1:236:A:LYS:HD3  | 1:246:A:ARG:HG2  | 6        | 0.16          |
| (2,1653) | 1:236:A:LYS:HD2  | 1:246:A:ARG:HG2  | 9        | 0.16          |
| (2,1653) | 1:236:A:LYS:HD3  | 1:246:A:ARG:HG2  | 9        | 0.16          |
| (2,1653) | 1:236:A:LYS:HD2  | 1:246:A:ARG:HG2  | 18       | 0.16          |
| (2,1653) | 1:236:A:LYS:HD3  | 1:246:A:ARG:HG2  | 18       | 0.16          |
| (2,1651) | 1:236:A:LYS:HD2  | 1:237:A:GLY:H    | 15       | 0.16          |
| (2,1651) | 1:236:A:LYS:HD3  | 1:237:A:GLY:H    | 15       | 0.16          |
| (2,1633) | 1:232:A:LYS:HG2  | 1:253:A:VAL:H    | 5        | 0.16          |
| (2,1633) | 1:232:A:LYS:HG3  | 1:253:A:VAL:H    | 5        | 0.16          |
| (2,1525) | 1:209:A:LYS:HE2  | 1:222:A:ALA:HB1  | 5        | 0.16          |
| (2,1525) | 1:209:A:LYS:HE2  | 1:222:A:ALA:HB2  | 5        | 0.16          |
| (2,1525) | 1:209:A:LYS:HE2  | 1:222:A:ALA:HB3  | 5        | 0.16          |
| (2,1525) | 1:209:A:LYS:HE3  | 1:222:A:ALA:HB1  | 5        | 0.16          |
| (2,1525) | 1:209:A:LYS:HE3  | 1:222:A:ALA:HB2  | 5        | 0.16          |
| (2,1525) | 1:209:A:LYS:HE3  | 1:222:A:ALA:HB3  | 5        | 0.16          |
| (2,1470) | 1:202:A:PRO:HB3  | 1:205:A:VAL:HG11 | 4        | 0.16          |
| (2,1470) | 1:202:A:PRO:HB3  | 1:205:A:VAL:HG12 | 4        | 0.16          |
| (2,1470) | 1:202:A:PRO:HB3  | 1:205:A:VAL:HG13 | 4        | 0.16          |
| (2,1470) | 1:202:A:PRO:HB3  | 1:205:A:VAL:HG21 | 4        | 0.16          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,1470) | 1:202:A:PRO:HB3  | 1:205:A:VAL:HG22 | 4        | 0.16          |
| (2,1470) | 1:202:A:PRO:HB3  | 1:205:A:VAL:HG23 | 4        | 0.16          |
| (2,1435) | 1:199:A:VAL:HG11 | 1:200:A:PRO:HG2  | 6        | 0.16          |
| (2,1435) | 1:199:A:VAL:HG12 | 1:200:A:PRO:HG2  | 6        | 0.16          |
| (2,1435) | 1:199:A:VAL:HG13 | 1:200:A:PRO:HG2  | 6        | 0.16          |
| (2,1435) | 1:199:A:VAL:HG21 | 1:200:A:PRO:HG2  | 6        | 0.16          |
| (2,1435) | 1:199:A:VAL:HG22 | 1:200:A:PRO:HG2  | 6        | 0.16          |
| (2,1435) | 1:199:A:VAL:HG23 | 1:200:A:PRO:HG2  | 6        | 0.16          |
| (2,1315) | 1:221:A:VAL:HG11 | 1:233:A:LEU:HD11 | 12       | 0.16          |
| (2,1315) | 1:221:A:VAL:HG11 | 1:233:A:LEU:HD12 | 12       | 0.16          |
| (2,1315) | 1:221:A:VAL:HG11 | 1:233:A:LEU:HD13 | 12       | 0.16          |
| (2,1315) | 1:221:A:VAL:HG12 | 1:233:A:LEU:HD11 | 12       | 0.16          |
| (2,1315) | 1:221:A:VAL:HG12 | 1:233:A:LEU:HD12 | 12       | 0.16          |
| (2,1315) | 1:221:A:VAL:HG12 | 1:233:A:LEU:HD13 | 12       | 0.16          |
| (2,1315) | 1:221:A:VAL:HG13 | 1:233:A:LEU:HD11 | 12       | 0.16          |
| (2,1315) | 1:221:A:VAL:HG13 | 1:233:A:LEU:HD12 | 12       | 0.16          |
| (2,1315) | 1:221:A:VAL:HG13 | 1:233:A:LEU:HD13 | 12       | 0.16          |
| (2,1311) | 1:233:A:LEU:HD11 | 1:235:A:LEU:HD11 | 7        | 0.16          |
| (2,1311) | 1:233:A:LEU:HD11 | 1:235:A:LEU:HD12 | 7        | 0.16          |
| (2,1311) | 1:233:A:LEU:HD11 | 1:235:A:LEU:HD13 | 7        | 0.16          |
| (2,1311) | 1:233:A:LEU:HD12 | 1:235:A:LEU:HD11 | 7        | 0.16          |
| (2,1311) | 1:233:A:LEU:HD12 | 1:235:A:LEU:HD12 | 7        | 0.16          |
| (2,1311) | 1:233:A:LEU:HD12 | 1:235:A:LEU:HD13 | 7        | 0.16          |
| (2,1311) | 1:233:A:LEU:HD13 | 1:235:A:LEU:HD11 | 7        | 0.16          |
| (2,1311) | 1:233:A:LEU:HD13 | 1:235:A:LEU:HD12 | 7        | 0.16          |
| (2,1311) | 1:233:A:LEU:HD13 | 1:235:A:LEU:HD13 | 7        | 0.16          |
| (2,1311) | 1:233:A:LEU:HD11 | 1:235:A:LEU:HD11 | 11       | 0.16          |
| (2,1311) | 1:233:A:LEU:HD11 | 1:235:A:LEU:HD12 | 11       | 0.16          |
| (2,1311) | 1:233:A:LEU:HD11 | 1:235:A:LEU:HD13 | 11       | 0.16          |
| (2,1311) | 1:233:A:LEU:HD12 | 1:235:A:LEU:HD11 | 11       | 0.16          |
| (2,1311) | 1:233:A:LEU:HD12 | 1:235:A:LEU:HD12 | 11       | 0.16          |
| (2,1311) | 1:233:A:LEU:HD12 | 1:235:A:LEU:HD13 | 11       | 0.16          |
| (2,1311) | 1:233:A:LEU:HD13 | 1:235:A:LEU:HD11 | 11       | 0.16          |
| (2,1311) | 1:233:A:LEU:HD13 | 1:235:A:LEU:HD12 | 11       | 0.16          |
| (2,1311) | 1:233:A:LEU:HD13 | 1:235:A:LEU:HD13 | 11       | 0.16          |
| (2,1311) | 1:233:A:LEU:HD11 | 1:235:A:LEU:HD11 | 12       | 0.16          |
| (2,1311) | 1:233:A:LEU:HD11 | 1:235:A:LEU:HD12 | 12       | 0.16          |
| (2,1311) | 1:233:A:LEU:HD11 | 1:235:A:LEU:HD13 | 12       | 0.16          |
| (2,1311) | 1:233:A:LEU:HD12 | 1:235:A:LEU:HD11 | 12       | 0.16          |
| (2,1311) | 1:233:A:LEU:HD12 | 1:235:A:LEU:HD12 | 12       | 0.16          |
| (2,1311) | 1:233:A:LEU:HD12 | 1:235:A:LEU:HD13 | 12       | 0.16          |
| (2,1311) | 1:233:A:LEU:HD13 | 1:235:A:LEU:HD11 | 12       | 0.16          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,1311) | 1:233:A:LEU:HD13 | 1:235:A:LEU:HD12 | 12       | 0.16          |
| (2,1311) | 1:233:A:LEU:HD13 | 1:235:A:LEU:HD13 | 12       | 0.16          |
| (2,1311) | 1:233:A:LEU:HD11 | 1:235:A:LEU:HD11 | 16       | 0.16          |
| (2,1311) | 1:233:A:LEU:HD11 | 1:235:A:LEU:HD12 | 16       | 0.16          |
| (2,1311) | 1:233:A:LEU:HD11 | 1:235:A:LEU:HD13 | 16       | 0.16          |
| (2,1311) | 1:233:A:LEU:HD12 | 1:235:A:LEU:HD11 | 16       | 0.16          |
| (2,1311) | 1:233:A:LEU:HD12 | 1:235:A:LEU:HD12 | 16       | 0.16          |
| (2,1311) | 1:233:A:LEU:HD12 | 1:235:A:LEU:HD13 | 16       | 0.16          |
| (2,1311) | 1:233:A:LEU:HD13 | 1:235:A:LEU:HD11 | 16       | 0.16          |
| (2,1311) | 1:233:A:LEU:HD13 | 1:235:A:LEU:HD12 | 16       | 0.16          |
| (2,1311) | 1:233:A:LEU:HD13 | 1:235:A:LEU:HD13 | 16       | 0.16          |
| (2,1311) | 1:233:A:LEU:HD11 | 1:235:A:LEU:HD11 | 19       | 0.16          |
| (2,1311) | 1:233:A:LEU:HD11 | 1:235:A:LEU:HD12 | 19       | 0.16          |
| (2,1311) | 1:233:A:LEU:HD11 | 1:235:A:LEU:HD13 | 19       | 0.16          |
| (2,1311) | 1:233:A:LEU:HD12 | 1:235:A:LEU:HD11 | 19       | 0.16          |
| (2,1311) | 1:233:A:LEU:HD12 | 1:235:A:LEU:HD12 | 19       | 0.16          |
| (2,1311) | 1:233:A:LEU:HD12 | 1:235:A:LEU:HD13 | 19       | 0.16          |
| (2,1311) | 1:233:A:LEU:HD13 | 1:235:A:LEU:HD11 | 19       | 0.16          |
| (2,1311) | 1:233:A:LEU:HD13 | 1:235:A:LEU:HD12 | 19       | 0.16          |
| (2,1311) | 1:233:A:LEU:HD13 | 1:235:A:LEU:HD13 | 19       | 0.16          |
| (2,1213) | 1:231:A:ARG:HD3  | 1:232:A:LYS:H    | 8        | 0.16          |
| (2,1213) | 1:231:A:ARG:HD3  | 1:232:A:LYS:H    | 19       | 0.16          |
| (2,937)  | 1:250:A:TYR:HD2  | 1:251:A:LEU:H    | 7        | 0.16          |
| (2,633)  | 1:197:A:LEU:HB3  | 1:210:A:VAL:HG21 | 9        | 0.16          |
| (2,633)  | 1:197:A:LEU:HB3  | 1:210:A:VAL:HG22 | 9        | 0.16          |
| (2,633)  | 1:197:A:LEU:HB3  | 1:210:A:VAL:HG23 | 9        | 0.16          |
| (2,433)  | 1:241:A:PRO:HA   | 1:246:A:ARG:HA   | 14       | 0.16          |
| (2,395)  | 1:194:A:TYR:HD2  | 1:195:A:ALA:HB1  | 15       | 0.16          |
| (2,395)  | 1:194:A:TYR:HD2  | 1:195:A:ALA:HB2  | 15       | 0.16          |
| (2,395)  | 1:194:A:TYR:HD2  | 1:195:A:ALA:HB3  | 15       | 0.16          |
| (2,390)  | 1:196:A:THR:HG21 | 1:252:A:GLU:HA   | 8        | 0.16          |
| (2,390)  | 1:196:A:THR:HG22 | 1:252:A:GLU:HA   | 8        | 0.16          |
| (2,390)  | 1:196:A:THR:HG23 | 1:252:A:GLU:HA   | 8        | 0.16          |
| (2,292)  | 1:191:A:GLN:HB3  | 1:243:A:PRO:HG3  | 9        | 0.16          |
| (2,247)  | 1:199:A:VAL:HA   | 1:203:A:ILE:HD11 | 4        | 0.16          |
| (2,247)  | 1:199:A:VAL:HA   | 1:203:A:ILE:HD12 | 4        | 0.16          |
| (2,247)  | 1:199:A:VAL:HA   | 1:203:A:ILE:HD13 | 4        | 0.16          |
| (2,247)  | 1:199:A:VAL:HA   | 1:203:A:ILE:HD11 | 16       | 0.16          |
| (2,247)  | 1:199:A:VAL:HA   | 1:203:A:ILE:HD12 | 16       | 0.16          |
| (2,247)  | 1:199:A:VAL:HA   | 1:203:A:ILE:HD13 | 16       | 0.16          |
| (2,151)  | 1:193:A:LEU:HD21 | 1:194:A:TYR:HB2  | 16       | 0.16          |
| (2,151)  | 1:193:A:LEU:HD22 | 1:194:A:TYR:HB2  | 16       | 0.16          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,151)  | 1:193:A:LEU:HD23 | 1:194:A:TYR:HB2  | 16       | 0.16          |
| (2,108)  | 1:210:A:VAL:HB   | 1:212:A:ALA:HB1  | 8        | 0.16          |
| (2,108)  | 1:210:A:VAL:HB   | 1:212:A:ALA:HB2  | 8        | 0.16          |
| (2,108)  | 1:210:A:VAL:HB   | 1:212:A:ALA:HB3  | 8        | 0.16          |
| (2,91)   | 1:170:A:THR:HB   | 1:219:A:VAL:HG21 | 10       | 0.16          |
| (2,91)   | 1:170:A:THR:HB   | 1:219:A:VAL:HG22 | 10       | 0.16          |
| (2,91)   | 1:170:A:THR:HB   | 1:219:A:VAL:HG23 | 10       | 0.16          |
| (1,21)   | 1:247:A:GLY:H    | 1:240:A:PHE:O    | 16       | 0.16          |
| (1,21)   | 1:247:A:GLY:H    | 1:240:A:PHE:O    | 19       | 0.16          |
| (2,1681) | 1:173:A:PHE:HD2  | 1:235:A:LEU:HD11 | 3        | 0.15          |
| (2,1681) | 1:173:A:PHE:HD2  | 1:235:A:LEU:HD12 | 3        | 0.15          |
| (2,1681) | 1:173:A:PHE:HD2  | 1:235:A:LEU:HD13 | 3        | 0.15          |
| (2,1681) | 1:173:A:PHE:HD2  | 1:235:A:LEU:HD11 | 7        | 0.15          |
| (2,1681) | 1:173:A:PHE:HD2  | 1:235:A:LEU:HD12 | 7        | 0.15          |
| (2,1681) | 1:173:A:PHE:HD2  | 1:235:A:LEU:HD13 | 7        | 0.15          |
| (2,1681) | 1:173:A:PHE:HD2  | 1:235:A:LEU:HD11 | 20       | 0.15          |
| (2,1681) | 1:173:A:PHE:HD2  | 1:235:A:LEU:HD12 | 20       | 0.15          |
| (2,1681) | 1:173:A:PHE:HD2  | 1:235:A:LEU:HD13 | 20       | 0.15          |
| (2,1651) | 1:236:A:LYS:HD2  | 1:237:A:GLY:H    | 5        | 0.15          |
| (2,1651) | 1:236:A:LYS:HD3  | 1:237:A:GLY:H    | 5        | 0.15          |
| (2,1639) | 1:232:A:LYS:HE2  | 1:252:A:GLU:HA   | 19       | 0.15          |
| (2,1639) | 1:232:A:LYS:HE3  | 1:252:A:GLU:HA   | 19       | 0.15          |
| (2,1578) | 1:219:A:VAL:HG21 | 1:238:A:LYS:HD2  | 6        | 0.15          |
| (2,1578) | 1:219:A:VAL:HG21 | 1:238:A:LYS:HD3  | 6        | 0.15          |
| (2,1578) | 1:219:A:VAL:HG22 | 1:238:A:LYS:HD2  | 6        | 0.15          |
| (2,1578) | 1:219:A:VAL:HG22 | 1:238:A:LYS:HD3  | 6        | 0.15          |
| (2,1578) | 1:219:A:VAL:HG23 | 1:238:A:LYS:HD2  | 6        | 0.15          |
| (2,1578) | 1:219:A:VAL:HG23 | 1:238:A:LYS:HD3  | 6        | 0.15          |
| (2,1435) | 1:199:A:VAL:HG11 | 1:200:A:PRO:HG2  | 1        | 0.15          |
| (2,1435) | 1:199:A:VAL:HG12 | 1:200:A:PRO:HG2  | 1        | 0.15          |
| (2,1435) | 1:199:A:VAL:HG13 | 1:200:A:PRO:HG2  | 1        | 0.15          |
| (2,1435) | 1:199:A:VAL:HG21 | 1:200:A:PRO:HG2  | 1        | 0.15          |
| (2,1435) | 1:199:A:VAL:HG22 | 1:200:A:PRO:HG2  | 1        | 0.15          |
| (2,1435) | 1:199:A:VAL:HG23 | 1:200:A:PRO:HG2  | 1        | 0.15          |
| (2,1435) | 1:199:A:VAL:HG11 | 1:200:A:PRO:HG2  | 12       | 0.15          |
| (2,1435) | 1:199:A:VAL:HG12 | 1:200:A:PRO:HG2  | 12       | 0.15          |
| (2,1435) | 1:199:A:VAL:HG13 | 1:200:A:PRO:HG2  | 12       | 0.15          |
| (2,1435) | 1:199:A:VAL:HG21 | 1:200:A:PRO:HG2  | 12       | 0.15          |
| (2,1435) | 1:199:A:VAL:HG22 | 1:200:A:PRO:HG2  | 12       | 0.15          |
| (2,1435) | 1:199:A:VAL:HG23 | 1:200:A:PRO:HG2  | 12       | 0.15          |
| (2,1435) | 1:199:A:VAL:HG11 | 1:200:A:PRO:HG2  | 13       | 0.15          |
| (2,1435) | 1:199:A:VAL:HG12 | 1:200:A:PRO:HG2  | 13       | 0.15          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,1435) | 1:199:A:VAL:HG13 | 1:200:A:PRO:HG2  | 13       | 0.15          |
| (2,1435) | 1:199:A:VAL:HG21 | 1:200:A:PRO:HG2  | 13       | 0.15          |
| (2,1435) | 1:199:A:VAL:HG22 | 1:200:A:PRO:HG2  | 13       | 0.15          |
| (2,1435) | 1:199:A:VAL:HG23 | 1:200:A:PRO:HG2  | 13       | 0.15          |
| (2,1315) | 1:221:A:VAL:HG11 | 1:233:A:LEU:HD11 | 14       | 0.15          |
| (2,1315) | 1:221:A:VAL:HG11 | 1:233:A:LEU:HD12 | 14       | 0.15          |
| (2,1315) | 1:221:A:VAL:HG11 | 1:233:A:LEU:HD13 | 14       | 0.15          |
| (2,1315) | 1:221:A:VAL:HG12 | 1:233:A:LEU:HD11 | 14       | 0.15          |
| (2,1315) | 1:221:A:VAL:HG12 | 1:233:A:LEU:HD12 | 14       | 0.15          |
| (2,1315) | 1:221:A:VAL:HG12 | 1:233:A:LEU:HD13 | 14       | 0.15          |
| (2,1315) | 1:221:A:VAL:HG13 | 1:233:A:LEU:HD11 | 14       | 0.15          |
| (2,1315) | 1:221:A:VAL:HG13 | 1:233:A:LEU:HD12 | 14       | 0.15          |
| (2,1315) | 1:221:A:VAL:HG13 | 1:233:A:LEU:HD13 | 14       | 0.15          |
| (2,997)  | 1:242:A:GLY:H    | 1:243:A:PRO:HD3  | 11       | 0.15          |
| (2,778)  | 1:189:A:GLY:HA3  | 1:242:A:GLY:HA3  | 8        | 0.15          |
| (2,687)  | 1:197:A:LEU:HD21 | 1:212:A:ALA:H    | 19       | 0.15          |
| (2,687)  | 1:197:A:LEU:HD22 | 1:212:A:ALA:H    | 19       | 0.15          |
| (2,687)  | 1:197:A:LEU:HD23 | 1:212:A:ALA:H    | 19       | 0.15          |
| (2,633)  | 1:197:A:LEU:HB3  | 1:210:A:VAL:HG21 | 20       | 0.15          |
| (2,633)  | 1:197:A:LEU:HB3  | 1:210:A:VAL:HG22 | 20       | 0.15          |
| (2,633)  | 1:197:A:LEU:HB3  | 1:210:A:VAL:HG23 | 20       | 0.15          |
| (2,396)  | 1:225:A:PRO:HG2  | 1:226:A:ARG:HG3  | 3        | 0.15          |
| (2,395)  | 1:194:A:TYR:HD2  | 1:195:A:ALA:HB1  | 9        | 0.15          |
| (2,395)  | 1:194:A:TYR:HD2  | 1:195:A:ALA:HB2  | 9        | 0.15          |
| (2,395)  | 1:194:A:TYR:HD2  | 1:195:A:ALA:HB3  | 9        | 0.15          |
| (2,395)  | 1:194:A:TYR:HD2  | 1:195:A:ALA:HB1  | 14       | 0.15          |
| (2,395)  | 1:194:A:TYR:HD2  | 1:195:A:ALA:HB2  | 14       | 0.15          |
| (2,395)  | 1:194:A:TYR:HD2  | 1:195:A:ALA:HB3  | 14       | 0.15          |
| (2,332)  | 1:231:A:ARG:HD3  | 1:253:A:VAL:HG11 | 2        | 0.15          |
| (2,332)  | 1:231:A:ARG:HD3  | 1:253:A:VAL:HG12 | 2        | 0.15          |
| (2,332)  | 1:231:A:ARG:HD3  | 1:253:A:VAL:HG13 | 2        | 0.15          |
| (2,247)  | 1:199:A:VAL:HA   | 1:203:A:ILE:HD11 | 2        | 0.15          |
| (2,247)  | 1:199:A:VAL:HA   | 1:203:A:ILE:HD12 | 2        | 0.15          |
| (2,247)  | 1:199:A:VAL:HA   | 1:203:A:ILE:HD13 | 2        | 0.15          |
| (2,247)  | 1:199:A:VAL:HA   | 1:203:A:ILE:HD11 | 5        | 0.15          |
| (2,247)  | 1:199:A:VAL:HA   | 1:203:A:ILE:HD12 | 5        | 0.15          |
| (2,247)  | 1:199:A:VAL:HA   | 1:203:A:ILE:HD13 | 5        | 0.15          |
| (2,247)  | 1:199:A:VAL:HA   | 1:203:A:ILE:HD11 | 8        | 0.15          |
| (2,247)  | 1:199:A:VAL:HA   | 1:203:A:ILE:HD12 | 8        | 0.15          |
| (2,247)  | 1:199:A:VAL:HA   | 1:203:A:ILE:HD13 | 8        | 0.15          |
| (2,202)  | 1:197:A:LEU:HA   | 1:210:A:VAL:HG11 | 4        | 0.15          |
| (2,202)  | 1:197:A:LEU:HA   | 1:210:A:VAL:HG12 | 4        | 0.15          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,202)  | 1:197:A:LEU:HA   | 1:210:A:VAL:HG13 | 4        | 0.15          |
| (2,202)  | 1:197:A:LEU:HA   | 1:210:A:VAL:HG11 | 5        | 0.15          |
| (2,202)  | 1:197:A:LEU:HA   | 1:210:A:VAL:HG12 | 5        | 0.15          |
| (2,202)  | 1:197:A:LEU:HA   | 1:210:A:VAL:HG13 | 5        | 0.15          |
| (2,202)  | 1:197:A:LEU:HA   | 1:210:A:VAL:HG11 | 7        | 0.15          |
| (2,202)  | 1:197:A:LEU:HA   | 1:210:A:VAL:HG12 | 7        | 0.15          |
| (2,202)  | 1:197:A:LEU:HA   | 1:210:A:VAL:HG13 | 7        | 0.15          |
| (2,151)  | 1:193:A:LEU:HD21 | 1:194:A:TYR:HB2  | 3        | 0.15          |
| (2,151)  | 1:193:A:LEU:HD22 | 1:194:A:TYR:HB2  | 3        | 0.15          |
| (2,151)  | 1:193:A:LEU:HD23 | 1:194:A:TYR:HB2  | 3        | 0.15          |
| (2,91)   | 1:170:A:THR:HB   | 1:219:A:VAL:HG21 | 6        | 0.15          |
| (2,91)   | 1:170:A:THR:HB   | 1:219:A:VAL:HG22 | 6        | 0.15          |
| (2,91)   | 1:170:A:THR:HB   | 1:219:A:VAL:HG23 | 6        | 0.15          |
| (2,91)   | 1:170:A:THR:HB   | 1:219:A:VAL:HG21 | 13       | 0.15          |
| (2,91)   | 1:170:A:THR:HB   | 1:219:A:VAL:HG22 | 13       | 0.15          |
| (2,91)   | 1:170:A:THR:HB   | 1:219:A:VAL:HG23 | 13       | 0.15          |
| (2,34)   | 1:194:A:TYR:HD2  | 1:249:A:LEU:HD11 | 2        | 0.15          |
| (2,34)   | 1:194:A:TYR:HD2  | 1:249:A:LEU:HD12 | 2        | 0.15          |
| (2,34)   | 1:194:A:TYR:HD2  | 1:249:A:LEU:HD13 | 2        | 0.15          |
| (2,1681) | 1:173:A:PHE:HD2  | 1:235:A:LEU:HD11 | 11       | 0.14          |
| (2,1681) | 1:173:A:PHE:HD2  | 1:235:A:LEU:HD12 | 11       | 0.14          |
| (2,1681) | 1:173:A:PHE:HD2  | 1:235:A:LEU:HD13 | 11       | 0.14          |
| (2,1677) | 1:179:A:ALA:HA   | 1:231:A:ARG:HA   | 6        | 0.14          |
| (2,1663) | 1:241:A:PRO:HB2  | 1:245:A:GLY:H    | 20       | 0.14          |
| (2,1663) | 1:241:A:PRO:HB3  | 1:245:A:GLY:H    | 20       | 0.14          |
| (2,1657) | 1:238:A:LYS:H    | 1:238:A:LYS:HE2  | 6        | 0.14          |
| (2,1657) | 1:238:A:LYS:H    | 1:238:A:LYS:HE3  | 6        | 0.14          |
| (2,1654) | 1:236:A:LYS:HE2  | 1:237:A:GLY:H    | 12       | 0.14          |
| (2,1654) | 1:236:A:LYS:HE3  | 1:237:A:GLY:H    | 12       | 0.14          |
| (2,1651) | 1:236:A:LYS:HD2  | 1:237:A:GLY:H    | 2        | 0.14          |
| (2,1651) | 1:236:A:LYS:HD3  | 1:237:A:GLY:H    | 2        | 0.14          |
| (2,1638) | 1:232:A:LYS:HE2  | 1:233:A:LEU:H    | 15       | 0.14          |
| (2,1638) | 1:232:A:LYS:HE3  | 1:233:A:LEU:H    | 15       | 0.14          |
| (2,1633) | 1:232:A:LYS:HG2  | 1:253:A:VAL:H    | 11       | 0.14          |
| (2,1633) | 1:232:A:LYS:HG3  | 1:253:A:VAL:H    | 11       | 0.14          |
| (2,1633) | 1:232:A:LYS:HG2  | 1:253:A:VAL:H    | 20       | 0.14          |
| (2,1633) | 1:232:A:LYS:HG3  | 1:253:A:VAL:H    | 20       | 0.14          |
| (2,1625) | 1:232:A:LYS:HB2  | 1:232:A:LYS:HE2  | 7        | 0.14          |
| (2,1625) | 1:232:A:LYS:HB2  | 1:232:A:LYS:HE3  | 7        | 0.14          |
| (2,1578) | 1:219:A:VAL:HG21 | 1:238:A:LYS:HD2  | 18       | 0.14          |
| (2,1578) | 1:219:A:VAL:HG21 | 1:238:A:LYS:HD3  | 18       | 0.14          |
| (2,1578) | 1:219:A:VAL:HG22 | 1:238:A:LYS:HD2  | 18       | 0.14          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,1578) | 1:219:A:VAL:HG22 | 1:238:A:LYS:HD3  | 18       | 0.14          |
| (2,1578) | 1:219:A:VAL:HG23 | 1:238:A:LYS:HD2  | 18       | 0.14          |
| (2,1578) | 1:219:A:VAL:HG23 | 1:238:A:LYS:HD3  | 18       | 0.14          |
| (2,1525) | 1:209:A:LYS:HE2  | 1:222:A:ALA:HB1  | 12       | 0.14          |
| (2,1525) | 1:209:A:LYS:HE2  | 1:222:A:ALA:HB2  | 12       | 0.14          |
| (2,1525) | 1:209:A:LYS:HE2  | 1:222:A:ALA:HB3  | 12       | 0.14          |
| (2,1525) | 1:209:A:LYS:HE3  | 1:222:A:ALA:HB1  | 12       | 0.14          |
| (2,1525) | 1:209:A:LYS:HE3  | 1:222:A:ALA:HB2  | 12       | 0.14          |
| (2,1525) | 1:209:A:LYS:HE3  | 1:222:A:ALA:HB3  | 12       | 0.14          |
| (2,1470) | 1:202:A:PRO:HB3  | 1:205:A:VAL:HG11 | 8        | 0.14          |
| (2,1470) | 1:202:A:PRO:HB3  | 1:205:A:VAL:HG12 | 8        | 0.14          |
| (2,1470) | 1:202:A:PRO:HB3  | 1:205:A:VAL:HG13 | 8        | 0.14          |
| (2,1470) | 1:202:A:PRO:HB3  | 1:205:A:VAL:HG21 | 8        | 0.14          |
| (2,1470) | 1:202:A:PRO:HB3  | 1:205:A:VAL:HG22 | 8        | 0.14          |
| (2,1470) | 1:202:A:PRO:HB3  | 1:205:A:VAL:HG23 | 8        | 0.14          |
| (2,1435) | 1:199:A:VAL:HG11 | 1:200:A:PRO:HG2  | 7        | 0.14          |
| (2,1435) | 1:199:A:VAL:HG12 | 1:200:A:PRO:HG2  | 7        | 0.14          |
| (2,1435) | 1:199:A:VAL:HG13 | 1:200:A:PRO:HG2  | 7        | 0.14          |
| (2,1435) | 1:199:A:VAL:HG21 | 1:200:A:PRO:HG2  | 7        | 0.14          |
| (2,1435) | 1:199:A:VAL:HG22 | 1:200:A:PRO:HG2  | 7        | 0.14          |
| (2,1435) | 1:199:A:VAL:HG23 | 1:200:A:PRO:HG2  | 7        | 0.14          |
| (2,1435) | 1:199:A:VAL:HG11 | 1:200:A:PRO:HG2  | 9        | 0.14          |
| (2,1435) | 1:199:A:VAL:HG12 | 1:200:A:PRO:HG2  | 9        | 0.14          |
| (2,1435) | 1:199:A:VAL:HG13 | 1:200:A:PRO:HG2  | 9        | 0.14          |
| (2,1435) | 1:199:A:VAL:HG21 | 1:200:A:PRO:HG2  | 9        | 0.14          |
| (2,1435) | 1:199:A:VAL:HG22 | 1:200:A:PRO:HG2  | 9        | 0.14          |
| (2,1435) | 1:199:A:VAL:HG23 | 1:200:A:PRO:HG2  | 9        | 0.14          |
| (2,1435) | 1:199:A:VAL:HG11 | 1:200:A:PRO:HG2  | 18       | 0.14          |
| (2,1435) | 1:199:A:VAL:HG12 | 1:200:A:PRO:HG2  | 18       | 0.14          |
| (2,1435) | 1:199:A:VAL:HG13 | 1:200:A:PRO:HG2  | 18       | 0.14          |
| (2,1435) | 1:199:A:VAL:HG21 | 1:200:A:PRO:HG2  | 18       | 0.14          |
| (2,1435) | 1:199:A:VAL:HG22 | 1:200:A:PRO:HG2  | 18       | 0.14          |
| (2,1435) | 1:199:A:VAL:HG23 | 1:200:A:PRO:HG2  | 18       | 0.14          |
| (2,1363) | 1:172:A:LEU:HD21 | 1:178:A:ALA:HB1  | 15       | 0.14          |
| (2,1363) | 1:172:A:LEU:HD21 | 1:178:A:ALA:HB2  | 15       | 0.14          |
| (2,1363) | 1:172:A:LEU:HD21 | 1:178:A:ALA:HB3  | 15       | 0.14          |
| (2,1363) | 1:172:A:LEU:HD22 | 1:178:A:ALA:HB1  | 15       | 0.14          |
| (2,1363) | 1:172:A:LEU:HD22 | 1:178:A:ALA:HB2  | 15       | 0.14          |
| (2,1363) | 1:172:A:LEU:HD22 | 1:178:A:ALA:HB3  | 15       | 0.14          |
| (2,1363) | 1:172:A:LEU:HD23 | 1:178:A:ALA:HB1  | 15       | 0.14          |
| (2,1363) | 1:172:A:LEU:HD23 | 1:178:A:ALA:HB2  | 15       | 0.14          |
| (2,1363) | 1:172:A:LEU:HD23 | 1:178:A:ALA:HB3  | 15       | 0.14          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,1298) | 1:223:A:VAL:HG21 | 1:224:A:PRO:HG2  | 7        | 0.14          |
| (2,1298) | 1:223:A:VAL:HG22 | 1:224:A:PRO:HG2  | 7        | 0.14          |
| (2,1298) | 1:223:A:VAL:HG23 | 1:224:A:PRO:HG2  | 7        | 0.14          |
| (2,1284) | 1:195:A:ALA:H    | 1:250:A:TYR:HD1  | 7        | 0.14          |
| (2,1213) | 1:231:A:ARG:HD3  | 1:232:A:LYS:H    | 14       | 0.14          |
| (2,1050) | 1:231:A:ARG:H    | 1:253:A:VAL:HG11 | 12       | 0.14          |
| (2,1050) | 1:231:A:ARG:H    | 1:253:A:VAL:HG12 | 12       | 0.14          |
| (2,1050) | 1:231:A:ARG:H    | 1:253:A:VAL:HG13 | 12       | 0.14          |
| (2,1006) | 1:230:A:GLY:H    | 1:255:A:ILE:HG13 | 13       | 0.14          |
| (2,739)  | 1:225:A:PRO:HB3  | 1:226:A:ARG:HG2  | 13       | 0.14          |
| (2,732)  | 1:197:A:LEU:HD21 | 1:251:A:LEU:HD11 | 13       | 0.14          |
| (2,732)  | 1:197:A:LEU:HD21 | 1:251:A:LEU:HD12 | 13       | 0.14          |
| (2,732)  | 1:197:A:LEU:HD21 | 1:251:A:LEU:HD13 | 13       | 0.14          |
| (2,732)  | 1:197:A:LEU:HD22 | 1:251:A:LEU:HD11 | 13       | 0.14          |
| (2,732)  | 1:197:A:LEU:HD22 | 1:251:A:LEU:HD12 | 13       | 0.14          |
| (2,732)  | 1:197:A:LEU:HD22 | 1:251:A:LEU:HD13 | 13       | 0.14          |
| (2,732)  | 1:197:A:LEU:HD23 | 1:251:A:LEU:HD11 | 13       | 0.14          |
| (2,732)  | 1:197:A:LEU:HD23 | 1:251:A:LEU:HD12 | 13       | 0.14          |
| (2,732)  | 1:197:A:LEU:HD23 | 1:251:A:LEU:HD13 | 13       | 0.14          |
| (2,553)  | 1:193:A:LEU:HB3  | 1:249:A:LEU:HD21 | 2        | 0.14          |
| (2,553)  | 1:193:A:LEU:HB3  | 1:249:A:LEU:HD22 | 2        | 0.14          |
| (2,553)  | 1:193:A:LEU:HB3  | 1:249:A:LEU:HD23 | 2        | 0.14          |
| (2,553)  | 1:193:A:LEU:HB3  | 1:249:A:LEU:HD21 | 4        | 0.14          |
| (2,553)  | 1:193:A:LEU:HB3  | 1:249:A:LEU:HD22 | 4        | 0.14          |
| (2,553)  | 1:193:A:LEU:HB3  | 1:249:A:LEU:HD23 | 4        | 0.14          |
| (2,553)  | 1:193:A:LEU:HB3  | 1:249:A:LEU:HD21 | 9        | 0.14          |
| (2,553)  | 1:193:A:LEU:HB3  | 1:249:A:LEU:HD22 | 9        | 0.14          |
| (2,553)  | 1:193:A:LEU:HB3  | 1:249:A:LEU:HD23 | 9        | 0.14          |
| (2,553)  | 1:193:A:LEU:HB3  | 1:249:A:LEU:HD21 | 11       | 0.14          |
| (2,553)  | 1:193:A:LEU:HB3  | 1:249:A:LEU:HD22 | 11       | 0.14          |
| (2,553)  | 1:193:A:LEU:HB3  | 1:249:A:LEU:HD23 | 11       | 0.14          |
| (2,553)  | 1:193:A:LEU:HB3  | 1:249:A:LEU:HD21 | 16       | 0.14          |
| (2,553)  | 1:193:A:LEU:HB3  | 1:249:A:LEU:HD22 | 16       | 0.14          |
| (2,553)  | 1:193:A:LEU:HB3  | 1:249:A:LEU:HD23 | 16       | 0.14          |
| (2,474)  | 1:180:A:GLY:H    | 1:231:A:ARG:HD2  | 13       | 0.14          |
| (2,395)  | 1:194:A:TYR:HD2  | 1:195:A:ALA:HB1  | 4        | 0.14          |
| (2,395)  | 1:194:A:TYR:HD2  | 1:195:A:ALA:HB2  | 4        | 0.14          |
| (2,395)  | 1:194:A:TYR:HD2  | 1:195:A:ALA:HB3  | 4        | 0.14          |
| (2,395)  | 1:194:A:TYR:HD2  | 1:195:A:ALA:HB1  | 11       | 0.14          |
| (2,395)  | 1:194:A:TYR:HD2  | 1:195:A:ALA:HB2  | 11       | 0.14          |
| (2,395)  | 1:194:A:TYR:HD2  | 1:195:A:ALA:HB3  | 11       | 0.14          |
| (2,395)  | 1:194:A:TYR:HD2  | 1:195:A:ALA:HB1  | 12       | 0.14          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,395)  | 1:194:A:TYR:HD2  | 1:195:A:ALA:HB2  | 12       | 0.14          |
| (2,395)  | 1:194:A:TYR:HD2  | 1:195:A:ALA:HB3  | 12       | 0.14          |
| (2,395)  | 1:194:A:TYR:HD2  | 1:195:A:ALA:HB1  | 16       | 0.14          |
| (2,395)  | 1:194:A:TYR:HD2  | 1:195:A:ALA:HB2  | 16       | 0.14          |
| (2,395)  | 1:194:A:TYR:HD2  | 1:195:A:ALA:HB3  | 16       | 0.14          |
| (2,247)  | 1:199:A:VAL:HA   | 1:203:A:ILE:HD11 | 9        | 0.14          |
| (2,247)  | 1:199:A:VAL:HA   | 1:203:A:ILE:HD12 | 9        | 0.14          |
| (2,247)  | 1:199:A:VAL:HA   | 1:203:A:ILE:HD13 | 9        | 0.14          |
| (2,247)  | 1:199:A:VAL:HA   | 1:203:A:ILE:HD11 | 11       | 0.14          |
| (2,247)  | 1:199:A:VAL:HA   | 1:203:A:ILE:HD12 | 11       | 0.14          |
| (2,247)  | 1:199:A:VAL:HA   | 1:203:A:ILE:HD13 | 11       | 0.14          |
| (2,247)  | 1:199:A:VAL:HA   | 1:203:A:ILE:HD11 | 18       | 0.14          |
| (2,247)  | 1:199:A:VAL:HA   | 1:203:A:ILE:HD12 | 18       | 0.14          |
| (2,247)  | 1:199:A:VAL:HA   | 1:203:A:ILE:HD13 | 18       | 0.14          |
| (2,151)  | 1:193:A:LEU:HD21 | 1:194:A:TYR:HB2  | 7        | 0.14          |
| (2,151)  | 1:193:A:LEU:HD22 | 1:194:A:TYR:HB2  | 7        | 0.14          |
| (2,151)  | 1:193:A:LEU:HD23 | 1:194:A:TYR:HB2  | 7        | 0.14          |
| (2,91)   | 1:170:A:THR:HB   | 1:219:A:VAL:HG21 | 5        | 0.14          |
| (2,91)   | 1:170:A:THR:HB   | 1:219:A:VAL:HG22 | 5        | 0.14          |
| (2,91)   | 1:170:A:THR:HB   | 1:219:A:VAL:HG23 | 5        | 0.14          |
| (2,34)   | 1:194:A:TYR:HD2  | 1:249:A:LEU:HD11 | 19       | 0.14          |
| (2,34)   | 1:194:A:TYR:HD2  | 1:249:A:LEU:HD12 | 19       | 0.14          |
| (2,34)   | 1:194:A:TYR:HD2  | 1:249:A:LEU:HD13 | 19       | 0.14          |
| (2,1684) | 1:172:A:LEU:HG   | 1:219:A:VAL:HG11 | 20       | 0.13          |
| (2,1684) | 1:172:A:LEU:HG   | 1:219:A:VAL:HG12 | 20       | 0.13          |
| (2,1684) | 1:172:A:LEU:HG   | 1:219:A:VAL:HG13 | 20       | 0.13          |
| (2,1684) | 1:172:A:LEU:HG   | 1:219:A:VAL:HG21 | 20       | 0.13          |
| (2,1684) | 1:172:A:LEU:HG   | 1:219:A:VAL:HG22 | 20       | 0.13          |
| (2,1684) | 1:172:A:LEU:HG   | 1:219:A:VAL:HG23 | 20       | 0.13          |
| (2,1681) | 1:173:A:PHE:HD2  | 1:235:A:LEU:HD11 | 5        | 0.13          |
| (2,1681) | 1:173:A:PHE:HD2  | 1:235:A:LEU:HD12 | 5        | 0.13          |
| (2,1681) | 1:173:A:PHE:HD2  | 1:235:A:LEU:HD13 | 5        | 0.13          |
| (2,1663) | 1:241:A:PRO:HB2  | 1:245:A:GLY:H    | 7        | 0.13          |
| (2,1663) | 1:241:A:PRO:HB3  | 1:245:A:GLY:H    | 7        | 0.13          |
| (2,1663) | 1:241:A:PRO:HB2  | 1:245:A:GLY:H    | 12       | 0.13          |
| (2,1663) | 1:241:A:PRO:HB3  | 1:245:A:GLY:H    | 12       | 0.13          |
| (2,1578) | 1:219:A:VAL:HG21 | 1:238:A:LYS:HD2  | 15       | 0.13          |
| (2,1578) | 1:219:A:VAL:HG21 | 1:238:A:LYS:HD3  | 15       | 0.13          |
| (2,1578) | 1:219:A:VAL:HG22 | 1:238:A:LYS:HD2  | 15       | 0.13          |
| (2,1578) | 1:219:A:VAL:HG22 | 1:238:A:LYS:HD3  | 15       | 0.13          |
| (2,1578) | 1:219:A:VAL:HG23 | 1:238:A:LYS:HD2  | 15       | 0.13          |
| (2,1578) | 1:219:A:VAL:HG23 | 1:238:A:LYS:HD3  | 15       | 0.13          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,1578) | 1:219:A:VAL:HG21 | 1:238:A:LYS:HD2  | 16       | 0.13          |
| (2,1578) | 1:219:A:VAL:HG21 | 1:238:A:LYS:HD3  | 16       | 0.13          |
| (2,1578) | 1:219:A:VAL:HG22 | 1:238:A:LYS:HD2  | 16       | 0.13          |
| (2,1578) | 1:219:A:VAL:HG22 | 1:238:A:LYS:HD3  | 16       | 0.13          |
| (2,1578) | 1:219:A:VAL:HG23 | 1:238:A:LYS:HD2  | 16       | 0.13          |
| (2,1578) | 1:219:A:VAL:HG23 | 1:238:A:LYS:HD3  | 16       | 0.13          |
| (2,1525) | 1:209:A:LYS:HE2  | 1:222:A:ALA:HB1  | 4        | 0.13          |
| (2,1525) | 1:209:A:LYS:HE2  | 1:222:A:ALA:HB2  | 4        | 0.13          |
| (2,1525) | 1:209:A:LYS:HE2  | 1:222:A:ALA:HB3  | 4        | 0.13          |
| (2,1525) | 1:209:A:LYS:HE3  | 1:222:A:ALA:HB1  | 4        | 0.13          |
| (2,1525) | 1:209:A:LYS:HE3  | 1:222:A:ALA:HB2  | 4        | 0.13          |
| (2,1525) | 1:209:A:LYS:HE3  | 1:222:A:ALA:HB3  | 4        | 0.13          |
| (2,1470) | 1:202:A:PRO:HB3  | 1:205:A:VAL:HG11 | 7        | 0.13          |
| (2,1470) | 1:202:A:PRO:HB3  | 1:205:A:VAL:HG12 | 7        | 0.13          |
| (2,1470) | 1:202:A:PRO:HB3  | 1:205:A:VAL:HG13 | 7        | 0.13          |
| (2,1470) | 1:202:A:PRO:HB3  | 1:205:A:VAL:HG21 | 7        | 0.13          |
| (2,1470) | 1:202:A:PRO:HB3  | 1:205:A:VAL:HG22 | 7        | 0.13          |
| (2,1470) | 1:202:A:PRO:HB3  | 1:205:A:VAL:HG23 | 7        | 0.13          |
| (2,1435) | 1:199:A:VAL:HG11 | 1:200:A:PRO:HG2  | 2        | 0.13          |
| (2,1435) | 1:199:A:VAL:HG12 | 1:200:A:PRO:HG2  | 2        | 0.13          |
| (2,1435) | 1:199:A:VAL:HG13 | 1:200:A:PRO:HG2  | 2        | 0.13          |
| (2,1435) | 1:199:A:VAL:HG21 | 1:200:A:PRO:HG2  | 2        | 0.13          |
| (2,1435) | 1:199:A:VAL:HG22 | 1:200:A:PRO:HG2  | 2        | 0.13          |
| (2,1435) | 1:199:A:VAL:HG23 | 1:200:A:PRO:HG2  | 2        | 0.13          |
| (2,1435) | 1:199:A:VAL:HG11 | 1:200:A:PRO:HG2  | 3        | 0.13          |
| (2,1435) | 1:199:A:VAL:HG12 | 1:200:A:PRO:HG2  | 3        | 0.13          |
| (2,1435) | 1:199:A:VAL:HG13 | 1:200:A:PRO:HG2  | 3        | 0.13          |
| (2,1435) | 1:199:A:VAL:HG21 | 1:200:A:PRO:HG2  | 3        | 0.13          |
| (2,1435) | 1:199:A:VAL:HG22 | 1:200:A:PRO:HG2  | 3        | 0.13          |
| (2,1435) | 1:199:A:VAL:HG23 | 1:200:A:PRO:HG2  | 3        | 0.13          |
| (2,1435) | 1:199:A:VAL:HG11 | 1:200:A:PRO:HG2  | 14       | 0.13          |
| (2,1435) | 1:199:A:VAL:HG12 | 1:200:A:PRO:HG2  | 14       | 0.13          |
| (2,1435) | 1:199:A:VAL:HG13 | 1:200:A:PRO:HG2  | 14       | 0.13          |
| (2,1435) | 1:199:A:VAL:HG21 | 1:200:A:PRO:HG2  | 14       | 0.13          |
| (2,1435) | 1:199:A:VAL:HG22 | 1:200:A:PRO:HG2  | 14       | 0.13          |
| (2,1435) | 1:199:A:VAL:HG23 | 1:200:A:PRO:HG2  | 14       | 0.13          |
| (2,1435) | 1:199:A:VAL:HG11 | 1:200:A:PRO:HG2  | 19       | 0.13          |
| (2,1435) | 1:199:A:VAL:HG12 | 1:200:A:PRO:HG2  | 19       | 0.13          |
| (2,1435) | 1:199:A:VAL:HG13 | 1:200:A:PRO:HG2  | 19       | 0.13          |
| (2,1435) | 1:199:A:VAL:HG21 | 1:200:A:PRO:HG2  | 19       | 0.13          |
| (2,1435) | 1:199:A:VAL:HG22 | 1:200:A:PRO:HG2  | 19       | 0.13          |
| (2,1435) | 1:199:A:VAL:HG23 | 1:200:A:PRO:HG2  | 19       | 0.13          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,1435) | 1:199:A:VAL:HG11 | 1:200:A:PRO:HG2  | 20       | 0.13          |
| (2,1435) | 1:199:A:VAL:HG12 | 1:200:A:PRO:HG2  | 20       | 0.13          |
| (2,1435) | 1:199:A:VAL:HG13 | 1:200:A:PRO:HG2  | 20       | 0.13          |
| (2,1435) | 1:199:A:VAL:HG21 | 1:200:A:PRO:HG2  | 20       | 0.13          |
| (2,1435) | 1:199:A:VAL:HG22 | 1:200:A:PRO:HG2  | 20       | 0.13          |
| (2,1435) | 1:199:A:VAL:HG23 | 1:200:A:PRO:HG2  | 20       | 0.13          |
| (2,1381) | 1:169:A:GLN:HG2  | 1:170:A:THR:HG21 | 4        | 0.13          |
| (2,1381) | 1:169:A:GLN:HG2  | 1:170:A:THR:HG22 | 4        | 0.13          |
| (2,1381) | 1:169:A:GLN:HG2  | 1:170:A:THR:HG23 | 4        | 0.13          |
| (2,1381) | 1:169:A:GLN:HG3  | 1:170:A:THR:HG21 | 4        | 0.13          |
| (2,1381) | 1:169:A:GLN:HG3  | 1:170:A:THR:HG22 | 4        | 0.13          |
| (2,1381) | 1:169:A:GLN:HG3  | 1:170:A:THR:HG23 | 4        | 0.13          |
| (2,1366) | 1:176:A:MET:HE1  | 1:178:A:ALA:HB1  | 8        | 0.13          |
| (2,1366) | 1:176:A:MET:HE1  | 1:178:A:ALA:HB2  | 8        | 0.13          |
| (2,1366) | 1:176:A:MET:HE1  | 1:178:A:ALA:HB3  | 8        | 0.13          |
| (2,1366) | 1:176:A:MET:HE2  | 1:178:A:ALA:HB1  | 8        | 0.13          |
| (2,1366) | 1:176:A:MET:HE2  | 1:178:A:ALA:HB2  | 8        | 0.13          |
| (2,1366) | 1:176:A:MET:HE2  | 1:178:A:ALA:HB3  | 8        | 0.13          |
| (2,1366) | 1:176:A:MET:HE3  | 1:178:A:ALA:HB1  | 8        | 0.13          |
| (2,1366) | 1:176:A:MET:HE3  | 1:178:A:ALA:HB2  | 8        | 0.13          |
| (2,1366) | 1:176:A:MET:HE3  | 1:178:A:ALA:HB3  | 8        | 0.13          |
| (2,1337) | 1:175:A:THR:HG21 | 1:222:A:ALA:HB1  | 8        | 0.13          |
| (2,1337) | 1:175:A:THR:HG21 | 1:222:A:ALA:HB2  | 8        | 0.13          |
| (2,1337) | 1:175:A:THR:HG21 | 1:222:A:ALA:HB3  | 8        | 0.13          |
| (2,1337) | 1:175:A:THR:HG22 | 1:222:A:ALA:HB1  | 8        | 0.13          |
| (2,1337) | 1:175:A:THR:HG22 | 1:222:A:ALA:HB2  | 8        | 0.13          |
| (2,1337) | 1:175:A:THR:HG22 | 1:222:A:ALA:HB3  | 8        | 0.13          |
| (2,1337) | 1:175:A:THR:HG23 | 1:222:A:ALA:HB1  | 8        | 0.13          |
| (2,1337) | 1:175:A:THR:HG23 | 1:222:A:ALA:HB2  | 8        | 0.13          |
| (2,1337) | 1:175:A:THR:HG23 | 1:222:A:ALA:HB3  | 8        | 0.13          |
| (2,1284) | 1:195:A:ALA:H    | 1:250:A:TYR:HD1  | 3        | 0.13          |
| (2,1213) | 1:231:A:ARG:HD3  | 1:232:A:LYS:H    | 4        | 0.13          |
| (2,1213) | 1:231:A:ARG:HD3  | 1:232:A:LYS:H    | 18       | 0.13          |
| (2,1006) | 1:230:A:GLY:H    | 1:255:A:ILE:HG13 | 5        | 0.13          |
| (2,754)  | 1:211:A:ARG:HA   | 1:218:A:PRO:HB2  | 3        | 0.13          |
| (2,739)  | 1:225:A:PRO:HB3  | 1:226:A:ARG:HG2  | 1        | 0.13          |
| (2,739)  | 1:225:A:PRO:HB3  | 1:226:A:ARG:HG2  | 5        | 0.13          |
| (2,739)  | 1:225:A:PRO:HB3  | 1:226:A:ARG:HG2  | 7        | 0.13          |
| (2,732)  | 1:197:A:LEU:HD21 | 1:251:A:LEU:HD11 | 2        | 0.13          |
| (2,732)  | 1:197:A:LEU:HD21 | 1:251:A:LEU:HD12 | 2        | 0.13          |
| (2,732)  | 1:197:A:LEU:HD21 | 1:251:A:LEU:HD13 | 2        | 0.13          |
| (2,732)  | 1:197:A:LEU:HD22 | 1:251:A:LEU:HD11 | 2        | 0.13          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (2,732) | 1:197:A:LEU:HD22 | 1:251:A:LEU:HD12 | 2        | 0.13          |
| (2,732) | 1:197:A:LEU:HD22 | 1:251:A:LEU:HD13 | 2        | 0.13          |
| (2,732) | 1:197:A:LEU:HD23 | 1:251:A:LEU:HD11 | 2        | 0.13          |
| (2,732) | 1:197:A:LEU:HD23 | 1:251:A:LEU:HD12 | 2        | 0.13          |
| (2,732) | 1:197:A:LEU:HD23 | 1:251:A:LEU:HD13 | 2        | 0.13          |
| (2,687) | 1:197:A:LEU:HD21 | 1:212:A:ALA:H    | 16       | 0.13          |
| (2,687) | 1:197:A:LEU:HD22 | 1:212:A:ALA:H    | 16       | 0.13          |
| (2,687) | 1:197:A:LEU:HD23 | 1:212:A:ALA:H    | 16       | 0.13          |
| (2,633) | 1:197:A:LEU:HB3  | 1:210:A:VAL:HG21 | 19       | 0.13          |
| (2,633) | 1:197:A:LEU:HB3  | 1:210:A:VAL:HG22 | 19       | 0.13          |
| (2,633) | 1:197:A:LEU:HB3  | 1:210:A:VAL:HG23 | 19       | 0.13          |
| (2,553) | 1:193:A:LEU:HB3  | 1:249:A:LEU:HD21 | 19       | 0.13          |
| (2,553) | 1:193:A:LEU:HB3  | 1:249:A:LEU:HD22 | 19       | 0.13          |
| (2,553) | 1:193:A:LEU:HB3  | 1:249:A:LEU:HD23 | 19       | 0.13          |
| (2,488) | 1:170:A:THR:HG21 | 1:171:A:ASP:HA   | 12       | 0.13          |
| (2,488) | 1:170:A:THR:HG22 | 1:171:A:ASP:HA   | 12       | 0.13          |
| (2,488) | 1:170:A:THR:HG23 | 1:171:A:ASP:HA   | 12       | 0.13          |
| (2,481) | 1:231:A:ARG:HD2  | 1:253:A:VAL:HG11 | 19       | 0.13          |
| (2,481) | 1:231:A:ARG:HD2  | 1:253:A:VAL:HG12 | 19       | 0.13          |
| (2,481) | 1:231:A:ARG:HD2  | 1:253:A:VAL:HG13 | 19       | 0.13          |
| (2,396) | 1:225:A:PRO:HG2  | 1:226:A:ARG:HG3  | 8        | 0.13          |
| (2,390) | 1:196:A:THR:HG21 | 1:252:A:GLU:HA   | 7        | 0.13          |
| (2,390) | 1:196:A:THR:HG22 | 1:252:A:GLU:HA   | 7        | 0.13          |
| (2,390) | 1:196:A:THR:HG23 | 1:252:A:GLU:HA   | 7        | 0.13          |
| (2,390) | 1:196:A:THR:HG21 | 1:252:A:GLU:HA   | 11       | 0.13          |
| (2,390) | 1:196:A:THR:HG22 | 1:252:A:GLU:HA   | 11       | 0.13          |
| (2,390) | 1:196:A:THR:HG23 | 1:252:A:GLU:HA   | 11       | 0.13          |
| (2,387) | 1:196:A:THR:HG21 | 1:252:A:GLU:H    | 10       | 0.13          |
| (2,387) | 1:196:A:THR:HG22 | 1:252:A:GLU:H    | 10       | 0.13          |
| (2,387) | 1:196:A:THR:HG23 | 1:252:A:GLU:H    | 10       | 0.13          |
| (2,382) | 1:198:A:ASP:HA   | 1:254:A:ARG:HB3  | 16       | 0.13          |
| (2,335) | 1:204:A:ALA:HB1  | 1:228:A:GLN:H    | 10       | 0.13          |
| (2,335) | 1:204:A:ALA:HB2  | 1:228:A:GLN:H    | 10       | 0.13          |
| (2,335) | 1:204:A:ALA:HB3  | 1:228:A:GLN:H    | 10       | 0.13          |
| (2,292) | 1:191:A:GLN:HB3  | 1:243:A:PRO:HG3  | 15       | 0.13          |
| (2,202) | 1:197:A:LEU:HA   | 1:210:A:VAL:HG11 | 14       | 0.13          |
| (2,202) | 1:197:A:LEU:HA   | 1:210:A:VAL:HG12 | 14       | 0.13          |
| (2,202) | 1:197:A:LEU:HA   | 1:210:A:VAL:HG13 | 14       | 0.13          |
| (2,197) | 1:174:A:TYR:HB3  | 1:234:A:ARG:HB2  | 6        | 0.13          |
| (2,180) | 1:249:A:LEU:HA   | 1:250:A:TYR:HD2  | 5        | 0.13          |
| (2,91)  | 1:170:A:THR:HB   | 1:219:A:VAL:HG21 | 12       | 0.13          |
| (2,91)  | 1:170:A:THR:HB   | 1:219:A:VAL:HG22 | 12       | 0.13          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,91)   | 1:170:A:THR:HB   | 1:219:A:VAL:HG23 | 12       | 0.13          |
| (1,21)   | 1:247:A:GLY:H    | 1:240:A:PHE:O    | 11       | 0.13          |
| (1,21)   | 1:247:A:GLY:H    | 1:240:A:PHE:O    | 12       | 0.13          |
| (2,1684) | 1:172:A:LEU:HG   | 1:219:A:VAL:HG11 | 8        | 0.12          |
| (2,1684) | 1:172:A:LEU:HG   | 1:219:A:VAL:HG12 | 8        | 0.12          |
| (2,1684) | 1:172:A:LEU:HG   | 1:219:A:VAL:HG13 | 8        | 0.12          |
| (2,1684) | 1:172:A:LEU:HG   | 1:219:A:VAL:HG21 | 8        | 0.12          |
| (2,1684) | 1:172:A:LEU:HG   | 1:219:A:VAL:HG22 | 8        | 0.12          |
| (2,1684) | 1:172:A:LEU:HG   | 1:219:A:VAL:HG23 | 8        | 0.12          |
| (2,1681) | 1:173:A:PHE:HD2  | 1:235:A:LEU:HD11 | 10       | 0.12          |
| (2,1681) | 1:173:A:PHE:HD2  | 1:235:A:LEU:HD12 | 10       | 0.12          |
| (2,1681) | 1:173:A:PHE:HD2  | 1:235:A:LEU:HD13 | 10       | 0.12          |
| (2,1681) | 1:173:A:PHE:HD2  | 1:235:A:LEU:HD11 | 19       | 0.12          |
| (2,1681) | 1:173:A:PHE:HD2  | 1:235:A:LEU:HD12 | 19       | 0.12          |
| (2,1681) | 1:173:A:PHE:HD2  | 1:235:A:LEU:HD13 | 19       | 0.12          |
| (2,1678) | 1:173:A:PHE:HE2  | 1:235:A:LEU:HD21 | 5        | 0.12          |
| (2,1678) | 1:173:A:PHE:HE2  | 1:235:A:LEU:HD22 | 5        | 0.12          |
| (2,1678) | 1:173:A:PHE:HE2  | 1:235:A:LEU:HD23 | 5        | 0.12          |
| (2,1639) | 1:232:A:LYS:HE2  | 1:252:A:GLU:HA   | 17       | 0.12          |
| (2,1639) | 1:232:A:LYS:HE3  | 1:252:A:GLU:HA   | 17       | 0.12          |
| (2,1639) | 1:232:A:LYS:HE2  | 1:252:A:GLU:HA   | 18       | 0.12          |
| (2,1639) | 1:232:A:LYS:HE3  | 1:252:A:GLU:HA   | 18       | 0.12          |
| (2,1525) | 1:209:A:LYS:HE2  | 1:222:A:ALA:HB1  | 1        | 0.12          |
| (2,1525) | 1:209:A:LYS:HE2  | 1:222:A:ALA:HB2  | 1        | 0.12          |
| (2,1525) | 1:209:A:LYS:HE2  | 1:222:A:ALA:HB3  | 1        | 0.12          |
| (2,1525) | 1:209:A:LYS:HE3  | 1:222:A:ALA:HB1  | 1        | 0.12          |
| (2,1525) | 1:209:A:LYS:HE3  | 1:222:A:ALA:HB2  | 1        | 0.12          |
| (2,1525) | 1:209:A:LYS:HE3  | 1:222:A:ALA:HB3  | 1        | 0.12          |
| (2,1525) | 1:209:A:LYS:HE2  | 1:222:A:ALA:HB1  | 14       | 0.12          |
| (2,1525) | 1:209:A:LYS:HE2  | 1:222:A:ALA:HB2  | 14       | 0.12          |
| (2,1525) | 1:209:A:LYS:HE2  | 1:222:A:ALA:HB3  | 14       | 0.12          |
| (2,1525) | 1:209:A:LYS:HE3  | 1:222:A:ALA:HB1  | 14       | 0.12          |
| (2,1525) | 1:209:A:LYS:HE3  | 1:222:A:ALA:HB2  | 14       | 0.12          |
| (2,1525) | 1:209:A:LYS:HE3  | 1:222:A:ALA:HB3  | 14       | 0.12          |
| (2,1525) | 1:209:A:LYS:HE2  | 1:222:A:ALA:HB1  | 20       | 0.12          |
| (2,1525) | 1:209:A:LYS:HE2  | 1:222:A:ALA:HB2  | 20       | 0.12          |
| (2,1525) | 1:209:A:LYS:HE2  | 1:222:A:ALA:HB3  | 20       | 0.12          |
| (2,1525) | 1:209:A:LYS:HE3  | 1:222:A:ALA:HB1  | 20       | 0.12          |
| (2,1525) | 1:209:A:LYS:HE3  | 1:222:A:ALA:HB2  | 20       | 0.12          |
| (2,1525) | 1:209:A:LYS:HE3  | 1:222:A:ALA:HB3  | 20       | 0.12          |
| (2,1435) | 1:199:A:VAL:HG11 | 1:200:A:PRO:HG2  | 11       | 0.12          |
| (2,1435) | 1:199:A:VAL:HG12 | 1:200:A:PRO:HG2  | 11       | 0.12          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,1435) | 1:199:A:VAL:HG13 | 1:200:A:PRO:HG2  | 11       | 0.12          |
| (2,1435) | 1:199:A:VAL:HG21 | 1:200:A:PRO:HG2  | 11       | 0.12          |
| (2,1435) | 1:199:A:VAL:HG22 | 1:200:A:PRO:HG2  | 11       | 0.12          |
| (2,1435) | 1:199:A:VAL:HG23 | 1:200:A:PRO:HG2  | 11       | 0.12          |
| (2,1435) | 1:199:A:VAL:HG11 | 1:200:A:PRO:HG2  | 17       | 0.12          |
| (2,1435) | 1:199:A:VAL:HG12 | 1:200:A:PRO:HG2  | 17       | 0.12          |
| (2,1435) | 1:199:A:VAL:HG13 | 1:200:A:PRO:HG2  | 17       | 0.12          |
| (2,1435) | 1:199:A:VAL:HG21 | 1:200:A:PRO:HG2  | 17       | 0.12          |
| (2,1435) | 1:199:A:VAL:HG22 | 1:200:A:PRO:HG2  | 17       | 0.12          |
| (2,1435) | 1:199:A:VAL:HG23 | 1:200:A:PRO:HG2  | 17       | 0.12          |
| (2,1311) | 1:233:A:LEU:HD11 | 1:235:A:LEU:HD11 | 2        | 0.12          |
| (2,1311) | 1:233:A:LEU:HD11 | 1:235:A:LEU:HD12 | 2        | 0.12          |
| (2,1311) | 1:233:A:LEU:HD11 | 1:235:A:LEU:HD13 | 2        | 0.12          |
| (2,1311) | 1:233:A:LEU:HD12 | 1:235:A:LEU:HD11 | 2        | 0.12          |
| (2,1311) | 1:233:A:LEU:HD12 | 1:235:A:LEU:HD12 | 2        | 0.12          |
| (2,1311) | 1:233:A:LEU:HD12 | 1:235:A:LEU:HD13 | 2        | 0.12          |
| (2,1311) | 1:233:A:LEU:HD13 | 1:235:A:LEU:HD11 | 2        | 0.12          |
| (2,1311) | 1:233:A:LEU:HD13 | 1:235:A:LEU:HD12 | 2        | 0.12          |
| (2,1311) | 1:233:A:LEU:HD13 | 1:235:A:LEU:HD13 | 2        | 0.12          |
| (2,1303) | 1:235:A:LEU:HD11 | 1:238:A:LYS:HG3  | 18       | 0.12          |
| (2,1303) | 1:235:A:LEU:HD12 | 1:238:A:LYS:HG3  | 18       | 0.12          |
| (2,1303) | 1:235:A:LEU:HD13 | 1:238:A:LYS:HG3  | 18       | 0.12          |
| (2,1096) | 1:240:A:PHE:H    | 1:247:A:GLY:H    | 20       | 0.12          |
| (2,1006) | 1:230:A:GLY:H    | 1:255:A:ILE:HG13 | 6        | 0.12          |
| (2,937)  | 1:250:A:TYR:HD2  | 1:251:A:LEU:H    | 9        | 0.12          |
| (2,924)  | 1:235:A:LEU:HD21 | 1:236:A:LYS:H    | 5        | 0.12          |
| (2,924)  | 1:235:A:LEU:HD22 | 1:236:A:LYS:H    | 5        | 0.12          |
| (2,924)  | 1:235:A:LEU:HD23 | 1:236:A:LYS:H    | 5        | 0.12          |
| (2,924)  | 1:235:A:LEU:HD21 | 1:236:A:LYS:H    | 11       | 0.12          |
| (2,924)  | 1:235:A:LEU:HD22 | 1:236:A:LYS:H    | 11       | 0.12          |
| (2,924)  | 1:235:A:LEU:HD23 | 1:236:A:LYS:H    | 11       | 0.12          |
| (2,924)  | 1:235:A:LEU:HD21 | 1:236:A:LYS:H    | 15       | 0.12          |
| (2,924)  | 1:235:A:LEU:HD22 | 1:236:A:LYS:H    | 15       | 0.12          |
| (2,924)  | 1:235:A:LEU:HD23 | 1:236:A:LYS:H    | 15       | 0.12          |
| (2,778)  | 1:189:A:GLY:HA3  | 1:242:A:GLY:HA3  | 6        | 0.12          |
| (2,778)  | 1:189:A:GLY:HA3  | 1:242:A:GLY:HA3  | 10       | 0.12          |
| (2,778)  | 1:189:A:GLY:HA3  | 1:242:A:GLY:HA3  | 19       | 0.12          |
| (2,773)  | 1:228:A:GLN:HG3  | 1:255:A:ILE:HG21 | 6        | 0.12          |
| (2,773)  | 1:228:A:GLN:HG3  | 1:255:A:ILE:HG22 | 6        | 0.12          |
| (2,773)  | 1:228:A:GLN:HG3  | 1:255:A:ILE:HG23 | 6        | 0.12          |
| (2,739)  | 1:225:A:PRO:HB3  | 1:226:A:ARG:HG2  | 9        | 0.12          |
| (2,739)  | 1:225:A:PRO:HB3  | 1:226:A:ARG:HG2  | 20       | 0.12          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (2,732) | 1:197:A:LEU:HD21 | 1:251:A:LEU:HD11 | 1        | 0.12          |
| (2,732) | 1:197:A:LEU:HD21 | 1:251:A:LEU:HD12 | 1        | 0.12          |
| (2,732) | 1:197:A:LEU:HD21 | 1:251:A:LEU:HD13 | 1        | 0.12          |
| (2,732) | 1:197:A:LEU:HD22 | 1:251:A:LEU:HD11 | 1        | 0.12          |
| (2,732) | 1:197:A:LEU:HD22 | 1:251:A:LEU:HD12 | 1        | 0.12          |
| (2,732) | 1:197:A:LEU:HD22 | 1:251:A:LEU:HD13 | 1        | 0.12          |
| (2,732) | 1:197:A:LEU:HD23 | 1:251:A:LEU:HD11 | 1        | 0.12          |
| (2,732) | 1:197:A:LEU:HD23 | 1:251:A:LEU:HD12 | 1        | 0.12          |
| (2,732) | 1:197:A:LEU:HD23 | 1:251:A:LEU:HD13 | 1        | 0.12          |
| (2,732) | 1:197:A:LEU:HD21 | 1:251:A:LEU:HD11 | 18       | 0.12          |
| (2,732) | 1:197:A:LEU:HD21 | 1:251:A:LEU:HD12 | 18       | 0.12          |
| (2,732) | 1:197:A:LEU:HD21 | 1:251:A:LEU:HD13 | 18       | 0.12          |
| (2,732) | 1:197:A:LEU:HD22 | 1:251:A:LEU:HD11 | 18       | 0.12          |
| (2,732) | 1:197:A:LEU:HD22 | 1:251:A:LEU:HD12 | 18       | 0.12          |
| (2,732) | 1:197:A:LEU:HD22 | 1:251:A:LEU:HD13 | 18       | 0.12          |
| (2,732) | 1:197:A:LEU:HD23 | 1:251:A:LEU:HD11 | 18       | 0.12          |
| (2,732) | 1:197:A:LEU:HD23 | 1:251:A:LEU:HD12 | 18       | 0.12          |
| (2,732) | 1:197:A:LEU:HD23 | 1:251:A:LEU:HD13 | 18       | 0.12          |
| (2,726) | 1:174:A:TYR:HB3  | 1:251:A:LEU:HD11 | 4        | 0.12          |
| (2,726) | 1:174:A:TYR:HB3  | 1:251:A:LEU:HD12 | 4        | 0.12          |
| (2,726) | 1:174:A:TYR:HB3  | 1:251:A:LEU:HD13 | 4        | 0.12          |
| (2,726) | 1:174:A:TYR:HB3  | 1:251:A:LEU:HD11 | 5        | 0.12          |
| (2,726) | 1:174:A:TYR:HB3  | 1:251:A:LEU:HD12 | 5        | 0.12          |
| (2,726) | 1:174:A:TYR:HB3  | 1:251:A:LEU:HD13 | 5        | 0.12          |
| (2,633) | 1:197:A:LEU:HB3  | 1:210:A:VAL:HG21 | 3        | 0.12          |
| (2,633) | 1:197:A:LEU:HB3  | 1:210:A:VAL:HG22 | 3        | 0.12          |
| (2,633) | 1:197:A:LEU:HB3  | 1:210:A:VAL:HG23 | 3        | 0.12          |
| (2,564) | 1:178:A:ALA:HB1  | 1:233:A:LEU:HB3  | 12       | 0.12          |
| (2,564) | 1:178:A:ALA:HB2  | 1:233:A:LEU:HB3  | 12       | 0.12          |
| (2,564) | 1:178:A:ALA:HB3  | 1:233:A:LEU:HB3  | 12       | 0.12          |
| (2,553) | 1:193:A:LEU:HB3  | 1:249:A:LEU:HD21 | 12       | 0.12          |
| (2,553) | 1:193:A:LEU:HB3  | 1:249:A:LEU:HD22 | 12       | 0.12          |
| (2,553) | 1:193:A:LEU:HB3  | 1:249:A:LEU:HD23 | 12       | 0.12          |
| (2,474) | 1:180:A:GLY:H    | 1:231:A:ARG:HD2  | 6        | 0.12          |
| (2,395) | 1:194:A:TYR:HD2  | 1:195:A:ALA:HB1  | 6        | 0.12          |
| (2,395) | 1:194:A:TYR:HD2  | 1:195:A:ALA:HB2  | 6        | 0.12          |
| (2,395) | 1:194:A:TYR:HD2  | 1:195:A:ALA:HB3  | 6        | 0.12          |
| (2,247) | 1:199:A:VAL:HA   | 1:203:A:ILE:HD11 | 13       | 0.12          |
| (2,247) | 1:199:A:VAL:HA   | 1:203:A:ILE:HD12 | 13       | 0.12          |
| (2,247) | 1:199:A:VAL:HA   | 1:203:A:ILE:HD13 | 13       | 0.12          |
| (2,247) | 1:199:A:VAL:HA   | 1:203:A:ILE:HD11 | 19       | 0.12          |
| (2,247) | 1:199:A:VAL:HA   | 1:203:A:ILE:HD12 | 19       | 0.12          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,247)  | 1:199:A:VAL:HA   | 1:203:A:ILE:HD13 | 19       | 0.12          |
| (2,202)  | 1:197:A:LEU:HA   | 1:210:A:VAL:HG11 | 13       | 0.12          |
| (2,202)  | 1:197:A:LEU:HA   | 1:210:A:VAL:HG12 | 13       | 0.12          |
| (2,202)  | 1:197:A:LEU:HA   | 1:210:A:VAL:HG13 | 13       | 0.12          |
| (2,202)  | 1:197:A:LEU:HA   | 1:210:A:VAL:HG11 | 16       | 0.12          |
| (2,202)  | 1:197:A:LEU:HA   | 1:210:A:VAL:HG12 | 16       | 0.12          |
| (2,202)  | 1:197:A:LEU:HA   | 1:210:A:VAL:HG13 | 16       | 0.12          |
| (2,162)  | 1:176:A:MET:HE1  | 1:177:A:LYS:HA   | 20       | 0.12          |
| (2,162)  | 1:176:A:MET:HE2  | 1:177:A:LYS:HA   | 20       | 0.12          |
| (2,162)  | 1:176:A:MET:HE3  | 1:177:A:LYS:HA   | 20       | 0.12          |
| (2,36)   | 1:170:A:THR:HG21 | 1:173:A:PHE:HD1  | 2        | 0.12          |
| (2,36)   | 1:170:A:THR:HG22 | 1:173:A:PHE:HD1  | 2        | 0.12          |
| (2,36)   | 1:170:A:THR:HG23 | 1:173:A:PHE:HD1  | 2        | 0.12          |
| (1,21)   | 1:247:A:GLY:H    | 1:240:A:PHE:O    | 3        | 0.12          |
| (1,19)   | 1:239:A:GLY:H    | 1:247:A:GLY:O    | 12       | 0.12          |
| (2,1653) | 1:236:A:LYS:HD2  | 1:246:A:ARG:HG2  | 13       | 0.11          |
| (2,1653) | 1:236:A:LYS:HD3  | 1:246:A:ARG:HG2  | 13       | 0.11          |
| (2,1651) | 1:236:A:LYS:HD2  | 1:237:A:GLY:H    | 7        | 0.11          |
| (2,1651) | 1:236:A:LYS:HD3  | 1:237:A:GLY:H    | 7        | 0.11          |
| (2,1651) | 1:236:A:LYS:HD2  | 1:237:A:GLY:H    | 12       | 0.11          |
| (2,1651) | 1:236:A:LYS:HD3  | 1:237:A:GLY:H    | 12       | 0.11          |
| (2,1639) | 1:232:A:LYS:HE2  | 1:252:A:GLU:HA   | 2        | 0.11          |
| (2,1639) | 1:232:A:LYS:HE3  | 1:252:A:GLU:HA   | 2        | 0.11          |
| (2,1639) | 1:232:A:LYS:HE2  | 1:252:A:GLU:HA   | 10       | 0.11          |
| (2,1639) | 1:232:A:LYS:HE3  | 1:252:A:GLU:HA   | 10       | 0.11          |
| (2,1578) | 1:219:A:VAL:HG21 | 1:238:A:LYS:HD2  | 7        | 0.11          |
| (2,1578) | 1:219:A:VAL:HG21 | 1:238:A:LYS:HD3  | 7        | 0.11          |
| (2,1578) | 1:219:A:VAL:HG22 | 1:238:A:LYS:HD2  | 7        | 0.11          |
| (2,1578) | 1:219:A:VAL:HG22 | 1:238:A:LYS:HD3  | 7        | 0.11          |
| (2,1578) | 1:219:A:VAL:HG23 | 1:238:A:LYS:HD2  | 7        | 0.11          |
| (2,1578) | 1:219:A:VAL:HG23 | 1:238:A:LYS:HD3  | 7        | 0.11          |
| (2,1435) | 1:199:A:VAL:HG11 | 1:200:A:PRO:HG2  | 4        | 0.11          |
| (2,1435) | 1:199:A:VAL:HG12 | 1:200:A:PRO:HG2  | 4        | 0.11          |
| (2,1435) | 1:199:A:VAL:HG13 | 1:200:A:PRO:HG2  | 4        | 0.11          |
| (2,1435) | 1:199:A:VAL:HG21 | 1:200:A:PRO:HG2  | 4        | 0.11          |
| (2,1435) | 1:199:A:VAL:HG22 | 1:200:A:PRO:HG2  | 4        | 0.11          |
| (2,1435) | 1:199:A:VAL:HG23 | 1:200:A:PRO:HG2  | 4        | 0.11          |
| (2,1435) | 1:199:A:VAL:HG11 | 1:200:A:PRO:HG2  | 5        | 0.11          |
| (2,1435) | 1:199:A:VAL:HG12 | 1:200:A:PRO:HG2  | 5        | 0.11          |
| (2,1435) | 1:199:A:VAL:HG13 | 1:200:A:PRO:HG2  | 5        | 0.11          |
| (2,1435) | 1:199:A:VAL:HG21 | 1:200:A:PRO:HG2  | 5        | 0.11          |
| (2,1435) | 1:199:A:VAL:HG22 | 1:200:A:PRO:HG2  | 5        | 0.11          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,1435) | 1:199:A:VAL:HG23 | 1:200:A:PRO:HG2  | 5        | 0.11          |
| (2,1435) | 1:199:A:VAL:HG11 | 1:200:A:PRO:HG2  | 8        | 0.11          |
| (2,1435) | 1:199:A:VAL:HG12 | 1:200:A:PRO:HG2  | 8        | 0.11          |
| (2,1435) | 1:199:A:VAL:HG13 | 1:200:A:PRO:HG2  | 8        | 0.11          |
| (2,1435) | 1:199:A:VAL:HG21 | 1:200:A:PRO:HG2  | 8        | 0.11          |
| (2,1435) | 1:199:A:VAL:HG22 | 1:200:A:PRO:HG2  | 8        | 0.11          |
| (2,1435) | 1:199:A:VAL:HG23 | 1:200:A:PRO:HG2  | 8        | 0.11          |
| (2,1435) | 1:199:A:VAL:HG11 | 1:200:A:PRO:HG2  | 15       | 0.11          |
| (2,1435) | 1:199:A:VAL:HG12 | 1:200:A:PRO:HG2  | 15       | 0.11          |
| (2,1435) | 1:199:A:VAL:HG13 | 1:200:A:PRO:HG2  | 15       | 0.11          |
| (2,1435) | 1:199:A:VAL:HG21 | 1:200:A:PRO:HG2  | 15       | 0.11          |
| (2,1435) | 1:199:A:VAL:HG22 | 1:200:A:PRO:HG2  | 15       | 0.11          |
| (2,1435) | 1:199:A:VAL:HG23 | 1:200:A:PRO:HG2  | 15       | 0.11          |
| (2,1435) | 1:199:A:VAL:HG11 | 1:200:A:PRO:HG2  | 16       | 0.11          |
| (2,1435) | 1:199:A:VAL:HG12 | 1:200:A:PRO:HG2  | 16       | 0.11          |
| (2,1435) | 1:199:A:VAL:HG13 | 1:200:A:PRO:HG2  | 16       | 0.11          |
| (2,1435) | 1:199:A:VAL:HG21 | 1:200:A:PRO:HG2  | 16       | 0.11          |
| (2,1435) | 1:199:A:VAL:HG22 | 1:200:A:PRO:HG2  | 16       | 0.11          |
| (2,1435) | 1:199:A:VAL:HG23 | 1:200:A:PRO:HG2  | 16       | 0.11          |
| (2,1315) | 1:221:A:VAL:HG11 | 1:233:A:LEU:HD11 | 17       | 0.11          |
| (2,1315) | 1:221:A:VAL:HG11 | 1:233:A:LEU:HD12 | 17       | 0.11          |
| (2,1315) | 1:221:A:VAL:HG11 | 1:233:A:LEU:HD13 | 17       | 0.11          |
| (2,1315) | 1:221:A:VAL:HG12 | 1:233:A:LEU:HD11 | 17       | 0.11          |
| (2,1315) | 1:221:A:VAL:HG12 | 1:233:A:LEU:HD12 | 17       | 0.11          |
| (2,1315) | 1:221:A:VAL:HG12 | 1:233:A:LEU:HD13 | 17       | 0.11          |
| (2,1315) | 1:221:A:VAL:HG13 | 1:233:A:LEU:HD11 | 17       | 0.11          |
| (2,1315) | 1:221:A:VAL:HG13 | 1:233:A:LEU:HD12 | 17       | 0.11          |
| (2,1315) | 1:221:A:VAL:HG13 | 1:233:A:LEU:HD13 | 17       | 0.11          |
| (2,1213) | 1:231:A:ARG:HD3  | 1:232:A:LYS:H    | 6        | 0.11          |
| (2,1050) | 1:231:A:ARG:H    | 1:253:A:VAL:HG11 | 14       | 0.11          |
| (2,1050) | 1:231:A:ARG:H    | 1:253:A:VAL:HG12 | 14       | 0.11          |
| (2,1050) | 1:231:A:ARG:H    | 1:253:A:VAL:HG13 | 14       | 0.11          |
| (2,1006) | 1:230:A:GLY:H    | 1:255:A:ILE:HG13 | 1        | 0.11          |
| (2,1006) | 1:230:A:GLY:H    | 1:255:A:ILE:HG13 | 10       | 0.11          |
| (2,1006) | 1:230:A:GLY:H    | 1:255:A:ILE:HG13 | 12       | 0.11          |
| (2,828)  | 1:228:A:GLN:H    | 1:231:A:ARG:HB2  | 7        | 0.11          |
| (2,828)  | 1:228:A:GLN:H    | 1:231:A:ARG:HB2  | 19       | 0.11          |
| (2,773)  | 1:228:A:GLN:HG3  | 1:255:A:ILE:HG21 | 13       | 0.11          |
| (2,773)  | 1:228:A:GLN:HG3  | 1:255:A:ILE:HG22 | 13       | 0.11          |
| (2,773)  | 1:228:A:GLN:HG3  | 1:255:A:ILE:HG23 | 13       | 0.11          |
| (2,773)  | 1:228:A:GLN:HG3  | 1:255:A:ILE:HG21 | 15       | 0.11          |
| (2,773)  | 1:228:A:GLN:HG3  | 1:255:A:ILE:HG22 | 15       | 0.11          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (2,773) | 1:228:A:GLN:HG3  | 1:255:A:ILE:HG23 | 15       | 0.11          |
| (2,773) | 1:228:A:GLN:HG3  | 1:255:A:ILE:HG21 | 19       | 0.11          |
| (2,773) | 1:228:A:GLN:HG3  | 1:255:A:ILE:HG22 | 19       | 0.11          |
| (2,773) | 1:228:A:GLN:HG3  | 1:255:A:ILE:HG23 | 19       | 0.11          |
| (2,739) | 1:225:A:PRO:HB3  | 1:226:A:ARG:HG2  | 6        | 0.11          |
| (2,739) | 1:225:A:PRO:HB3  | 1:226:A:ARG:HG2  | 10       | 0.11          |
| (2,732) | 1:197:A:LEU:HD21 | 1:251:A:LEU:HD11 | 7        | 0.11          |
| (2,732) | 1:197:A:LEU:HD21 | 1:251:A:LEU:HD12 | 7        | 0.11          |
| (2,732) | 1:197:A:LEU:HD21 | 1:251:A:LEU:HD13 | 7        | 0.11          |
| (2,732) | 1:197:A:LEU:HD22 | 1:251:A:LEU:HD11 | 7        | 0.11          |
| (2,732) | 1:197:A:LEU:HD22 | 1:251:A:LEU:HD12 | 7        | 0.11          |
| (2,732) | 1:197:A:LEU:HD22 | 1:251:A:LEU:HD13 | 7        | 0.11          |
| (2,732) | 1:197:A:LEU:HD23 | 1:251:A:LEU:HD11 | 7        | 0.11          |
| (2,732) | 1:197:A:LEU:HD23 | 1:251:A:LEU:HD12 | 7        | 0.11          |
| (2,732) | 1:197:A:LEU:HD23 | 1:251:A:LEU:HD13 | 7        | 0.11          |
| (2,732) | 1:197:A:LEU:HD21 | 1:251:A:LEU:HD11 | 20       | 0.11          |
| (2,732) | 1:197:A:LEU:HD21 | 1:251:A:LEU:HD12 | 20       | 0.11          |
| (2,732) | 1:197:A:LEU:HD21 | 1:251:A:LEU:HD13 | 20       | 0.11          |
| (2,732) | 1:197:A:LEU:HD22 | 1:251:A:LEU:HD11 | 20       | 0.11          |
| (2,732) | 1:197:A:LEU:HD22 | 1:251:A:LEU:HD12 | 20       | 0.11          |
| (2,732) | 1:197:A:LEU:HD22 | 1:251:A:LEU:HD13 | 20       | 0.11          |
| (2,732) | 1:197:A:LEU:HD23 | 1:251:A:LEU:HD11 | 20       | 0.11          |
| (2,732) | 1:197:A:LEU:HD23 | 1:251:A:LEU:HD12 | 20       | 0.11          |
| (2,732) | 1:197:A:LEU:HD23 | 1:251:A:LEU:HD13 | 20       | 0.11          |
| (2,726) | 1:174:A:TYR:HB3  | 1:251:A:LEU:HD11 | 16       | 0.11          |
| (2,726) | 1:174:A:TYR:HB3  | 1:251:A:LEU:HD12 | 16       | 0.11          |
| (2,726) | 1:174:A:TYR:HB3  | 1:251:A:LEU:HD13 | 16       | 0.11          |
| (2,601) | 1:170:A:THR:H    | 1:219:A:VAL:HG21 | 20       | 0.11          |
| (2,601) | 1:170:A:THR:H    | 1:219:A:VAL:HG22 | 20       | 0.11          |
| (2,601) | 1:170:A:THR:H    | 1:219:A:VAL:HG23 | 20       | 0.11          |
| (2,553) | 1:193:A:LEU:HB3  | 1:249:A:LEU:HD21 | 20       | 0.11          |
| (2,553) | 1:193:A:LEU:HB3  | 1:249:A:LEU:HD22 | 20       | 0.11          |
| (2,553) | 1:193:A:LEU:HB3  | 1:249:A:LEU:HD23 | 20       | 0.11          |
| (2,523) | 1:215:A:LEU:HD21 | 1:240:A:PHE:HD2  | 8        | 0.11          |
| (2,523) | 1:215:A:LEU:HD22 | 1:240:A:PHE:HD2  | 8        | 0.11          |
| (2,523) | 1:215:A:LEU:HD23 | 1:240:A:PHE:HD2  | 8        | 0.11          |
| (2,487) | 1:173:A:PHE:H    | 1:175:A:THR:HG21 | 18       | 0.11          |
| (2,487) | 1:173:A:PHE:H    | 1:175:A:THR:HG22 | 18       | 0.11          |
| (2,487) | 1:173:A:PHE:H    | 1:175:A:THR:HG23 | 18       | 0.11          |
| (2,412) | 1:225:A:PRO:HA   | 1:226:A:ARG:HG2  | 19       | 0.11          |
| (2,395) | 1:194:A:TYR:HD2  | 1:195:A:ALA:HB1  | 7        | 0.11          |
| (2,395) | 1:194:A:TYR:HD2  | 1:195:A:ALA:HB2  | 7        | 0.11          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,395)  | 1:194:A:TYR:HD2  | 1:195:A:ALA:HB3  | 7        | 0.11          |
| (2,390)  | 1:196:A:THR:HG21 | 1:252:A:GLU:HA   | 9        | 0.11          |
| (2,390)  | 1:196:A:THR:HG22 | 1:252:A:GLU:HA   | 9        | 0.11          |
| (2,390)  | 1:196:A:THR:HG23 | 1:252:A:GLU:HA   | 9        | 0.11          |
| (2,382)  | 1:198:A:ASP:HA   | 1:254:A:ARG:HB3  | 12       | 0.11          |
| (2,332)  | 1:231:A:ARG:HD3  | 1:253:A:VAL:HG11 | 9        | 0.11          |
| (2,332)  | 1:231:A:ARG:HD3  | 1:253:A:VAL:HG12 | 9        | 0.11          |
| (2,332)  | 1:231:A:ARG:HD3  | 1:253:A:VAL:HG13 | 9        | 0.11          |
| (2,332)  | 1:231:A:ARG:HD3  | 1:253:A:VAL:HG11 | 11       | 0.11          |
| (2,332)  | 1:231:A:ARG:HD3  | 1:253:A:VAL:HG12 | 11       | 0.11          |
| (2,332)  | 1:231:A:ARG:HD3  | 1:253:A:VAL:HG13 | 11       | 0.11          |
| (2,332)  | 1:231:A:ARG:HD3  | 1:253:A:VAL:HG11 | 15       | 0.11          |
| (2,332)  | 1:231:A:ARG:HD3  | 1:253:A:VAL:HG12 | 15       | 0.11          |
| (2,332)  | 1:231:A:ARG:HD3  | 1:253:A:VAL:HG13 | 15       | 0.11          |
| (2,324)  | 1:225:A:PRO:HD2  | 1:226:A:ARG:HG3  | 9        | 0.11          |
| (2,202)  | 1:197:A:LEU:HA   | 1:210:A:VAL:HG11 | 1        | 0.11          |
| (2,202)  | 1:197:A:LEU:HA   | 1:210:A:VAL:HG12 | 1        | 0.11          |
| (2,202)  | 1:197:A:LEU:HA   | 1:210:A:VAL:HG13 | 1        | 0.11          |
| (2,202)  | 1:197:A:LEU:HA   | 1:210:A:VAL:HG11 | 20       | 0.11          |
| (2,202)  | 1:197:A:LEU:HA   | 1:210:A:VAL:HG12 | 20       | 0.11          |
| (2,202)  | 1:197:A:LEU:HA   | 1:210:A:VAL:HG13 | 20       | 0.11          |
| (2,151)  | 1:193:A:LEU:HD21 | 1:194:A:TYR:HB2  | 5        | 0.11          |
| (2,151)  | 1:193:A:LEU:HD22 | 1:194:A:TYR:HB2  | 5        | 0.11          |
| (2,151)  | 1:193:A:LEU:HD23 | 1:194:A:TYR:HB2  | 5        | 0.11          |
| (2,151)  | 1:193:A:LEU:HD21 | 1:194:A:TYR:HB2  | 11       | 0.11          |
| (2,151)  | 1:193:A:LEU:HD22 | 1:194:A:TYR:HB2  | 11       | 0.11          |
| (2,151)  | 1:193:A:LEU:HD23 | 1:194:A:TYR:HB2  | 11       | 0.11          |
| (2,68)   | 1:179:A:ALA:HB1  | 1:226:A:ARG:HB2  | 2        | 0.11          |
| (2,68)   | 1:179:A:ALA:HB2  | 1:226:A:ARG:HB2  | 2        | 0.11          |
| (2,68)   | 1:179:A:ALA:HB3  | 1:226:A:ARG:HB2  | 2        | 0.11          |
| (2,65)   | 1:243:A:PRO:HG3  | 1:247:A:GLY:HA2  | 7        | 0.11          |
| (2,65)   | 1:243:A:PRO:HG3  | 1:247:A:GLY:HA2  | 13       | 0.11          |
| (2,34)   | 1:194:A:TYR:HD2  | 1:249:A:LEU:HD11 | 3        | 0.11          |
| (2,34)   | 1:194:A:TYR:HD2  | 1:249:A:LEU:HD12 | 3        | 0.11          |
| (2,34)   | 1:194:A:TYR:HD2  | 1:249:A:LEU:HD13 | 3        | 0.11          |
| (1,21)   | 1:247:A:GLY:H    | 1:240:A:PHE:O    | 1        | 0.11          |
| (1,21)   | 1:247:A:GLY:H    | 1:240:A:PHE:O    | 5        | 0.11          |
| (2,1684) | 1:172:A:LEU:HG   | 1:219:A:VAL:HG11 | 1        | 0.1           |
| (2,1684) | 1:172:A:LEU:HG   | 1:219:A:VAL:HG12 | 1        | 0.1           |
| (2,1684) | 1:172:A:LEU:HG   | 1:219:A:VAL:HG13 | 1        | 0.1           |
| (2,1684) | 1:172:A:LEU:HG   | 1:219:A:VAL:HG21 | 1        | 0.1           |
| (2,1684) | 1:172:A:LEU:HG   | 1:219:A:VAL:HG22 | 1        | 0.1           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,1684) | 1:172:A:LEU:HG   | 1:219:A:VAL:HG23 | 1        | 0.1           |
| (2,1663) | 1:241:A:PRO:HB2  | 1:245:A:GLY:H    | 11       | 0.1           |
| (2,1663) | 1:241:A:PRO:HB3  | 1:245:A:GLY:H    | 11       | 0.1           |
| (2,1663) | 1:241:A:PRO:HB2  | 1:245:A:GLY:H    | 19       | 0.1           |
| (2,1663) | 1:241:A:PRO:HB3  | 1:245:A:GLY:H    | 19       | 0.1           |
| (2,1653) | 1:236:A:LYS:HD2  | 1:246:A:ARG:HG2  | 20       | 0.1           |
| (2,1653) | 1:236:A:LYS:HD3  | 1:246:A:ARG:HG2  | 20       | 0.1           |
| (2,1651) | 1:236:A:LYS:HD2  | 1:237:A:GLY:H    | 13       | 0.1           |
| (2,1651) | 1:236:A:LYS:HD3  | 1:237:A:GLY:H    | 13       | 0.1           |
| (2,1639) | 1:232:A:LYS:HE2  | 1:252:A:GLU:HA   | 12       | 0.1           |
| (2,1639) | 1:232:A:LYS:HE3  | 1:252:A:GLU:HA   | 12       | 0.1           |
| (2,1633) | 1:232:A:LYS:HG2  | 1:253:A:VAL:H    | 7        | 0.1           |
| (2,1633) | 1:232:A:LYS:HG3  | 1:253:A:VAL:H    | 7        | 0.1           |
| (2,1579) | 1:219:A:VAL:HG21 | 1:238:A:LYS:HE2  | 4        | 0.1           |
| (2,1579) | 1:219:A:VAL:HG21 | 1:238:A:LYS:HE3  | 4        | 0.1           |
| (2,1579) | 1:219:A:VAL:HG22 | 1:238:A:LYS:HE2  | 4        | 0.1           |
| (2,1579) | 1:219:A:VAL:HG22 | 1:238:A:LYS:HE3  | 4        | 0.1           |
| (2,1579) | 1:219:A:VAL:HG23 | 1:238:A:LYS:HE2  | 4        | 0.1           |
| (2,1579) | 1:219:A:VAL:HG23 | 1:238:A:LYS:HE3  | 4        | 0.1           |
| (2,1302) | 1:172:A:LEU:HD11 | 1:175:A:THR:HG21 | 3        | 0.1           |
| (2,1302) | 1:172:A:LEU:HD11 | 1:175:A:THR:HG22 | 3        | 0.1           |
| (2,1302) | 1:172:A:LEU:HD11 | 1:175:A:THR:HG23 | 3        | 0.1           |
| (2,1302) | 1:172:A:LEU:HD12 | 1:175:A:THR:HG21 | 3        | 0.1           |
| (2,1302) | 1:172:A:LEU:HD12 | 1:175:A:THR:HG22 | 3        | 0.1           |
| (2,1302) | 1:172:A:LEU:HD12 | 1:175:A:THR:HG23 | 3        | 0.1           |
| (2,1302) | 1:172:A:LEU:HD13 | 1:175:A:THR:HG21 | 3        | 0.1           |
| (2,1302) | 1:172:A:LEU:HD13 | 1:175:A:THR:HG22 | 3        | 0.1           |
| (2,1302) | 1:172:A:LEU:HD13 | 1:175:A:THR:HG23 | 3        | 0.1           |
| (2,1298) | 1:223:A:VAL:HG21 | 1:224:A:PRO:HG2  | 14       | 0.1           |
| (2,1298) | 1:223:A:VAL:HG22 | 1:224:A:PRO:HG2  | 14       | 0.1           |
| (2,1298) | 1:223:A:VAL:HG23 | 1:224:A:PRO:HG2  | 14       | 0.1           |
| (2,1298) | 1:223:A:VAL:HG21 | 1:224:A:PRO:HG2  | 20       | 0.1           |
| (2,1298) | 1:223:A:VAL:HG22 | 1:224:A:PRO:HG2  | 20       | 0.1           |
| (2,1298) | 1:223:A:VAL:HG23 | 1:224:A:PRO:HG2  | 20       | 0.1           |
| (2,1284) | 1:195:A:ALA:H    | 1:250:A:TYR:HD1  | 15       | 0.1           |
| (2,1262) | 1:205:A:VAL:HG21 | 1:226:A:ARG:H    | 6        | 0.1           |
| (2,1262) | 1:205:A:VAL:HG22 | 1:226:A:ARG:H    | 6        | 0.1           |
| (2,1262) | 1:205:A:VAL:HG23 | 1:226:A:ARG:H    | 6        | 0.1           |
| (2,1050) | 1:231:A:ARG:H    | 1:253:A:VAL:HG11 | 19       | 0.1           |
| (2,1050) | 1:231:A:ARG:H    | 1:253:A:VAL:HG12 | 19       | 0.1           |
| (2,1050) | 1:231:A:ARG:H    | 1:253:A:VAL:HG13 | 19       | 0.1           |
| (2,937)  | 1:250:A:TYR:HD2  | 1:251:A:LEU:H    | 17       | 0.1           |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (2,924) | 1:235:A:LEU:HD21 | 1:236:A:LYS:H    | 19       | 0.1           |
| (2,924) | 1:235:A:LEU:HD22 | 1:236:A:LYS:H    | 19       | 0.1           |
| (2,924) | 1:235:A:LEU:HD23 | 1:236:A:LYS:H    | 19       | 0.1           |
| (2,739) | 1:225:A:PRO:HB3  | 1:226:A:ARG:HG2  | 12       | 0.1           |
| (2,726) | 1:174:A:TYR:HB3  | 1:251:A:LEU:HD11 | 3        | 0.1           |
| (2,726) | 1:174:A:TYR:HB3  | 1:251:A:LEU:HD12 | 3        | 0.1           |
| (2,726) | 1:174:A:TYR:HB3  | 1:251:A:LEU:HD13 | 3        | 0.1           |
| (2,553) | 1:193:A:LEU:HB3  | 1:249:A:LEU:HD21 | 7        | 0.1           |
| (2,553) | 1:193:A:LEU:HB3  | 1:249:A:LEU:HD22 | 7        | 0.1           |
| (2,553) | 1:193:A:LEU:HB3  | 1:249:A:LEU:HD23 | 7        | 0.1           |
| (2,500) | 1:200:A:PRO:HB3  | 1:203:A:ILE:H    | 4        | 0.1           |
| (2,487) | 1:173:A:PHE:H    | 1:175:A:THR:HG21 | 17       | 0.1           |
| (2,487) | 1:173:A:PHE:H    | 1:175:A:THR:HG22 | 17       | 0.1           |
| (2,487) | 1:173:A:PHE:H    | 1:175:A:THR:HG23 | 17       | 0.1           |
| (2,395) | 1:194:A:TYR:HD2  | 1:195:A:ALA:HB1  | 18       | 0.1           |
| (2,395) | 1:194:A:TYR:HD2  | 1:195:A:ALA:HB2  | 18       | 0.1           |
| (2,395) | 1:194:A:TYR:HD2  | 1:195:A:ALA:HB3  | 18       | 0.1           |
| (2,378) | 1:219:A:VAL:HG11 | 1:238:A:LYS:HG3  | 2        | 0.1           |
| (2,378) | 1:219:A:VAL:HG12 | 1:238:A:LYS:HG3  | 2        | 0.1           |
| (2,378) | 1:219:A:VAL:HG13 | 1:238:A:LYS:HG3  | 2        | 0.1           |
| (2,151) | 1:193:A:LEU:HD21 | 1:194:A:TYR:HB2  | 15       | 0.1           |
| (2,151) | 1:193:A:LEU:HD22 | 1:194:A:TYR:HB2  | 15       | 0.1           |
| (2,151) | 1:193:A:LEU:HD23 | 1:194:A:TYR:HB2  | 15       | 0.1           |

## 10 Dihedral-angle violation analysis ⓘ

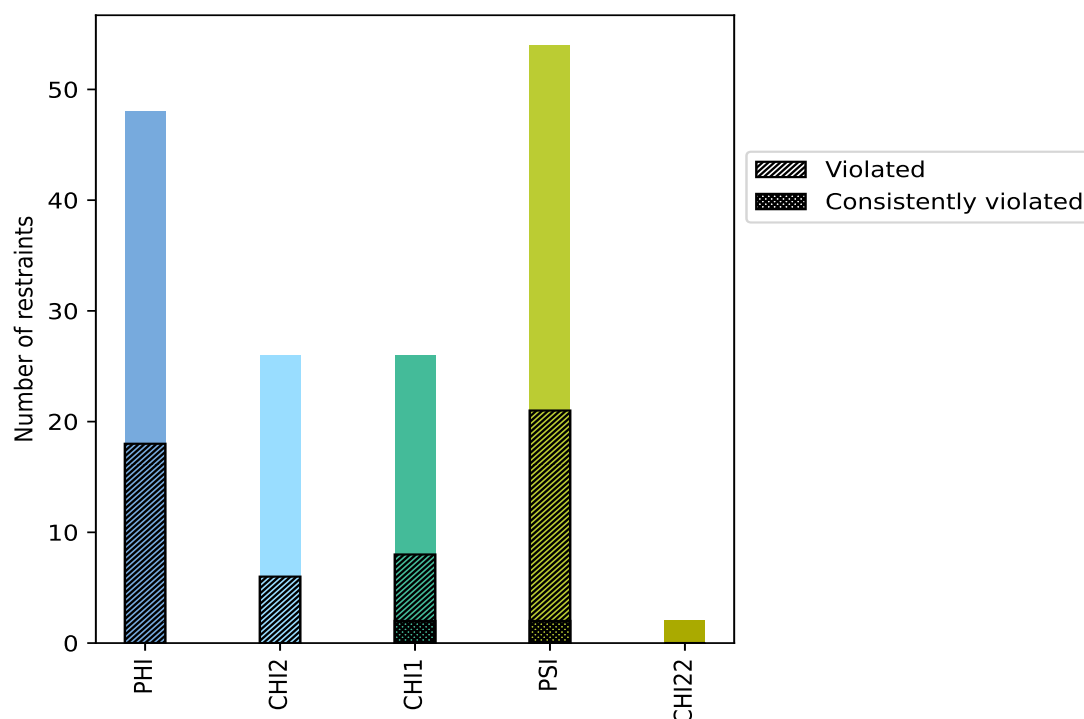
### 10.1 Summary of dihedral-angle violations ⓘ

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        | 48    | 30.8           | 18                    | 37.5           | 11.5           | 0                                  | 0.0            | 0.0            |
| CHI2       | 26    | 16.7           | 6                     | 23.1           | 3.8            | 0                                  | 0.0            | 0.0            |
| CHI1       | 26    | 16.7           | 8                     | 30.8           | 5.1            | 2                                  | 7.7            | 1.3            |
| PSI        | 54    | 34.6           | 21                    | 38.9           | 13.5           | 2                                  | 3.7            | 1.3            |
| CHI22      | 2     | 1.3            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Total      | 156   | 100.0          | 53                    | 34.0           | 34.0           | 4                                  | 2.6            | 2.6            |

<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 ⓘ



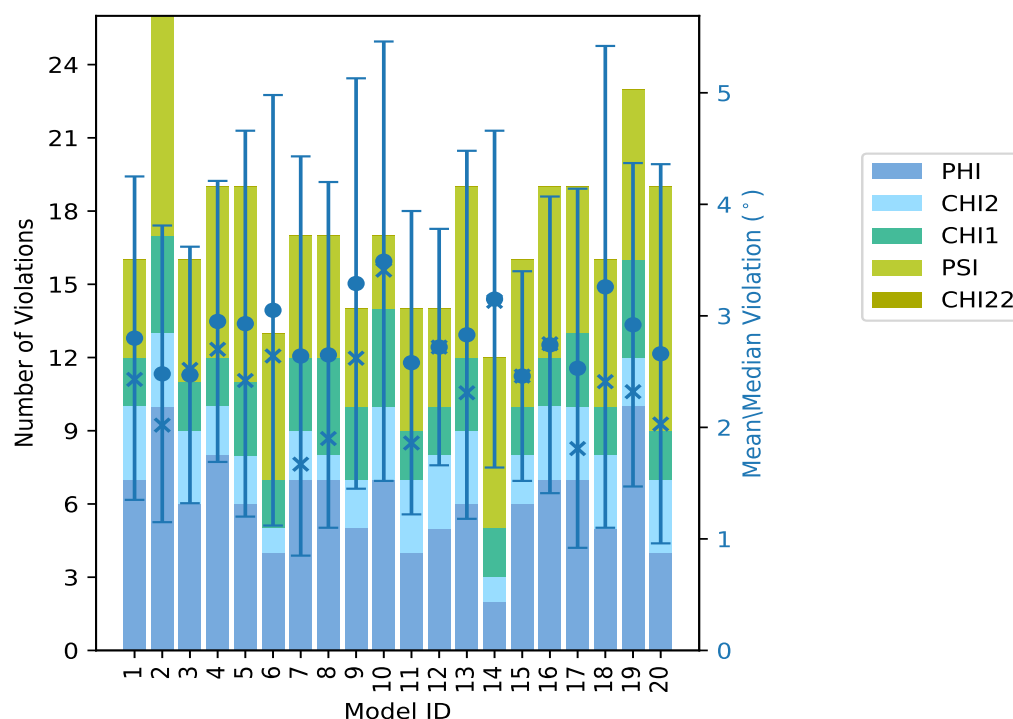
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

## 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                  | CHI2 | CHI1 | PSI | CHI22 | Total |          |         |        |            |
| 1        | 7                    | 3    | 2    | 4   | 0     | 16    | 2.8      | 6.7     | 1.45   | 2.43       |
| 2        | 10                   | 3    | 4    | 9   | 0     | 26    | 2.48     | 5.8     | 1.33   | 2.02       |
| 3        | 6                    | 3    | 2    | 5   | 0     | 16    | 2.47     | 4.65    | 1.15   | 2.52       |
| 4        | 8                    | 2    | 2    | 7   | 0     | 19    | 2.95     | 5.88    | 1.26   | 2.7        |
| 5        | 6                    | 2    | 3    | 8   | 0     | 19    | 2.93     | 7.33    | 1.73   | 2.42       |
| 6        | 4                    | 1    | 2    | 6   | 0     | 13    | 3.05     | 8.43    | 1.93   | 2.64       |
| 7        | 7                    | 2    | 3    | 5   | 0     | 17    | 2.64     | 7.31    | 1.79   | 1.67       |
| 8        | 7                    | 1    | 4    | 5   | 0     | 17    | 2.65     | 5.51    | 1.55   | 1.9        |
| 9        | 5                    | 2    | 3    | 4   | 0     | 14    | 3.29     | 7.31    | 1.84   | 2.62       |
| 10       | 7                    | 3    | 4    | 3   | 0     | 17    | 3.49     | 8.63    | 1.97   | 3.41       |
| 11       | 4                    | 3    | 2    | 5   | 0     | 14    | 2.58     | 5.36    | 1.36   | 1.86       |
| 12       | 5                    | 3    | 2    | 4   | 0     | 14    | 2.72     | 4.37    | 1.06   | 2.72       |
| 13       | 6                    | 3    | 3    | 7   | 0     | 19    | 2.83     | 6.97    | 1.65   | 2.31       |
| 14       | 2                    | 1    | 2    | 7   | 0     | 12    | 3.15     | 6.02    | 1.51   | 3.13       |
| 15       | 6                    | 2    | 2    | 6   | 0     | 16    | 2.46     | 4.74    | 0.94   | 2.46       |
| 16       | 7                    | 3    | 2    | 7   | 0     | 19    | 2.74     | 6.63    | 1.33   | 2.75       |
| 17       | 7                    | 3    | 3    | 6   | 0     | 19    | 2.53     | 7.04    | 1.61   | 1.81       |
| 18       | 5                    | 3    | 2    | 6   | 0     | 16    | 3.26     | 9.62    | 2.16   | 2.41       |
| 19       | 10                   | 2    | 4    | 7   | 0     | 23    | 2.92     | 5.98    | 1.45   | 2.32       |
| 20       | 4                    | 3    | 2    | 10  | 0     | 19    | 2.66     | 7.82    | 1.7    | 2.03       |

### 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                           | CHI2 | CHI1 | PSI | CHI22 | Total | Count <sup>1</sup>       | %    |
| 3                             | 1    | 2    | 5   | 0     | 11    | 1                        | 5.0  |
| 2                             | 0    | 1    | 4   | 0     | 7     | 2                        | 10.0 |
| 1                             | 0    | 3    | 3   | 0     | 7     | 3                        | 15.0 |
| 0                             | 1    | 0    | 2   | 0     | 3     | 4                        | 20.0 |
| 3                             | 1    | 0    | 0   | 0     | 4     | 5                        | 25.0 |
| 2                             | 0    | 0    | 2   | 0     | 4     | 6                        | 30.0 |
| 0                             | 0    | 0    | 0   | 0     | 0     | 7                        | 35.0 |
| 1                             | 1    | 0    | 0   | 0     | 2     | 8                        | 40.0 |
| 1                             | 0    | 0    | 1   | 0     | 2     | 9                        | 45.0 |
| 0                             | 0    | 0    | 0   | 0     | 0     | 10                       | 50.0 |
| 2                             | 1    | 0    | 0   | 0     | 3     | 11                       | 55.0 |

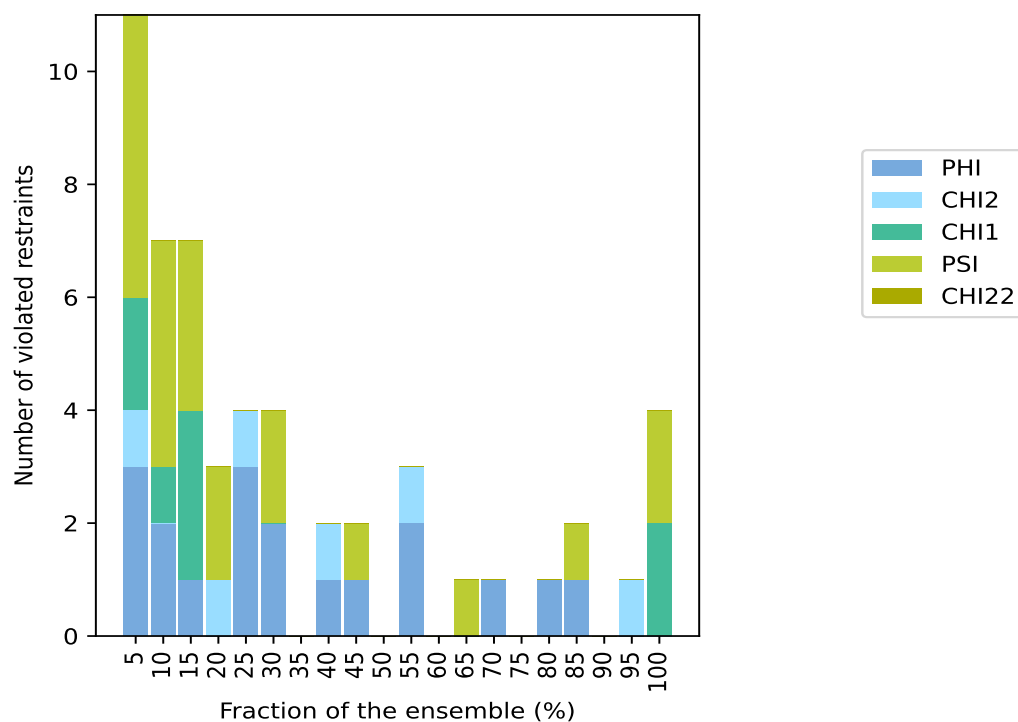
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| Number of violated restraints |      |      |     |       |       | Fraction of the ensemble |       |
|-------------------------------|------|------|-----|-------|-------|--------------------------|-------|
| PHI                           | CHI2 | CHI1 | PSI | CHI22 | Total | Count <sup>1</sup>       | %     |
| 0                             | 0    | 0    | 0   | 0     | 0     | 12                       | 60.0  |
| 0                             | 0    | 0    | 1   | 0     | 1     | 13                       | 65.0  |
| 1                             | 0    | 0    | 0   | 0     | 1     | 14                       | 70.0  |
| 0                             | 0    | 0    | 0   | 0     | 0     | 15                       | 75.0  |
| 1                             | 0    | 0    | 0   | 0     | 1     | 16                       | 80.0  |
| 1                             | 0    | 0    | 1   | 0     | 2     | 17                       | 85.0  |
| 0                             | 0    | 0    | 0   | 0     | 0     | 18                       | 90.0  |
| 0                             | 1    | 0    | 0   | 0     | 1     | 19                       | 95.0  |
| 0                             | 0    | 2    | 2   | 0     | 4     | 20                       | 100.0 |

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

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

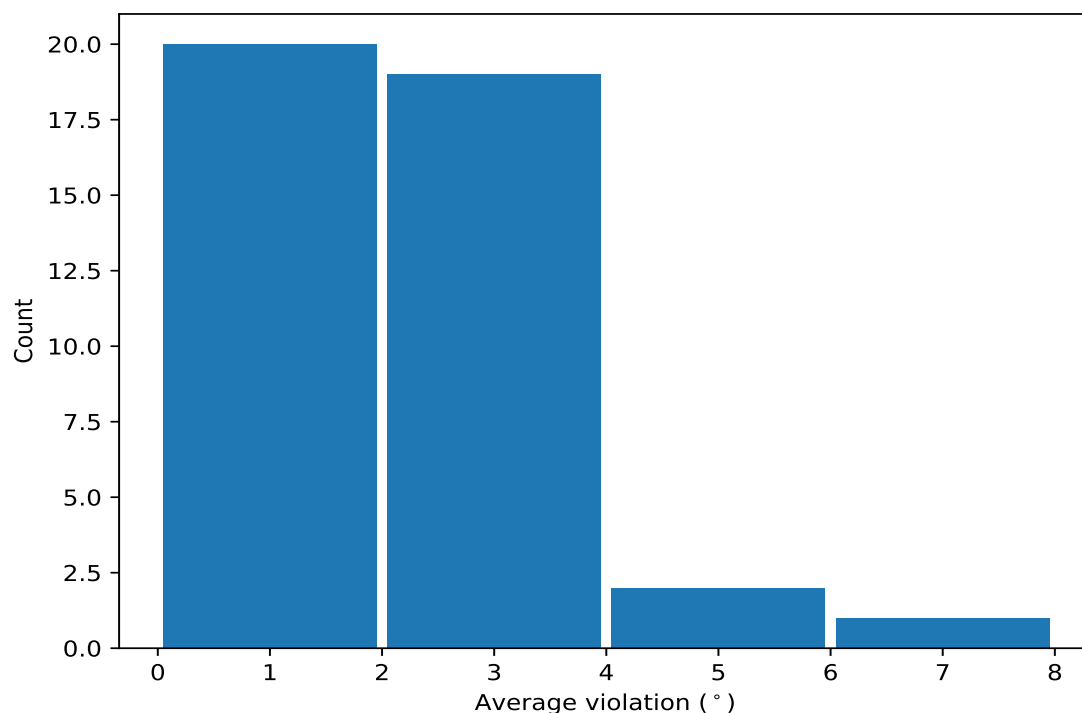


## 10.4 Most violated dihedral-angle restraints in the ensemble [i](#)

### 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 ⓘ

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> | Media |
|---------|----------------|----------------|----------------|-----------------|---------------------|------|-----------------|-------|
| (1,144) | 1:246:A:ARG:N  | 1:246:A:ARG:CA | 1:246:A:ARG:CB | 1:246:A:ARG:CG  | 20                  | 6.47 | 1.58            | 6.66  |
| (1,150) | 1:251:A:LEU:N  | 1:251:A:LEU:CA | 1:251:A:LEU:CB | 1:251:A:LEU:CG  | 20                  | 4.52 | 0.91            | 4.54  |
| (1,50)  | 1:220:A:GLU:N  | 1:220:A:GLU:CA | 1:220:A:GLU:C  | 1:221:A:VAL:N   | 20                  | 3.76 | 1.24            | 3.76  |
| (1,12)  | 1:197:A:LEU:N  | 1:197:A:LEU:CA | 1:197:A:LEU:C  | 1:198:A:ASP:N   | 20                  | 3.59 | 1.06            | 3.38  |
| (1,143) | 1:238:A:LYS:CA | 1:238:A:LYS:CB | 1:238:A:LYS:CG | 1:238:A:LYS:CD  | 19                  | 4.3  | 0.92            | 4.37  |
| (1,94)  | 1:251:A:LEU:N  | 1:251:A:LEU:CA | 1:251:A:LEU:C  | 1:252:A:GLU:N   | 17                  | 2.36 | 1.09            | 2.47  |
| (1,34)  | 1:211:A:ARG:C  | 1:212:A:ALA:N  | 1:212:A:ALA:CA | 1:212:A:ALA:C   | 17                  | 2.3  | 0.68            | 2.2   |
| (1,93)  | 1:250:A:TYR:C  | 1:251:A:LEU:N  | 1:251:A:LEU:CA | 1:251:A:LEU:C   | 16                  | 1.95 | 0.54            | 2.12  |
| (1,11)  | 1:196:A:THR:C  | 1:197:A:LEU:N  | 1:197:A:LEU:CA | 1:197:A:LEU:C   | 14                  | 3.08 | 1.09            | 2.94  |
| (1,84)  | 1:246:A:ARG:N  | 1:246:A:ARG:CA | 1:246:A:ARG:C  | 1:247:A:GLY:N   | 13                  | 2.12 | 0.98            | 1.62  |
| (1,141) | 1:236:A:LYS:CA | 1:236:A:LYS:CB | 1:236:A:LYS:CG | 1:236:A:LYS:CD  | 11                  | 2.41 | 0.95            | 2.09  |
| (1,91)  | 1:249:A:LEU:C  | 1:250:A:TYR:N  | 1:250:A:TYR:CA | 1:250:A:TYR:C   | 11                  | 1.94 | 0.76            | 1.72  |
| (1,28)  | 1:208:A:GLY:C  | 1:209:A:LYS:N  | 1:209:A:LYS:CA | 1:209:A:LYS:C   | 11                  | 1.67 | 0.68            | 1.4   |
| (1,15)  | 1:198:A:ASP:C  | 1:199:A:VAL:N  | 1:199:A:VAL:CA | 1:199:A:VAL:C   | 9                   | 2.11 | 0.47            | 1.95  |
| (1,8)   | 1:195:A:ALA:N  | 1:195:A:ALA:CA | 1:195:A:ALA:C  | 1:196:A:THR:N   | 9                   | 1.67 | 0.47            | 1.6   |
| (1,112) | 1:192:A:ASP:CA | 1:192:A:ASP:CB | 1:192:A:ASP:CG | 1:192:A:ASP:OD1 | 8                   | 2.59 | 0.79            | 2.33  |
| (1,55)  | 1:222:A:ALA:C  | 1:223:A:VAL:N  | 1:223:A:VAL:CA | 1:223:A:VAL:C   | 8                   | 1.56 | 0.52            | 1.46  |
| (1,89)  | 1:248:A:ASP:C  | 1:249:A:LEU:N  | 1:249:A:LEU:CA | 1:249:A:LEU:C   | 6                   | 2.42 | 0.89            | 2.33  |
| (1,48)  | 1:219:A:VAL:N  | 1:219:A:VAL:CA | 1:219:A:VAL:C  | 1:220:A:GLU:N   | 6                   | 2.0  | 0.96            | 1.8   |
| (1,62)  | 1:229:A:ALA:C  | 1:230:A:GLY:N  | 1:230:A:GLY:CA | 1:230:A:GLY:C   | 6                   | 1.73 | 0.54            | 1.81  |

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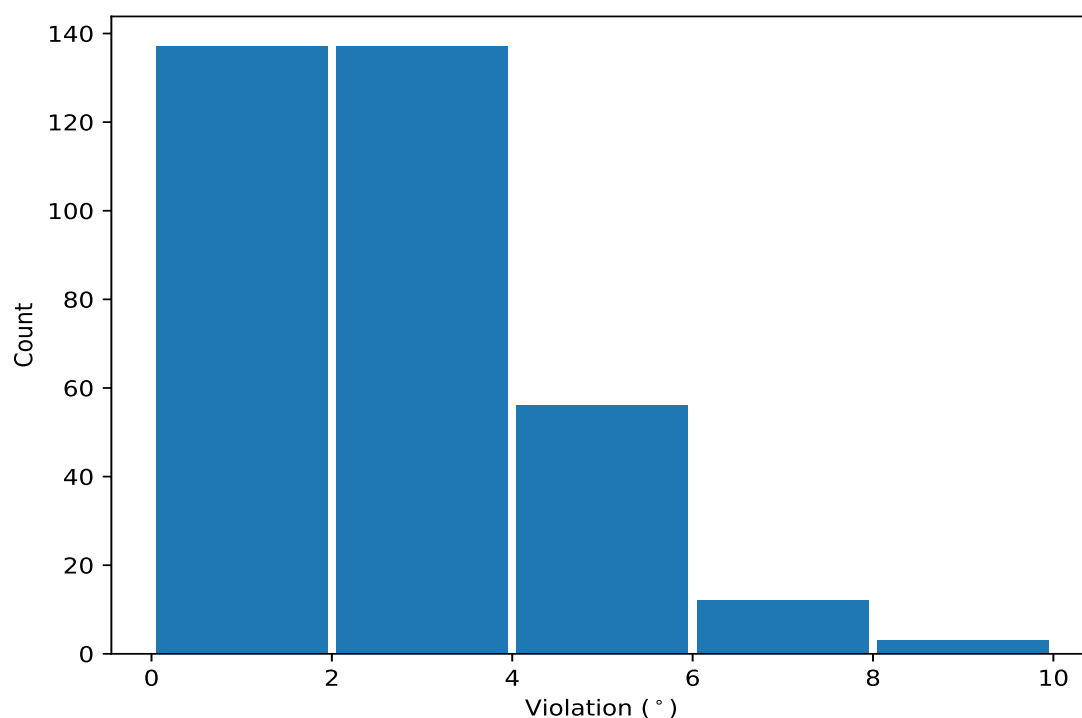
| Key     | Atom-1         | Atom-2         | Atom-3         | Atom-4          | Models <sup>1</sup> | Mean | SD <sup>2</sup> | Media |
|---------|----------------|----------------|----------------|-----------------|---------------------|------|-----------------|-------|
| (1,31)  | 1:210:A:VAL:N  | 1:210:A:VAL:CA | 1:210:A:VAL:C  | 1:211:A:ARG:N   | 6                   | 1.73 | 0.54            | 1.89  |
| (1,83)  | 1:245:A:GLY:C  | 1:246:A:ARG:N  | 1:246:A:ARG:CA | 1:246:A:ARG:C   | 5                   | 2.67 | 0.91            | 3.0   |
| (1,147) | 1:248:A:ASP:CA | 1:248:A:ASP:CB | 1:248:A:ASP:CG | 1:248:A:ASP:OD1 | 5                   | 2.63 | 0.97            | 2.73  |
| (1,1)   | 1:191:A:GLN:C  | 1:192:A:ASP:N  | 1:192:A:ASP:CA | 1:192:A:ASP:C   | 5                   | 1.87 | 0.36            | 1.82  |
| (1,66)  | 1:231:A:ARG:C  | 1:232:A:LYS:N  | 1:232:A:LYS:CA | 1:232:A:LYS:C   | 5                   | 1.67 | 0.49            | 1.5   |
| (1,43)  | 1:216:A:GLU:N  | 1:216:A:GLU:CA | 1:216:A:GLU:C  | 1:217:A:GLY:N   | 4                   | 3.8  | 1.31            | 3.59  |
| (1,107) | 1:173:A:PHE:CA | 1:173:A:PHE:CB | 1:173:A:PHE:CG | 1:173:A:PHE:CD1 | 4                   | 2.3  | 0.68            | 2.44  |
| (1,67)  | 1:232:A:LYS:N  | 1:232:A:LYS:CA | 1:232:A:LYS:C  | 1:233:A:LEU:N   | 4                   | 1.98 | 0.58            | 2.04  |
| (1,88)  | 1:248:A:ASP:N  | 1:248:A:ASP:CA | 1:248:A:ASP:C  | 1:249:A:LEU:N   | 3                   | 1.92 | 0.46            | 2.03  |
| (1,108) | 1:174:A:TYR:N  | 1:174:A:TYR:CA | 1:174:A:TYR:CB | 1:174:A:TYR:CG  | 3                   | 1.74 | 0.41            | 1.47  |
| (1,6)   | 1:194:A:TYR:N  | 1:194:A:TYR:CA | 1:194:A:TYR:C  | 1:195:A:ALA:N   | 3                   | 1.58 | 0.34            | 1.63  |
| (1,104) | 1:172:A:LEU:N  | 1:172:A:LEU:CA | 1:172:A:LEU:CB | 1:172:A:LEU:CG  | 3                   | 1.51 | 0.27            | 1.61  |
| (1,136) | 1:234:A:ARG:N  | 1:234:A:ARG:CA | 1:234:A:ARG:CB | 1:234:A:ARG:CG  | 3                   | 1.5  | 0.34            | 1.47  |
| (1,35)  | 1:212:A:ALA:N  | 1:212:A:ALA:CA | 1:212:A:ALA:C  | 1:213:A:MET:N   | 3                   | 1.3  | 0.06            | 1.29  |
| (1,101) | 1:254:A:ARG:C  | 1:255:A:ILE:N  | 1:255:A:ILE:CA | 1:255:A:ILE:C   | 3                   | 1.12 | 0.09            | 1.17  |
| (1,142) | 1:238:A:LYS:N  | 1:238:A:LYS:CA | 1:238:A:LYS:CB | 1:238:A:LYS:CG  | 2                   | 3.58 | 0.02            | 3.58  |
| (1,3)   | 1:192:A:ASP:C  | 1:193:A:LEU:N  | 1:193:A:LEU:CA | 1:193:A:LEU:C   | 2                   | 2.91 | 1.42            | 2.91  |
| (1,69)  | 1:233:A:LEU:N  | 1:233:A:LEU:CA | 1:233:A:LEU:C  | 1:234:A:ARG:N   | 2                   | 2.12 | 0.48            | 2.12  |
| (1,38)  | 1:213:A:MET:C  | 1:214:A:THR:N  | 1:214:A:THR:CA | 1:214:A:THR:C   | 2                   | 2.0  | 0.74            | 2.0   |
| (1,25)  | 1:205:A:VAL:N  | 1:205:A:VAL:CA | 1:205:A:VAL:C  | 1:206:A:VAL:N   | 2                   | 1.8  | 0.37            | 1.8   |
| (1,71)  | 1:234:A:ARG:N  | 1:234:A:ARG:CA | 1:234:A:ARG:C  | 1:235:A:LEU:N   | 2                   | 1.76 | 0.13            | 1.76  |
| (1,80)  | 1:241:A:PRO:N  | 1:241:A:PRO:CA | 1:241:A:PRO:C  | 1:242:A:GLY:N   | 2                   | 1.66 | 0.55            | 1.66  |

<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 ⓘ

### 10.5.1 Histogram : Distribution of violations ⓘ

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 (°) |
|---------|----------------|----------------|----------------|----------------|----------|---------------|
| (1,144) | 1:246:A:ARG:N  | 1:246:A:ARG:CA | 1:246:A:ARG:CB | 1:246:A:ARG:CG | 18       | 9.62          |
| (1,144) | 1:246:A:ARG:N  | 1:246:A:ARG:CA | 1:246:A:ARG:CB | 1:246:A:ARG:CG | 10       | 8.63          |
| (1,144) | 1:246:A:ARG:N  | 1:246:A:ARG:CA | 1:246:A:ARG:CB | 1:246:A:ARG:CG | 6        | 8.43          |
| (1,144) | 1:246:A:ARG:N  | 1:246:A:ARG:CA | 1:246:A:ARG:CB | 1:246:A:ARG:CG | 20       | 7.82          |
| (1,144) | 1:246:A:ARG:N  | 1:246:A:ARG:CA | 1:246:A:ARG:CB | 1:246:A:ARG:CG | 5        | 7.33          |
| (1,144) | 1:246:A:ARG:N  | 1:246:A:ARG:CA | 1:246:A:ARG:CB | 1:246:A:ARG:CG | 7        | 7.31          |
| (1,144) | 1:246:A:ARG:N  | 1:246:A:ARG:CA | 1:246:A:ARG:CB | 1:246:A:ARG:CG | 9        | 7.31          |
| (1,144) | 1:246:A:ARG:N  | 1:246:A:ARG:CA | 1:246:A:ARG:CB | 1:246:A:ARG:CG | 17       | 7.04          |
| (1,144) | 1:246:A:ARG:N  | 1:246:A:ARG:CA | 1:246:A:ARG:CB | 1:246:A:ARG:CG | 13       | 6.97          |
| (1,144) | 1:246:A:ARG:N  | 1:246:A:ARG:CA | 1:246:A:ARG:CB | 1:246:A:ARG:CG | 1        | 6.7           |
| (1,144) | 1:246:A:ARG:N  | 1:246:A:ARG:CA | 1:246:A:ARG:CB | 1:246:A:ARG:CG | 16       | 6.63          |
| (1,145) | 1:246:A:ARG:CA | 1:246:A:ARG:CB | 1:246:A:ARG:CG | 1:246:A:ARG:CD | 18       | 6.17          |
| (1,50)  | 1:220:A:GLU:N  | 1:220:A:GLU:CA | 1:220:A:GLU:C  | 1:221:A:VAL:N  | 9        | 6.17          |
| (1,12)  | 1:197:A:LEU:N  | 1:197:A:LEU:CA | 1:197:A:LEU:C  | 1:198:A:ASP:N  | 10       | 6.08          |
| (1,150) | 1:251:A:LEU:N  | 1:251:A:LEU:CA | 1:251:A:LEU:CB | 1:251:A:LEU:CG | 14       | 6.02          |
| (1,144) | 1:246:A:ARG:N  | 1:246:A:ARG:CA | 1:246:A:ARG:CB | 1:246:A:ARG:CG | 19       | 5.98          |
| (1,50)  | 1:220:A:GLU:N  | 1:220:A:GLU:CA | 1:220:A:GLU:C  | 1:221:A:VAL:N  | 10       | 5.91          |
| (1,144) | 1:246:A:ARG:N  | 1:246:A:ARG:CA | 1:246:A:ARG:CB | 1:246:A:ARG:CG | 4        | 5.88          |
| (1,150) | 1:251:A:LEU:N  | 1:251:A:LEU:CA | 1:251:A:LEU:CB | 1:251:A:LEU:CG | 18       | 5.8           |
| (1,144) | 1:246:A:ARG:N  | 1:246:A:ARG:CA | 1:246:A:ARG:CB | 1:246:A:ARG:CG | 2        | 5.8           |
| (1,43)  | 1:216:A:GLU:N  | 1:216:A:GLU:CA | 1:216:A:GLU:C  | 1:217:A:GLY:N  | 2        | 5.79          |

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| Key     | Atom-1         | Atom-2         | Atom-3         | Atom-4         | Model ID | Violation (°) |
|---------|----------------|----------------|----------------|----------------|----------|---------------|
| (1,143) | 1:238:A:LYS:CA | 1:238:A:LYS:CB | 1:238:A:LYS:CG | 1:238:A:LYS:CD | 5        | 5.76          |
| (1,150) | 1:251:A:LEU:N  | 1:251:A:LEU:CA | 1:251:A:LEU:CB | 1:251:A:LEU:CG | 7        | 5.74          |
| (1,11)  | 1:196:A:THR:C  | 1:197:A:LEU:N  | 1:197:A:LEU:CA | 1:197:A:LEU:C  | 13       | 5.64          |
| (1,144) | 1:246:A:ARG:N  | 1:246:A:ARG:CA | 1:246:A:ARG:CB | 1:246:A:ARG:CG | 8        | 5.51          |
| (1,150) | 1:251:A:LEU:N  | 1:251:A:LEU:CA | 1:251:A:LEU:CB | 1:251:A:LEU:CG | 5        | 5.49          |
| (1,50)  | 1:220:A:GLU:N  | 1:220:A:GLU:CA | 1:220:A:GLU:C  | 1:221:A:VAL:N  | 20       | 5.44          |
| (1,143) | 1:238:A:LYS:CA | 1:238:A:LYS:CB | 1:238:A:LYS:CG | 1:238:A:LYS:CD | 4        | 5.43          |
| (1,150) | 1:251:A:LEU:N  | 1:251:A:LEU:CA | 1:251:A:LEU:CB | 1:251:A:LEU:CG | 8        | 5.41          |
| (1,143) | 1:238:A:LYS:CA | 1:238:A:LYS:CB | 1:238:A:LYS:CG | 1:238:A:LYS:CD | 2        | 5.4           |
| (1,143) | 1:238:A:LYS:CA | 1:238:A:LYS:CB | 1:238:A:LYS:CG | 1:238:A:LYS:CD | 13       | 5.4           |
| (1,144) | 1:246:A:ARG:N  | 1:246:A:ARG:CA | 1:246:A:ARG:CB | 1:246:A:ARG:CG | 11       | 5.36          |
| (1,94)  | 1:251:A:LEU:N  | 1:251:A:LEU:CA | 1:251:A:LEU:C  | 1:252:A:GLU:N  | 19       | 5.29          |
| (1,144) | 1:246:A:ARG:N  | 1:246:A:ARG:CA | 1:246:A:ARG:CB | 1:246:A:ARG:CG | 14       | 5.24          |
| (1,150) | 1:251:A:LEU:N  | 1:251:A:LEU:CA | 1:251:A:LEU:CB | 1:251:A:LEU:CG | 9        | 5.22          |
| (1,150) | 1:251:A:LEU:N  | 1:251:A:LEU:CA | 1:251:A:LEU:CB | 1:251:A:LEU:CG | 19       | 5.16          |
| (1,143) | 1:238:A:LYS:CA | 1:238:A:LYS:CB | 1:238:A:LYS:CG | 1:238:A:LYS:CD | 19       | 5.1           |
| (1,143) | 1:238:A:LYS:CA | 1:238:A:LYS:CB | 1:238:A:LYS:CG | 1:238:A:LYS:CD | 8        | 5.01          |
| (1,12)  | 1:197:A:LEU:N  | 1:197:A:LEU:CA | 1:197:A:LEU:C  | 1:198:A:ASP:N  | 16       | 4.97          |
| (1,143) | 1:238:A:LYS:CA | 1:238:A:LYS:CB | 1:238:A:LYS:CG | 1:238:A:LYS:CD | 10       | 4.96          |
| (1,50)  | 1:220:A:GLU:N  | 1:220:A:GLU:CA | 1:220:A:GLU:C  | 1:221:A:VAL:N  | 6        | 4.91          |
| (1,11)  | 1:196:A:THR:C  | 1:197:A:LEU:N  | 1:197:A:LEU:CA | 1:197:A:LEU:C  | 7        | 4.86          |
| (1,12)  | 1:197:A:LEU:N  | 1:197:A:LEU:CA | 1:197:A:LEU:C  | 1:198:A:ASP:N  | 20       | 4.85          |
| (1,150) | 1:251:A:LEU:N  | 1:251:A:LEU:CA | 1:251:A:LEU:CB | 1:251:A:LEU:CG | 13       | 4.74          |
| (1,144) | 1:246:A:ARG:N  | 1:246:A:ARG:CA | 1:246:A:ARG:CB | 1:246:A:ARG:CG | 15       | 4.74          |
| (1,12)  | 1:197:A:LEU:N  | 1:197:A:LEU:CA | 1:197:A:LEU:C  | 1:198:A:ASP:N  | 17       | 4.71          |
| (1,144) | 1:246:A:ARG:N  | 1:246:A:ARG:CA | 1:246:A:ARG:CB | 1:246:A:ARG:CG | 3        | 4.65          |
| (1,150) | 1:251:A:LEU:N  | 1:251:A:LEU:CA | 1:251:A:LEU:CB | 1:251:A:LEU:CG | 1        | 4.63          |
| (1,12)  | 1:197:A:LEU:N  | 1:197:A:LEU:CA | 1:197:A:LEU:C  | 1:198:A:ASP:N  | 19       | 4.62          |
| (1,50)  | 1:220:A:GLU:N  | 1:220:A:GLU:CA | 1:220:A:GLU:C  | 1:221:A:VAL:N  | 17       | 4.6           |
| (1,50)  | 1:220:A:GLU:N  | 1:220:A:GLU:CA | 1:220:A:GLU:C  | 1:221:A:VAL:N  | 8        | 4.57          |
| (1,150) | 1:251:A:LEU:N  | 1:251:A:LEU:CA | 1:251:A:LEU:CB | 1:251:A:LEU:CG | 11       | 4.55          |
| (1,150) | 1:251:A:LEU:N  | 1:251:A:LEU:CA | 1:251:A:LEU:CB | 1:251:A:LEU:CG | 20       | 4.54          |
| (1,12)  | 1:197:A:LEU:N  | 1:197:A:LEU:CA | 1:197:A:LEU:C  | 1:198:A:ASP:N  | 14       | 4.54          |
| (1,143) | 1:238:A:LYS:CA | 1:238:A:LYS:CB | 1:238:A:LYS:CG | 1:238:A:LYS:CD | 11       | 4.5           |
| (1,143) | 1:238:A:LYS:CA | 1:238:A:LYS:CB | 1:238:A:LYS:CG | 1:238:A:LYS:CD | 9        | 4.4           |
| (1,143) | 1:238:A:LYS:CA | 1:238:A:LYS:CB | 1:238:A:LYS:CG | 1:238:A:LYS:CD | 7        | 4.37          |
| (1,12)  | 1:197:A:LEU:N  | 1:197:A:LEU:CA | 1:197:A:LEU:C  | 1:198:A:ASP:N  | 12       | 4.37          |
| (1,3)   | 1:192:A:ASP:C  | 1:193:A:LEU:N  | 1:193:A:LEU:CA | 1:193:A:LEU:C  | 5        | 4.33          |
| (1,84)  | 1:246:A:ARG:N  | 1:246:A:ARG:CA | 1:246:A:ARG:C  | 1:247:A:GLY:N  | 9        | 4.31          |
| (1,50)  | 1:220:A:GLU:N  | 1:220:A:GLU:CA | 1:220:A:GLU:C  | 1:221:A:VAL:N  | 1        | 4.31          |
| (1,150) | 1:251:A:LEU:N  | 1:251:A:LEU:CA | 1:251:A:LEU:CB | 1:251:A:LEU:CG | 6        | 4.26          |
| (1,150) | 1:251:A:LEU:N  | 1:251:A:LEU:CA | 1:251:A:LEU:CB | 1:251:A:LEU:CG | 3        | 4.22          |
| (1,143) | 1:238:A:LYS:CA | 1:238:A:LYS:CB | 1:238:A:LYS:CG | 1:238:A:LYS:CD | 14       | 4.21          |
| (1,150) | 1:251:A:LEU:N  | 1:251:A:LEU:CA | 1:251:A:LEU:CB | 1:251:A:LEU:CG | 12       | 4.2           |
| (1,50)  | 1:220:A:GLU:N  | 1:220:A:GLU:CA | 1:220:A:GLU:C  | 1:221:A:VAL:N  | 5        | 4.14          |
| (1,50)  | 1:220:A:GLU:N  | 1:220:A:GLU:CA | 1:220:A:GLU:C  | 1:221:A:VAL:N  | 4        | 4.11          |
| (1,143) | 1:238:A:LYS:CA | 1:238:A:LYS:CB | 1:238:A:LYS:CG | 1:238:A:LYS:CD | 16       | 4.07          |
| (1,94)  | 1:251:A:LEU:N  | 1:251:A:LEU:CA | 1:251:A:LEU:C  | 1:252:A:GLU:N  | 12       | 4.07          |
| (1,11)  | 1:196:A:THR:C  | 1:197:A:LEU:N  | 1:197:A:LEU:CA | 1:197:A:LEU:C  | 10       | 4.06          |
| (1,43)  | 1:216:A:GLU:N  | 1:216:A:GLU:CA | 1:216:A:GLU:C  | 1:217:A:GLY:N  | 4        | 4.02          |
| (1,141) | 1:236:A:LYS:CA | 1:236:A:LYS:CB | 1:236:A:LYS:CG | 1:236:A:LYS:CD | 10       | 3.97          |

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| Key     | Atom-1         | Atom-2         | Atom-3         | Atom-4          | Model ID | Violation (°) |
|---------|----------------|----------------|----------------|-----------------|----------|---------------|
| (1,150) | 1:251:A:LEU:N  | 1:251:A:LEU:CA | 1:251:A:LEU:CB | 1:251:A:LEU:CG  | 4        | 3.92          |
| (1,89)  | 1:248:A:ASP:C  | 1:249:A:LEU:N  | 1:249:A:LEU:CA | 1:249:A:LEU:C   | 6        | 3.92          |
| (1,48)  | 1:219:A:VAL:N  | 1:219:A:VAL:CA | 1:219:A:VAL:C  | 1:220:A:GLU:N   | 19       | 3.91          |
| (1,147) | 1:248:A:ASP:CA | 1:248:A:ASP:CB | 1:248:A:ASP:CG | 1:248:A:ASP:OD1 | 5        | 3.9           |
| (1,50)  | 1:220:A:GLU:N  | 1:220:A:GLU:CA | 1:220:A:GLU:C  | 1:221:A:VAL:N   | 18       | 3.89          |
| (1,83)  | 1:245:A:GLY:C  | 1:246:A:ARG:N  | 1:246:A:ARG:CA | 1:246:A:ARG:C   | 1        | 3.86          |
| (1,143) | 1:238:A:LYS:CA | 1:238:A:LYS:CB | 1:238:A:LYS:CG | 1:238:A:LYS:CD  | 12       | 3.84          |
| (1,112) | 1:192:A:ASP:CA | 1:192:A:ASP:CB | 1:192:A:ASP:CG | 1:192:A:ASP:OD1 | 17       | 3.82          |
| (1,141) | 1:236:A:LYS:CA | 1:236:A:LYS:CB | 1:236:A:LYS:CG | 1:236:A:LYS:CD  | 17       | 3.81          |
| (1,150) | 1:251:A:LEU:N  | 1:251:A:LEU:CA | 1:251:A:LEU:CB | 1:251:A:LEU:CG  | 2        | 3.73          |
| (1,12)  | 1:197:A:LEU:N  | 1:197:A:LEU:CA | 1:197:A:LEU:C  | 1:198:A:ASP:N   | 8        | 3.69          |
| (1,143) | 1:238:A:LYS:CA | 1:238:A:LYS:CB | 1:238:A:LYS:CG | 1:238:A:LYS:CD  | 1        | 3.63          |
| (1,143) | 1:238:A:LYS:CA | 1:238:A:LYS:CB | 1:238:A:LYS:CG | 1:238:A:LYS:CD  | 18       | 3.63          |
| (1,50)  | 1:220:A:GLU:N  | 1:220:A:GLU:CA | 1:220:A:GLU:C  | 1:221:A:VAL:N   | 19       | 3.62          |
| (1,142) | 1:238:A:LYS:N  | 1:238:A:LYS:CA | 1:238:A:LYS:CB | 1:238:A:LYS:CG  | 2        | 3.6           |
| (1,142) | 1:238:A:LYS:N  | 1:238:A:LYS:CA | 1:238:A:LYS:CB | 1:238:A:LYS:CG  | 19       | 3.57          |
| (1,84)  | 1:246:A:ARG:N  | 1:246:A:ARG:CA | 1:246:A:ARG:C  | 1:247:A:GLY:N   | 4        | 3.57          |
| (1,12)  | 1:197:A:LEU:N  | 1:197:A:LEU:CA | 1:197:A:LEU:C  | 1:198:A:ASP:N   | 15       | 3.57          |
| (1,112) | 1:192:A:ASP:CA | 1:192:A:ASP:CB | 1:192:A:ASP:CG | 1:192:A:ASP:OD1 | 10       | 3.54          |
| (1,143) | 1:238:A:LYS:CA | 1:238:A:LYS:CB | 1:238:A:LYS:CG | 1:238:A:LYS:CD  | 3        | 3.51          |
| (1,34)  | 1:211:A:ARG:C  | 1:212:A:ALA:N  | 1:212:A:ALA:CA | 1:212:A:ALA:C   | 19       | 3.5           |
| (1,150) | 1:251:A:LEU:N  | 1:251:A:LEU:CA | 1:251:A:LEU:CB | 1:251:A:LEU:CG  | 10       | 3.49          |
| (1,12)  | 1:197:A:LEU:N  | 1:197:A:LEU:CA | 1:197:A:LEU:C  | 1:198:A:ASP:N   | 11       | 3.45          |
| (1,147) | 1:248:A:ASP:CA | 1:248:A:ASP:CB | 1:248:A:ASP:CG | 1:248:A:ASP:OD1 | 13       | 3.44          |
| (1,34)  | 1:211:A:ARG:C  | 1:212:A:ALA:N  | 1:212:A:ALA:CA | 1:212:A:ALA:C   | 10       | 3.41          |
| (1,50)  | 1:220:A:GLU:N  | 1:220:A:GLU:CA | 1:220:A:GLU:C  | 1:221:A:VAL:N   | 15       | 3.32          |
| (1,141) | 1:236:A:LYS:CA | 1:236:A:LYS:CB | 1:236:A:LYS:CG | 1:236:A:LYS:CD  | 4        | 3.31          |
| (1,12)  | 1:197:A:LEU:N  | 1:197:A:LEU:CA | 1:197:A:LEU:C  | 1:198:A:ASP:N   | 18       | 3.3           |
| (1,28)  | 1:208:A:GLY:C  | 1:209:A:LYS:N  | 1:209:A:LYS:CA | 1:209:A:LYS:C   | 8        | 3.29          |
| (1,83)  | 1:245:A:GLY:C  | 1:246:A:ARG:N  | 1:246:A:ARG:CA | 1:246:A:ARG:C   | 3        | 3.28          |
| (1,112) | 1:192:A:ASP:CA | 1:192:A:ASP:CB | 1:192:A:ASP:CG | 1:192:A:ASP:OD1 | 3        | 3.27          |
| (1,143) | 1:238:A:LYS:CA | 1:238:A:LYS:CB | 1:238:A:LYS:CG | 1:238:A:LYS:CD  | 17       | 3.26          |
| (1,11)  | 1:196:A:THR:C  | 1:197:A:LEU:N  | 1:197:A:LEU:CA | 1:197:A:LEU:C   | 11       | 3.25          |
| (1,11)  | 1:196:A:THR:C  | 1:197:A:LEU:N  | 1:197:A:LEU:CA | 1:197:A:LEU:C   | 14       | 3.25          |
| (1,150) | 1:251:A:LEU:N  | 1:251:A:LEU:CA | 1:251:A:LEU:CB | 1:251:A:LEU:CG  | 15       | 3.2           |
| (1,94)  | 1:251:A:LEU:N  | 1:251:A:LEU:CA | 1:251:A:LEU:C  | 1:252:A:GLU:N   | 16       | 3.19          |
| (1,141) | 1:236:A:LYS:CA | 1:236:A:LYS:CB | 1:236:A:LYS:CG | 1:236:A:LYS:CD  | 6        | 3.17          |
| (1,94)  | 1:251:A:LEU:N  | 1:251:A:LEU:CA | 1:251:A:LEU:C  | 1:252:A:GLU:N   | 5        | 3.16          |
| (1,43)  | 1:216:A:GLU:N  | 1:216:A:GLU:CA | 1:216:A:GLU:C  | 1:217:A:GLY:N   | 14       | 3.16          |
| (1,50)  | 1:220:A:GLU:N  | 1:220:A:GLU:CA | 1:220:A:GLU:C  | 1:221:A:VAL:N   | 3        | 3.11          |
| (1,84)  | 1:246:A:ARG:N  | 1:246:A:ARG:CA | 1:246:A:ARG:C  | 1:247:A:GLY:N   | 14       | 3.1           |
| (1,91)  | 1:249:A:LEU:C  | 1:250:A:TYR:N  | 1:250:A:TYR:CA | 1:250:A:TYR:C   | 16       | 3.09          |
| (1,15)  | 1:198:A:ASP:C  | 1:199:A:VAL:N  | 1:199:A:VAL:CA | 1:199:A:VAL:C   | 3        | 3.09          |
| (1,34)  | 1:211:A:ARG:C  | 1:212:A:ALA:N  | 1:212:A:ALA:CA | 1:212:A:ALA:C   | 16       | 3.07          |
| (1,34)  | 1:211:A:ARG:C  | 1:212:A:ALA:N  | 1:212:A:ALA:CA | 1:212:A:ALA:C   | 2        | 3.06          |
| (1,11)  | 1:196:A:THR:C  | 1:197:A:LEU:N  | 1:197:A:LEU:CA | 1:197:A:LEU:C   | 12       | 3.06          |
| (1,91)  | 1:249:A:LEU:C  | 1:250:A:TYR:N  | 1:250:A:TYR:CA | 1:250:A:TYR:C   | 13       | 3.04          |
| (1,150) | 1:251:A:LEU:N  | 1:251:A:LEU:CA | 1:251:A:LEU:CB | 1:251:A:LEU:CG  | 16       | 3.02          |
| (1,150) | 1:251:A:LEU:N  | 1:251:A:LEU:CA | 1:251:A:LEU:CB | 1:251:A:LEU:CG  | 17       | 3.02          |
| (1,107) | 1:173:A:PHE:CA | 1:173:A:PHE:CB | 1:173:A:PHE:CG | 1:173:A:PHE:CD1 | 12       | 3.01          |
| (1,83)  | 1:245:A:GLY:C  | 1:246:A:ARG:N  | 1:246:A:ARG:CA | 1:246:A:ARG:C   | 16       | 3.0           |

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| Key     | Atom-1         | Atom-2         | Atom-3         | Atom-4          | Model ID | Violation (°) |
|---------|----------------|----------------|----------------|-----------------|----------|---------------|
| (1,93)  | 1:250:A:TYR:C  | 1:251:A:LEU:N  | 1:251:A:LEU:CA | 1:251:A:LEU:C   | 10       | 2.97          |
| (1,50)  | 1:220:A:GLU:N  | 1:220:A:GLU:CA | 1:220:A:GLU:C  | 1:221:A:VAL:N   | 12       | 2.96          |
| (1,12)  | 1:197:A:LEU:N  | 1:197:A:LEU:CA | 1:197:A:LEU:C  | 1:198:A:ASP:N   | 7        | 2.95          |
| (1,11)  | 1:196:A:THR:C  | 1:197:A:LEU:N  | 1:197:A:LEU:CA | 1:197:A:LEU:C   | 4        | 2.95          |
| (1,11)  | 1:196:A:THR:C  | 1:197:A:LEU:N  | 1:197:A:LEU:CA | 1:197:A:LEU:C   | 18       | 2.94          |
| (1,89)  | 1:248:A:ASP:C  | 1:249:A:LEU:N  | 1:249:A:LEU:CA | 1:249:A:LEU:C   | 4        | 2.93          |
| (1,50)  | 1:220:A:GLU:N  | 1:220:A:GLU:CA | 1:220:A:GLU:C  | 1:221:A:VAL:N   | 13       | 2.93          |
| (1,34)  | 1:211:A:ARG:C  | 1:212:A:ALA:N  | 1:212:A:ALA:CA | 1:212:A:ALA:C   | 3        | 2.93          |
| (1,50)  | 1:220:A:GLU:N  | 1:220:A:GLU:CA | 1:220:A:GLU:C  | 1:221:A:VAL:N   | 7        | 2.9           |
| (1,11)  | 1:196:A:THR:C  | 1:197:A:LEU:N  | 1:197:A:LEU:CA | 1:197:A:LEU:C   | 19       | 2.88          |
| (1,107) | 1:173:A:PHE:CA | 1:173:A:PHE:CB | 1:173:A:PHE:CG | 1:173:A:PHE:CD1 | 15       | 2.87          |
| (1,12)  | 1:197:A:LEU:N  | 1:197:A:LEU:CA | 1:197:A:LEU:C  | 1:198:A:ASP:N   | 6        | 2.86          |
| (1,34)  | 1:211:A:ARG:C  | 1:212:A:ALA:N  | 1:212:A:ALA:CA | 1:212:A:ALA:C   | 1        | 2.83          |
| (1,55)  | 1:222:A:ALA:C  | 1:223:A:VAL:N  | 1:223:A:VAL:CA | 1:223:A:VAL:C   | 9        | 2.81          |
| (1,12)  | 1:197:A:LEU:N  | 1:197:A:LEU:CA | 1:197:A:LEU:C  | 1:198:A:ASP:N   | 13       | 2.81          |
| (1,89)  | 1:248:A:ASP:C  | 1:249:A:LEU:N  | 1:249:A:LEU:CA | 1:249:A:LEU:C   | 9        | 2.79          |
| (1,143) | 1:238:A:LYS:CA | 1:238:A:LYS:CB | 1:238:A:LYS:CG | 1:238:A:LYS:CD  | 15       | 2.77          |
| (1,50)  | 1:220:A:GLU:N  | 1:220:A:GLU:CA | 1:220:A:GLU:C  | 1:221:A:VAL:N   | 16       | 2.77          |
| (1,67)  | 1:232:A:LYS:N  | 1:232:A:LYS:CA | 1:232:A:LYS:C  | 1:233:A:LEU:N   | 15       | 2.75          |
| (1,28)  | 1:208:A:GLY:C  | 1:209:A:LYS:N  | 1:209:A:LYS:CA | 1:209:A:LYS:C   | 16       | 2.75          |
| (1,91)  | 1:249:A:LEU:C  | 1:250:A:TYR:N  | 1:250:A:TYR:CA | 1:250:A:TYR:C   | 11       | 2.74          |
| (1,38)  | 1:213:A:MET:C  | 1:214:A:THR:N  | 1:214:A:THR:CA | 1:214:A:THR:C   | 2        | 2.74          |
| (1,147) | 1:248:A:ASP:CA | 1:248:A:ASP:CB | 1:248:A:ASP:CG | 1:248:A:ASP:OD1 | 20       | 2.73          |
| (1,12)  | 1:197:A:LEU:N  | 1:197:A:LEU:CA | 1:197:A:LEU:C  | 1:198:A:ASP:N   | 4        | 2.7           |
| (1,8)   | 1:195:A:ALA:N  | 1:195:A:ALA:CA | 1:195:A:ALA:C  | 1:196:A:THR:N   | 19       | 2.7           |
| (1,94)  | 1:251:A:LEU:N  | 1:251:A:LEU:CA | 1:251:A:LEU:C  | 1:252:A:GLU:N   | 6        | 2.64          |
| (1,84)  | 1:246:A:ARG:N  | 1:246:A:ARG:CA | 1:246:A:ARG:C  | 1:247:A:GLY:N   | 2        | 2.64          |
| (1,62)  | 1:229:A:ALA:C  | 1:230:A:GLY:N  | 1:230:A:GLY:CA | 1:230:A:GLY:C   | 1        | 2.64          |
| (1,15)  | 1:198:A:ASP:C  | 1:199:A:VAL:N  | 1:199:A:VAL:CA | 1:199:A:VAL:C   | 4        | 2.63          |
| (1,12)  | 1:197:A:LEU:N  | 1:197:A:LEU:CA | 1:197:A:LEU:C  | 1:198:A:ASP:N   | 2        | 2.63          |
| (1,12)  | 1:197:A:LEU:N  | 1:197:A:LEU:CA | 1:197:A:LEU:C  | 1:198:A:ASP:N   | 5        | 2.63          |
| (1,66)  | 1:231:A:ARG:C  | 1:232:A:LYS:N  | 1:232:A:LYS:CA | 1:232:A:LYS:C   | 10       | 2.62          |
| (1,69)  | 1:233:A:LEU:N  | 1:233:A:LEU:CA | 1:233:A:LEU:C  | 1:234:A:ARG:N   | 10       | 2.61          |
| (1,94)  | 1:251:A:LEU:N  | 1:251:A:LEU:CA | 1:251:A:LEU:C  | 1:252:A:GLU:N   | 18       | 2.59          |
| (1,84)  | 1:246:A:ARG:N  | 1:246:A:ARG:CA | 1:246:A:ARG:C  | 1:247:A:GLY:N   | 17       | 2.57          |
| (1,91)  | 1:249:A:LEU:C  | 1:250:A:TYR:N  | 1:250:A:TYR:CA | 1:250:A:TYR:C   | 20       | 2.52          |
| (1,93)  | 1:250:A:TYR:C  | 1:251:A:LEU:N  | 1:251:A:LEU:CA | 1:251:A:LEU:C   | 5        | 2.5           |
| (1,93)  | 1:250:A:TYR:C  | 1:251:A:LEU:N  | 1:251:A:LEU:CA | 1:251:A:LEU:C   | 13       | 2.5           |
| (1,143) | 1:238:A:LYS:CA | 1:238:A:LYS:CB | 1:238:A:LYS:CG | 1:238:A:LYS:CD  | 20       | 2.48          |
| (1,94)  | 1:251:A:LEU:N  | 1:251:A:LEU:CA | 1:251:A:LEU:C  | 1:252:A:GLU:N   | 8        | 2.48          |
| (1,94)  | 1:251:A:LEU:N  | 1:251:A:LEU:CA | 1:251:A:LEU:C  | 1:252:A:GLU:N   | 15       | 2.48          |
| (1,144) | 1:246:A:ARG:N  | 1:246:A:ARG:CA | 1:246:A:ARG:CB | 1:246:A:ARG:CG  | 12       | 2.47          |
| (1,94)  | 1:251:A:LEU:N  | 1:251:A:LEU:CA | 1:251:A:LEU:C  | 1:252:A:GLU:N   | 4        | 2.47          |
| (1,12)  | 1:197:A:LEU:N  | 1:197:A:LEU:CA | 1:197:A:LEU:C  | 1:198:A:ASP:N   | 9        | 2.45          |
| (1,31)  | 1:210:A:VAL:N  | 1:210:A:VAL:CA | 1:210:A:VAL:C  | 1:211:A:ARG:N   | 1        | 2.44          |
| (1,11)  | 1:196:A:THR:C  | 1:197:A:LEU:N  | 1:197:A:LEU:CA | 1:197:A:LEU:C   | 15       | 2.44          |
| (1,112) | 1:192:A:ASP:CA | 1:192:A:ASP:CB | 1:192:A:ASP:CG | 1:192:A:ASP:OD1 | 16       | 2.43          |
| (1,34)  | 1:211:A:ARG:C  | 1:212:A:ALA:N  | 1:212:A:ALA:CA | 1:212:A:ALA:C   | 9        | 2.43          |
| (1,88)  | 1:248:A:ASP:N  | 1:248:A:ASP:CA | 1:248:A:ASP:C  | 1:249:A:LEU:N   | 5        | 2.42          |
| (1,12)  | 1:197:A:LEU:N  | 1:197:A:LEU:CA | 1:197:A:LEU:C  | 1:198:A:ASP:N   | 1        | 2.42          |
| (1,15)  | 1:198:A:ASP:C  | 1:199:A:VAL:N  | 1:199:A:VAL:CA | 1:199:A:VAL:C   | 17       | 2.41          |

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| Key     | Atom-1         | Atom-2         | Atom-3         | Atom-4          | Model ID | Violation (°) |
|---------|----------------|----------------|----------------|-----------------|----------|---------------|
| (1,1)   | 1:191:A:GLN:C  | 1:192:A:ASP:N  | 1:192:A:ASP:CA | 1:192:A:ASP:C   | 16       | 2.41          |
| (1,141) | 1:236:A:LYS:CA | 1:236:A:LYS:CB | 1:236:A:LYS:CG | 1:236:A:LYS:CD  | 9        | 2.37          |
| (1,93)  | 1:250:A:TYR:C  | 1:251:A:LEU:N  | 1:251:A:LEU:CA | 1:251:A:LEU:C   | 15       | 2.35          |
| (1,93)  | 1:250:A:TYR:C  | 1:251:A:LEU:N  | 1:251:A:LEU:CA | 1:251:A:LEU:C   | 4        | 2.34          |
| (1,108) | 1:174:A:TYR:N  | 1:174:A:TYR:CA | 1:174:A:TYR:CB | 1:174:A:TYR:CG  | 19       | 2.32          |
| (1,94)  | 1:251:A:LEU:N  | 1:251:A:LEU:CA | 1:251:A:LEU:C  | 1:252:A:GLU:N   | 13       | 2.31          |
| (1,48)  | 1:219:A:VAL:N  | 1:219:A:VAL:CA | 1:219:A:VAL:C  | 1:220:A:GLU:N   | 7        | 2.26          |
| (1,93)  | 1:250:A:TYR:C  | 1:251:A:LEU:N  | 1:251:A:LEU:CA | 1:251:A:LEU:C   | 12       | 2.25          |
| (1,43)  | 1:216:A:GLU:N  | 1:216:A:GLU:CA | 1:216:A:GLU:C  | 1:217:A:GLY:N   | 19       | 2.23          |
| (1,112) | 1:192:A:ASP:CA | 1:192:A:ASP:CB | 1:192:A:ASP:CG | 1:192:A:ASP:OD1 | 18       | 2.22          |
| (1,34)  | 1:211:A:ARG:C  | 1:212:A:ALA:N  | 1:212:A:ALA:CA | 1:212:A:ALA:C   | 12       | 2.22          |
| (1,80)  | 1:241:A:PRO:N  | 1:241:A:PRO:CA | 1:241:A:PRO:C  | 1:242:A:GLY:N   | 2        | 2.21          |
| (1,79)  | 1:240:A:PHE:N  | 1:240:A:PHE:CA | 1:240:A:PHE:C  | 1:241:A:PRO:N   | 14       | 2.2           |
| (1,34)  | 1:211:A:ARG:C  | 1:212:A:ALA:N  | 1:212:A:ALA:CA | 1:212:A:ALA:C   | 6        | 2.2           |
| (1,25)  | 1:205:A:VAL:N  | 1:205:A:VAL:CA | 1:205:A:VAL:C  | 1:206:A:VAL:N   | 2        | 2.16          |
| (1,93)  | 1:250:A:TYR:C  | 1:251:A:LEU:N  | 1:251:A:LEU:CA | 1:251:A:LEU:C   | 19       | 2.14          |
| (1,112) | 1:192:A:ASP:CA | 1:192:A:ASP:CB | 1:192:A:ASP:CG | 1:192:A:ASP:OD1 | 19       | 2.13          |
| (1,93)  | 1:250:A:TYR:C  | 1:251:A:LEU:N  | 1:251:A:LEU:CA | 1:251:A:LEU:C   | 2        | 2.13          |
| (1,48)  | 1:219:A:VAL:N  | 1:219:A:VAL:CA | 1:219:A:VAL:C  | 1:220:A:GLU:N   | 20       | 2.13          |
| (1,11)  | 1:196:A:THR:C  | 1:197:A:LEU:N  | 1:197:A:LEU:CA | 1:197:A:LEU:C   | 1        | 2.13          |
| (1,12)  | 1:197:A:LEU:N  | 1:197:A:LEU:CA | 1:197:A:LEU:C  | 1:198:A:ASP:N   | 3        | 2.11          |
| (1,93)  | 1:250:A:TYR:C  | 1:251:A:LEU:N  | 1:251:A:LEU:CA | 1:251:A:LEU:C   | 1        | 2.1           |
| (1,31)  | 1:210:A:VAL:N  | 1:210:A:VAL:CA | 1:210:A:VAL:C  | 1:211:A:ARG:N   | 18       | 2.1           |
| (1,141) | 1:236:A:LYS:CA | 1:236:A:LYS:CB | 1:236:A:LYS:CG | 1:236:A:LYS:CD  | 3        | 2.09          |
| (1,1)   | 1:191:A:GLN:C  | 1:192:A:ASP:N  | 1:192:A:ASP:CA | 1:192:A:ASP:C   | 19       | 2.09          |
| (1,67)  | 1:232:A:LYS:N  | 1:232:A:LYS:CA | 1:232:A:LYS:C  | 1:233:A:LEU:N   | 20       | 2.06          |
| (1,34)  | 1:211:A:ARG:C  | 1:212:A:ALA:N  | 1:212:A:ALA:CA | 1:212:A:ALA:C   | 13       | 2.06          |
| (1,141) | 1:236:A:LYS:CA | 1:236:A:LYS:CB | 1:236:A:LYS:CG | 1:236:A:LYS:CD  | 2        | 2.05          |
| (1,50)  | 1:220:A:GLU:N  | 1:220:A:GLU:CA | 1:220:A:GLU:C  | 1:221:A:VAL:N   | 14       | 2.04          |
| (1,88)  | 1:248:A:ASP:N  | 1:248:A:ASP:CA | 1:248:A:ASP:C  | 1:249:A:LEU:N   | 20       | 2.03          |
| (1,31)  | 1:210:A:VAL:N  | 1:210:A:VAL:CA | 1:210:A:VAL:C  | 1:211:A:ARG:N   | 16       | 2.02          |
| (1,107) | 1:173:A:PHE:CA | 1:173:A:PHE:CB | 1:173:A:PHE:CG | 1:173:A:PHE:CD1 | 16       | 2.01          |
| (1,67)  | 1:232:A:LYS:N  | 1:232:A:LYS:CA | 1:232:A:LYS:C  | 1:233:A:LEU:N   | 5        | 2.01          |
| (1,8)   | 1:195:A:ALA:N  | 1:195:A:ALA:CA | 1:195:A:ALA:C  | 1:196:A:THR:N   | 2        | 2.0           |
| (1,15)  | 1:198:A:ASP:C  | 1:199:A:VAL:N  | 1:199:A:VAL:CA | 1:199:A:VAL:C   | 2        | 1.98          |
| (1,6)   | 1:194:A:TYR:N  | 1:194:A:TYR:CA | 1:194:A:TYR:C  | 1:195:A:ALA:N   | 13       | 1.98          |
| (1,50)  | 1:220:A:GLU:N  | 1:220:A:GLU:CA | 1:220:A:GLU:C  | 1:221:A:VAL:N   | 11       | 1.97          |
| (1,91)  | 1:249:A:LEU:C  | 1:250:A:TYR:N  | 1:250:A:TYR:CA | 1:250:A:TYR:C   | 4        | 1.96          |
| (1,62)  | 1:229:A:ALA:C  | 1:230:A:GLY:N  | 1:230:A:GLY:CA | 1:230:A:GLY:C   | 4        | 1.96          |
| (1,62)  | 1:229:A:ALA:C  | 1:230:A:GLY:N  | 1:230:A:GLY:CA | 1:230:A:GLY:C   | 10       | 1.95          |
| (1,15)  | 1:198:A:ASP:C  | 1:199:A:VAL:N  | 1:199:A:VAL:CA | 1:199:A:VAL:C   | 7        | 1.95          |
| (1,136) | 1:234:A:ARG:N  | 1:234:A:ARG:CA | 1:234:A:ARG:CB | 1:234:A:ARG:CG  | 8        | 1.93          |
| (1,11)  | 1:196:A:THR:C  | 1:197:A:LEU:N  | 1:197:A:LEU:CA | 1:197:A:LEU:C   | 2        | 1.91          |
| (1,8)   | 1:195:A:ALA:N  | 1:195:A:ALA:CA | 1:195:A:ALA:C  | 1:196:A:THR:N   | 4        | 1.91          |
| (1,11)  | 1:196:A:THR:C  | 1:197:A:LEU:N  | 1:197:A:LEU:CA | 1:197:A:LEU:C   | 8        | 1.9           |
| (1,71)  | 1:234:A:ARG:N  | 1:234:A:ARG:CA | 1:234:A:ARG:C  | 1:235:A:LEU:N   | 6        | 1.89          |
| (1,28)  | 1:208:A:GLY:C  | 1:209:A:LYS:N  | 1:209:A:LYS:CA | 1:209:A:LYS:C   | 18       | 1.89          |
| (1,34)  | 1:211:A:ARG:C  | 1:212:A:ALA:N  | 1:212:A:ALA:CA | 1:212:A:ALA:C   | 5        | 1.88          |
| (1,89)  | 1:248:A:ASP:C  | 1:249:A:LEU:N  | 1:249:A:LEU:CA | 1:249:A:LEU:C   | 2        | 1.87          |
| (1,15)  | 1:198:A:ASP:C  | 1:199:A:VAL:N  | 1:199:A:VAL:CA | 1:199:A:VAL:C   | 20       | 1.87          |
| (1,93)  | 1:250:A:TYR:C  | 1:251:A:LEU:N  | 1:251:A:LEU:CA | 1:251:A:LEU:C   | 8        | 1.85          |

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| Key     | Atom-1         | Atom-2         | Atom-3         | Atom-4          | Model ID | Violation (°) |
|---------|----------------|----------------|----------------|-----------------|----------|---------------|
| (1,15)  | 1:198:A:ASP:C  | 1:199:A:VAL:N  | 1:199:A:VAL:CA | 1:199:A:VAL:C   | 15       | 1.82          |
| (1,1)   | 1:191:A:GLN:C  | 1:192:A:ASP:N  | 1:192:A:ASP:CA | 1:192:A:ASP:C   | 18       | 1.82          |
| (1,34)  | 1:211:A:ARG:C  | 1:212:A:ALA:N  | 1:212:A:ALA:CA | 1:212:A:ALA:C   | 17       | 1.81          |
| (1,11)  | 1:196:A:THR:C  | 1:197:A:LEU:N  | 1:197:A:LEU:CA | 1:197:A:LEU:C   | 9        | 1.81          |
| (1,104) | 1:172:A:LEU:N  | 1:172:A:LEU:CA | 1:172:A:LEU:CB | 1:172:A:LEU:CG  | 13       | 1.79          |
| (1,8)   | 1:195:A:ALA:N  | 1:195:A:ALA:CA | 1:195:A:ALA:C  | 1:196:A:THR:N   | 5        | 1.78          |
| (1,31)  | 1:210:A:VAL:N  | 1:210:A:VAL:CA | 1:210:A:VAL:C  | 1:211:A:ARG:N   | 11       | 1.76          |
| (1,89)  | 1:248:A:ASP:C  | 1:249:A:LEU:N  | 1:249:A:LEU:CA | 1:249:A:LEU:C   | 18       | 1.75          |
| (1,112) | 1:192:A:ASP:CA | 1:192:A:ASP:CB | 1:192:A:ASP:CG | 1:192:A:ASP:OD1 | 11       | 1.73          |
| (1,91)  | 1:249:A:LEU:C  | 1:250:A:TYR:N  | 1:250:A:TYR:CA | 1:250:A:TYR:C   | 15       | 1.72          |
| (1,55)  | 1:222:A:ALA:C  | 1:223:A:VAL:N  | 1:223:A:VAL:CA | 1:223:A:VAL:C   | 10       | 1.7           |
| (1,15)  | 1:198:A:ASP:C  | 1:199:A:VAL:N  | 1:199:A:VAL:CA | 1:199:A:VAL:C   | 13       | 1.7           |
| (1,94)  | 1:251:A:LEU:N  | 1:251:A:LEU:CA | 1:251:A:LEU:C  | 1:252:A:GLU:N   | 11       | 1.67          |
| (1,94)  | 1:251:A:LEU:N  | 1:251:A:LEU:CA | 1:251:A:LEU:C  | 1:252:A:GLU:N   | 20       | 1.67          |
| (1,62)  | 1:229:A:ALA:C  | 1:230:A:GLY:N  | 1:230:A:GLY:CA | 1:230:A:GLY:C   | 5        | 1.67          |
| (1,1)   | 1:191:A:GLN:C  | 1:192:A:ASP:N  | 1:192:A:ASP:CA | 1:192:A:ASP:C   | 7        | 1.67          |
| (1,93)  | 1:250:A:TYR:C  | 1:251:A:LEU:N  | 1:251:A:LEU:CA | 1:251:A:LEU:C   | 7        | 1.65          |
| (1,91)  | 1:249:A:LEU:C  | 1:250:A:TYR:N  | 1:250:A:TYR:CA | 1:250:A:TYR:C   | 1        | 1.65          |
| (1,83)  | 1:245:A:GLY:C  | 1:246:A:ARG:N  | 1:246:A:ARG:CA | 1:246:A:ARG:C   | 2        | 1.65          |
| (1,84)  | 1:246:A:ARG:N  | 1:246:A:ARG:CA | 1:246:A:ARG:C  | 1:247:A:GLY:N   | 15       | 1.64          |
| (1,69)  | 1:233:A:LEU:N  | 1:233:A:LEU:CA | 1:233:A:LEU:C  | 1:234:A:ARG:N   | 18       | 1.64          |
| (1,141) | 1:236:A:LYS:CA | 1:236:A:LYS:CB | 1:236:A:LYS:CG | 1:236:A:LYS:CD  | 7        | 1.63          |
| (1,6)   | 1:194:A:TYR:N  | 1:194:A:TYR:CA | 1:194:A:TYR:C  | 1:195:A:ALA:N   | 20       | 1.63          |
| (1,96)  | 1:252:A:GLU:N  | 1:252:A:GLU:CA | 1:252:A:GLU:C  | 1:253:A:VAL:N   | 19       | 1.62          |
| (1,92)  | 1:250:A:TYR:N  | 1:250:A:TYR:CA | 1:250:A:TYR:C  | 1:251:A:LEU:N   | 20       | 1.62          |
| (1,84)  | 1:246:A:ARG:N  | 1:246:A:ARG:CA | 1:246:A:ARG:C  | 1:247:A:GLY:N   | 16       | 1.62          |
| (1,71)  | 1:234:A:ARG:N  | 1:234:A:ARG:CA | 1:234:A:ARG:C  | 1:235:A:LEU:N   | 20       | 1.62          |
| (1,34)  | 1:211:A:ARG:C  | 1:212:A:ALA:N  | 1:212:A:ALA:CA | 1:212:A:ALA:C   | 4        | 1.62          |
| (1,104) | 1:172:A:LEU:N  | 1:172:A:LEU:CA | 1:172:A:LEU:CB | 1:172:A:LEU:CG  | 9        | 1.61          |
| (1,50)  | 1:220:A:GLU:N  | 1:220:A:GLU:CA | 1:220:A:GLU:C  | 1:221:A:VAL:N   | 2        | 1.61          |
| (1,55)  | 1:222:A:ALA:C  | 1:223:A:VAL:N  | 1:223:A:VAL:CA | 1:223:A:VAL:C   | 19       | 1.6           |
| (1,8)   | 1:195:A:ALA:N  | 1:195:A:ALA:CA | 1:195:A:ALA:C  | 1:196:A:THR:N   | 13       | 1.6           |
| (1,141) | 1:236:A:LYS:CA | 1:236:A:LYS:CB | 1:236:A:LYS:CG | 1:236:A:LYS:CD  | 20       | 1.59          |
| (1,34)  | 1:211:A:ARG:C  | 1:212:A:ALA:N  | 1:212:A:ALA:CA | 1:212:A:ALA:C   | 14       | 1.59          |
| (1,112) | 1:192:A:ASP:CA | 1:192:A:ASP:CB | 1:192:A:ASP:CG | 1:192:A:ASP:OD1 | 12       | 1.58          |
| (1,66)  | 1:231:A:ARG:C  | 1:232:A:LYS:N  | 1:232:A:LYS:CA | 1:232:A:LYS:C   | 17       | 1.58          |
| (1,15)  | 1:198:A:ASP:C  | 1:199:A:VAL:N  | 1:199:A:VAL:CA | 1:199:A:VAL:C   | 8        | 1.58          |
| (1,93)  | 1:250:A:TYR:C  | 1:251:A:LEU:N  | 1:251:A:LEU:CA | 1:251:A:LEU:C   | 16       | 1.56          |
| (1,83)  | 1:245:A:GLY:C  | 1:246:A:ARG:N  | 1:246:A:ARG:CA | 1:246:A:ARG:C   | 19       | 1.56          |
| (1,28)  | 1:208:A:GLY:C  | 1:209:A:LYS:N  | 1:209:A:LYS:CA | 1:209:A:LYS:C   | 12       | 1.56          |
| (1,147) | 1:248:A:ASP:CA | 1:248:A:ASP:CB | 1:248:A:ASP:CG | 1:248:A:ASP:OD1 | 1        | 1.54          |
| (1,28)  | 1:208:A:GLY:C  | 1:209:A:LYS:N  | 1:209:A:LYS:CA | 1:209:A:LYS:C   | 2        | 1.54          |
| (1,147) | 1:248:A:ASP:CA | 1:248:A:ASP:CB | 1:248:A:ASP:CG | 1:248:A:ASP:OD1 | 2        | 1.52          |
| (1,55)  | 1:222:A:ALA:C  | 1:223:A:VAL:N  | 1:223:A:VAL:CA | 1:223:A:VAL:C   | 17       | 1.51          |
| (1,34)  | 1:211:A:ARG:C  | 1:212:A:ALA:N  | 1:212:A:ALA:CA | 1:212:A:ALA:C   | 15       | 1.51          |
| (1,66)  | 1:231:A:ARG:C  | 1:232:A:LYS:N  | 1:232:A:LYS:CA | 1:232:A:LYS:C   | 19       | 1.5           |
| (1,34)  | 1:211:A:ARG:C  | 1:212:A:ALA:N  | 1:212:A:ALA:CA | 1:212:A:ALA:C   | 8        | 1.49          |
| (1,3)   | 1:192:A:ASP:C  | 1:193:A:LEU:N  | 1:193:A:LEU:CA | 1:193:A:LEU:C   | 20       | 1.49          |
| (1,136) | 1:234:A:ARG:N  | 1:234:A:ARG:CA | 1:234:A:ARG:CB | 1:234:A:ARG:CG  | 5        | 1.47          |
| (1,108) | 1:174:A:TYR:N  | 1:174:A:TYR:CA | 1:174:A:TYR:CB | 1:174:A:TYR:CG  | 7        | 1.47          |
| (1,84)  | 1:246:A:ARG:N  | 1:246:A:ARG:CA | 1:246:A:ARG:C  | 1:247:A:GLY:N   | 11       | 1.47          |

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| Key     | Atom-1         | Atom-2         | Atom-3         | Atom-4          | Model ID | Violation (°) |
|---------|----------------|----------------|----------------|-----------------|----------|---------------|
| (1,48)  | 1:219:A:VAL:N  | 1:219:A:VAL:CA | 1:219:A:VAL:C  | 1:220:A:GLU:N   | 17       | 1.47          |
| (1,34)  | 1:211:A:ARG:C  | 1:212:A:ALA:N  | 1:212:A:ALA:CA | 1:212:A:ALA:C   | 18       | 1.47          |
| (1,8)   | 1:195:A:ALA:N  | 1:195:A:ALA:CA | 1:195:A:ALA:C  | 1:196:A:THR:N   | 6        | 1.47          |
| (1,95)  | 1:251:A:LEU:C  | 1:252:A:GLU:N  | 1:252:A:GLU:CA | 1:252:A:GLU:C   | 2        | 1.46          |
| (1,91)  | 1:249:A:LEU:C  | 1:250:A:TYR:N  | 1:250:A:TYR:CA | 1:250:A:TYR:C   | 5        | 1.45          |
| (1,84)  | 1:246:A:ARG:N  | 1:246:A:ARG:CA | 1:246:A:ARG:C  | 1:247:A:GLY:N   | 1        | 1.45          |
| (1,108) | 1:174:A:TYR:N  | 1:174:A:TYR:CA | 1:174:A:TYR:CB | 1:174:A:TYR:CG  | 8        | 1.44          |
| (1,106) | 1:173:A:PHE:N  | 1:173:A:PHE:CA | 1:173:A:PHE:CB | 1:173:A:PHE:CG  | 2        | 1.44          |
| (1,84)  | 1:246:A:ARG:N  | 1:246:A:ARG:CA | 1:246:A:ARG:C  | 1:247:A:GLY:N   | 12       | 1.43          |
| (1,25)  | 1:205:A:VAL:N  | 1:205:A:VAL:CA | 1:205:A:VAL:C  | 1:206:A:VAL:N   | 6        | 1.43          |
| (1,55)  | 1:222:A:ALA:C  | 1:223:A:VAL:N  | 1:223:A:VAL:CA | 1:223:A:VAL:C   | 4        | 1.41          |
| (1,66)  | 1:231:A:ARG:C  | 1:232:A:LYS:N  | 1:232:A:LYS:CA | 1:232:A:LYS:C   | 8        | 1.4           |
| (1,28)  | 1:208:A:GLY:C  | 1:209:A:LYS:N  | 1:209:A:LYS:CA | 1:209:A:LYS:C   | 19       | 1.4           |
| (1,35)  | 1:212:A:ALA:N  | 1:212:A:ALA:CA | 1:212:A:ALA:C  | 1:213:A:MET:N   | 18       | 1.38          |
| (1,4)   | 1:193:A:LEU:N  | 1:193:A:LEU:CA | 1:193:A:LEU:C  | 1:194:A:TYR:N   | 5        | 1.37          |
| (1,141) | 1:236:A:LYS:CA | 1:236:A:LYS:CB | 1:236:A:LYS:CG | 1:236:A:LYS:CD  | 13       | 1.36          |
| (1,1)   | 1:191:A:GLN:C  | 1:192:A:ASP:N  | 1:192:A:ASP:CA | 1:192:A:ASP:C   | 3        | 1.35          |
| (1,107) | 1:173:A:PHE:CA | 1:173:A:PHE:CB | 1:173:A:PHE:CG | 1:173:A:PHE:CD1 | 1        | 1.33          |
| (1,94)  | 1:251:A:LEU:N  | 1:251:A:LEU:CA | 1:251:A:LEU:C  | 1:252:A:GLU:N   | 9        | 1.32          |
| (1,93)  | 1:250:A:TYR:C  | 1:251:A:LEU:N  | 1:251:A:LEU:CA | 1:251:A:LEU:C   | 11       | 1.32          |
| (1,88)  | 1:248:A:ASP:N  | 1:248:A:ASP:CA | 1:248:A:ASP:C  | 1:249:A:LEU:N   | 16       | 1.32          |
| (1,93)  | 1:250:A:TYR:C  | 1:251:A:LEU:N  | 1:251:A:LEU:CA | 1:251:A:LEU:C   | 3        | 1.31          |
| (1,84)  | 1:246:A:ARG:N  | 1:246:A:ARG:CA | 1:246:A:ARG:C  | 1:247:A:GLY:N   | 7        | 1.31          |
| (1,8)   | 1:195:A:ALA:N  | 1:195:A:ALA:CA | 1:195:A:ALA:C  | 1:196:A:THR:N   | 7        | 1.31          |
| (1,35)  | 1:212:A:ALA:N  | 1:212:A:ALA:CA | 1:212:A:ALA:C  | 1:213:A:MET:N   | 20       | 1.29          |
| (1,94)  | 1:251:A:LEU:N  | 1:251:A:LEU:CA | 1:251:A:LEU:C  | 1:252:A:GLU:N   | 14       | 1.28          |
| (1,94)  | 1:251:A:LEU:N  | 1:251:A:LEU:CA | 1:251:A:LEU:C  | 1:252:A:GLU:N   | 2        | 1.26          |
| (1,89)  | 1:248:A:ASP:C  | 1:249:A:LEU:N  | 1:249:A:LEU:CA | 1:249:A:LEU:C   | 7        | 1.26          |
| (1,84)  | 1:246:A:ARG:N  | 1:246:A:ARG:CA | 1:246:A:ARG:C  | 1:247:A:GLY:N   | 13       | 1.26          |
| (1,55)  | 1:222:A:ALA:C  | 1:223:A:VAL:N  | 1:223:A:VAL:CA | 1:223:A:VAL:C   | 6        | 1.26          |
| (1,38)  | 1:213:A:MET:C  | 1:214:A:THR:N  | 1:214:A:THR:CA | 1:214:A:THR:C   | 19       | 1.26          |
| (1,66)  | 1:231:A:ARG:C  | 1:232:A:LYS:N  | 1:232:A:LYS:CA | 1:232:A:LYS:C   | 2        | 1.25          |
| (1,35)  | 1:212:A:ALA:N  | 1:212:A:ALA:CA | 1:212:A:ALA:C  | 1:213:A:MET:N   | 8        | 1.24          |
| (1,28)  | 1:208:A:GLY:C  | 1:209:A:LYS:N  | 1:209:A:LYS:CA | 1:209:A:LYS:C   | 6        | 1.24          |
| (1,48)  | 1:219:A:VAL:N  | 1:219:A:VAL:CA | 1:219:A:VAL:C  | 1:220:A:GLU:N   | 15       | 1.23          |
| (1,61)  | 1:229:A:ALA:N  | 1:229:A:ALA:CA | 1:229:A:ALA:C  | 1:230:A:GLY:N   | 16       | 1.21          |
| (1,8)   | 1:195:A:ALA:N  | 1:195:A:ALA:CA | 1:195:A:ALA:C  | 1:196:A:THR:N   | 14       | 1.21          |
| (1,101) | 1:254:A:ARG:C  | 1:255:A:ILE:N  | 1:255:A:ILE:CA | 1:255:A:ILE:C   | 11       | 1.2           |
| (1,93)  | 1:250:A:TYR:C  | 1:251:A:LEU:N  | 1:251:A:LEU:CA | 1:251:A:LEU:C   | 17       | 1.2           |
| (1,28)  | 1:208:A:GLY:C  | 1:209:A:LYS:N  | 1:209:A:LYS:CA | 1:209:A:LYS:C   | 3        | 1.19          |
| (1,28)  | 1:208:A:GLY:C  | 1:209:A:LYS:N  | 1:209:A:LYS:CA | 1:209:A:LYS:C   | 10       | 1.19          |
| (1,141) | 1:236:A:LYS:CA | 1:236:A:LYS:CB | 1:236:A:LYS:CG | 1:236:A:LYS:CD  | 11       | 1.18          |
| (1,84)  | 1:246:A:ARG:N  | 1:246:A:ARG:CA | 1:246:A:ARG:C  | 1:247:A:GLY:N   | 5        | 1.18          |
| (1,62)  | 1:229:A:ALA:C  | 1:230:A:GLY:N  | 1:230:A:GLY:CA | 1:230:A:GLY:C   | 8        | 1.18          |
| (1,101) | 1:254:A:ARG:C  | 1:255:A:ILE:N  | 1:255:A:ILE:CA | 1:255:A:ILE:C   | 7        | 1.17          |
| (1,32)  | 1:210:A:VAL:C  | 1:211:A:ARG:N  | 1:211:A:ARG:CA | 1:211:A:ARG:C   | 13       | 1.17          |
| (1,28)  | 1:208:A:GLY:C  | 1:209:A:LYS:N  | 1:209:A:LYS:CA | 1:209:A:LYS:C   | 20       | 1.17          |
| (1,55)  | 1:222:A:ALA:C  | 1:223:A:VAL:N  | 1:223:A:VAL:CA | 1:223:A:VAL:C   | 5        | 1.16          |
| (1,94)  | 1:251:A:LEU:N  | 1:251:A:LEU:CA | 1:251:A:LEU:C  | 1:252:A:GLU:N   | 17       | 1.15          |
| (1,104) | 1:172:A:LEU:N  | 1:172:A:LEU:CA | 1:172:A:LEU:CB | 1:172:A:LEU:CG  | 10       | 1.14          |
| (1,94)  | 1:251:A:LEU:N  | 1:251:A:LEU:CA | 1:251:A:LEU:C  | 1:252:A:GLU:N   | 3        | 1.14          |

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| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4         | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|----------------|----------|---------------|
| (1,6)   | 1:194:A:TYR:N | 1:194:A:TYR:CA | 1:194:A:TYR:C  | 1:195:A:ALA:N  | 3        | 1.14          |
| (1,67)  | 1:232:A:LYS:N | 1:232:A:LYS:CA | 1:232:A:LYS:C  | 1:233:A:LEU:N  | 13       | 1.12          |
| (1,28)  | 1:208:A:GLY:C | 1:209:A:LYS:N  | 1:209:A:LYS:CA | 1:209:A:LYS:C  | 1        | 1.11          |
| (1,80)  | 1:241:A:PRO:N | 1:241:A:PRO:CA | 1:241:A:PRO:C  | 1:242:A:GLY:N  | 3        | 1.1           |
| (1,136) | 1:234:A:ARG:N | 1:234:A:ARG:CA | 1:234:A:ARG:CB | 1:234:A:ARG:CG | 10       | 1.09          |
| (1,87)  | 1:247:A:GLY:C | 1:248:A:ASP:N  | 1:248:A:ASP:CA | 1:248:A:ASP:C  | 12       | 1.09          |
| (1,123) | 1:209:A:LYS:N | 1:209:A:LYS:CA | 1:209:A:LYS:CB | 1:209:A:LYS:CG | 17       | 1.07          |
| (1,8)   | 1:195:A:ALA:N | 1:195:A:ALA:CA | 1:195:A:ALA:C  | 1:196:A:THR:N  | 17       | 1.07          |
| (1,91)  | 1:249:A:LEU:C | 1:250:A:TYR:N  | 1:250:A:TYR:CA | 1:250:A:TYR:C  | 17       | 1.06          |
| (1,91)  | 1:249:A:LEU:C | 1:250:A:TYR:N  | 1:250:A:TYR:CA | 1:250:A:TYR:C  | 19       | 1.05          |
| (1,93)  | 1:250:A:TYR:C | 1:251:A:LEU:N  | 1:251:A:LEU:CA | 1:251:A:LEU:C  | 9        | 1.03          |
| (1,31)  | 1:210:A:VAL:N | 1:210:A:VAL:CA | 1:210:A:VAL:C  | 1:211:A:ARG:N  | 2        | 1.03          |
| (1,91)  | 1:249:A:LEU:C | 1:250:A:TYR:N  | 1:250:A:TYR:CA | 1:250:A:TYR:C  | 7        | 1.02          |
| (1,48)  | 1:219:A:VAL:N | 1:219:A:VAL:CA | 1:219:A:VAL:C  | 1:220:A:GLU:N  | 4        | 1.02          |
| (1,31)  | 1:210:A:VAL:N | 1:210:A:VAL:CA | 1:210:A:VAL:C  | 1:211:A:ARG:N  | 8        | 1.02          |
| (1,62)  | 1:229:A:ALA:C | 1:230:A:GLY:N  | 1:230:A:GLY:CA | 1:230:A:GLY:C  | 15       | 1.01          |
| (1,55)  | 1:222:A:ALA:C | 1:223:A:VAL:N  | 1:223:A:VAL:CA | 1:223:A:VAL:C  | 16       | 1.01          |
| (1,101) | 1:254:A:ARG:C | 1:255:A:ILE:N  | 1:255:A:ILE:CA | 1:255:A:ILE:C  | 17       | 1.0           |